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EiX-GNN: Concept-level eigencentality explainer for graph neural networks

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Abstract

Nowadays, deep prediction models, especially graph neural networks, have a major place in critical applications. In such context, those models need to be highly interpretable or being explainable by humans, and at the societal scope, this understanding may also be feasible for humans that do not have a strong prior knowledge in models and contexts that need to be explained. In the literature, explaining is a human knowledge transfer process regarding a phenomenon between an explainer and an explainee. We propose EiX-GNN (Eigencentality eXplainer for Graph Neural Networks) a new powerful method for explaining graph neural networks that encodes computationally this social explainer-to-explainee dependence underlying in the explanation process. To handle this dependency, we introduce the notion of explainee concept assimilability which allows explainer to adapt its explanation to explainee background or expectation. We lead a qualitative study to illustrate our explainee concept assimilability notion on real-world data as well as a qualitative study that compares, according to objective metrics established in the literature, fairness and compactness of our method with respect to performing state-of-the-art methods. It turns out that our method achieves strong results in both aspects.

1 Introduction

Graphs are widely used data structures involved in many real-world problems. Graph Neural Network (GNN) [Scarselli et al.(2009)Scarselli, Gori, Tsoi, Hagenbuchner, and Monfardini] are artificial neural networks suited for such data structure. For graph classification, node classification or link prediction tasks, GNN models have shown impressive performances [Defferrard et al.(2016)Defferrard, Bresson, and Vandergheynst, Zhang & Chen(2018)Zhang, Chen, and Yang, Ying et al.(2018)Ying, He, Chen, Eksombatchai, Hamilton, and Leskovec]. Regarding real-life deployment, GNN models have shown impressive results for drugs design [Bapst et al.(2020)Bapst, Keck, Groll, and Wenzel], web recommendations [Ying et al.(2018)Ying, He, Chen, Eksombatchai, Hamilton, and Leskovec] or traffic forecasting [Darrow-Pinion et al.(2021)Darrow-Pinion, She, Wong, Lange, Hester, Perez, Nunkesser, Lee, Guo, Wiltshire, Battaglia, and Wainwright]. A major drawback of those deep models is their occluded internal decisional processes, in particular in critical applications, it raises confidence, trustworthy, privacy and security concerns. Explainable Artificial Intelligence (XAI) is a set of methods that aims to tackle these issues by providing human-level meaningful insights about deep model internals by explaining how those models behave. Explaining, understanding, or interpreting, although they are different notions, are intrinsically human dependent and context-dependent. So, it turns out that they are social notions. One of those social requirements is that an explainer must adapt its explanation formulation according to the relative background of the explainee regarding the phenomenon to explain [Clough et al.(2019)Clough, Oksuz, Puyol-Antón, Ruijsink, King, and Schnabel, Kim et al.(2020)Kim, Wattenberg, Gilmer, Cai, Wexler, Viegas, and Sayres]. Several interesting XAI methods have been proposed for explaining graph neural network models but they often fail to take into account the social dependency when providing their explanations and rather focus only on the signal side of deep models to provide insights on deep model internals. In this contribution we provide a social-aware explaining method that leverages background knowledge variability that is inherent in any social-related process while maintaining high score regarding state-of-the-art objective assessment metrics. Firstly, we will frame the social context that the explanation process depends on. Then we will introduce our approach in accordance with the numerical formulation of the social context. Then we provide the relevancy of our method against compared methods with a qualitative objective study on real-world applications and a quantitative objective study regarding objective metrics widely used in the literature.

2 Related Work

GNN is firstly introduced by [Scarselli et al.(2009)Scarselli, Gori, Tsoi, Hagenbuchner, and Monfardini] with the message-passing scheme. They have been studied from the geometrical point of view and framed by [Bronstein et al.(2021)Bronstein, Bruna, Cohen, and Veličković], from this point of view, as the generalizing model of test-of-time models such as Convolutional Neural Network (CNN) that have achieved main results in computer vision [Krizhevsky et al.(2012)Krizhevsky, Sutskever, and Hinton, Russakovsky et al.(2015)Russakovsky, Deng, Su] or Transformers [Vaswani et al.(2017)Vaswani, Shazeer, Parmar, Uszkoreit, Jones, Gomez, Kaiser, and Polosukhin] in speech processing [Devlin et al.(2019)Devlin, Chang, Lee, and Toutanova]. Genuine GNN of [Scarselli et al.(2009)Scarselli] has been widely extended by [Satorras et al.(2021)Satorras, Hoogeboom, and Welling, Battaglia et al.(2018)Battaglia, Hamrick, Defferrard et al.(2016)Defferrard, Bresson, and Vandergheynst, Monti et al.(2018)Monti, Shchur, Bojchevski, Litany, Günnemann, Sanchez-Lengeling et al.(2020)Sanchez-Lengeling, Wei, Lee, Reif, Wang, Qian, McCloskey, Colwell, and Wiltschko, Gilmer et al.(2017)Gilmer, Schoenholz, Riley, Vinyals, and Dahl, Gori et al.(2005)Gori, Monfardini, and Scarselli] including Graph Convolutional Network (GCN) [Kipf & Welling(2017)Kipf and Welling] and Graph Attention Network (GAT) [Veličković et al.(2018)Veličković, Cucurull, Casanova, Romero, Liò, and Bengio] that also achieve numerous results in their own fields. Explaining methods are divided in several paradigms. The common approach is the model-based post-hoc local paradigm which consists in explaining each instance with including optimized deep model in the loop for furnishing explanations. Under this paradigm, a serious amount of explaining methods to GNN have emerged. Attribution methods scope is to provide relevance to features regarding their impact on the classification, often under a white-box approach [Battaglia et al.(2018)Battaglia, Hamrick, Bapst, Sanchez-Gonzalez, Pope et al.(2019)Pope, Kolouri, Rostami, Martin, and Hoffmann] that have model internal insights either thank to model parameters and local behavior or with relative contribution approach [Yeh et al.(2019)Yeh, Hsieh, Suggala, Inouye, and Perturbation-based methods act in a black-box flavor (i.e., completely blind from model internal for explaining) and their trouble model with node ablation procedure [Ying et al.(2019)Ying, Bourgeois, You, Zitnik, and Leskovec], or edges ablation [Luo et al.(2020)Luo, Cheng, Xu, Yu, Zong, Chen, and Zhang, Schlichtkrull(2021)] or counterfactual adjunctions [Lucic et al.(2022)Lucic, Hoeve, Tolomei, Rijke, and Silvestri]. Heuristic search methods have also proven to be relevant for explaining as well as generative model [Yuan et al.(2020)Yuan, Tang, Hu, and Ji]. Additionally, explaining methods suited for node classifiers has brought relevant results [Huang et al.(2022)Huang, Yamada, Vu & Thai(2020)Vu and Thai]. Assessing the quality of those methods also remains a core challenge for the XAI community and some metrics have been proposed. They deal with explanation fidelity towards explained deep models. As well, sparsity measure is used to show the explanation compactness. These metrics are actually derived from an informal formulation of desirable property explaining methods have to fulfill [Jacovi & Goldberg(2020)Jacovi and Goldberg, Jacovi & Goldberg(2021)Jacovi and Goldberg, Lipton(2018), Murdoch et al.(2019)Murdoch et al.]. All these approaches share a common assumption: explaining a deep classifier relies on finding relevant sub-structure on the instanced input that conserves the classifier behavior. Besides aforementioned methods show interesting results, they always miss the inherently and intrinsically social dependence of the explanation process [Kim et al.(2019)Kim, Wattenberg, Gilmer, Cai, Wexler, Viegas, and Sayres, Bas(1980), Kulesza et al.(2013)Kulesza, Stumpf, Brinker, Miller(2019)]. Notably that an explainer has to share his knowledge regarding a phenomenon to an explainee in an explainee-understandable manner in order to have an effective explanation process profitable for the explainee [Bechtel & Abrahamsen(2005)Bechtel and Abrahamsen, Glennan(2002), Chater & Oaksford(2006)Chater and Oaksford, Keil(2006)]. In this study, we first provide a relevant method that achieves stronger explanation results regarding state-of-the-art methods while fully encoding the explainee-knowledge dependency and more broadly the social context any explanation process in dependent on.

3 Problem formulation

Explaining helps human experts to inspect deep models, in order to show issues, blind spots or to prevent those models to potentially harm society. For explaining machine learning problems, the social context [Selbst et al.(2019)Selbst, Boyd, Friedler, Venkatasubramanian, and Vertes] and human being factor [noa(), Miller(2019)] are core elements. Indeed, this explanation process involves an alignment of mental models. That alignment is between what the machine learning model is doing and what the user thinks the model is doing. In order terms, to achieve this information trading it requires a set of arguments that conjointly machine and user are aware of and are able to deal with. Explaining machine learning model is thus a human-centric process and in order to provide meaningful insight on how the model behaves to the user, the explanation process must be adapted [Kim et al.(2019)Kim, Wattenberg, Gilmer, Cai, Wexler, Viegas, and Sayres, Clough et al.(2019)Clough, Oksuz, Puyol-Antón, R]. Note that it is easier to shape machine outcomes representation than to force humans to think in far different way that they are used to think. Consequently, it is the machine that has to be adapted to the user. But when a user wants to have insightful explanations, they have to be expressed regarding a specific granularity. Indeed a user with a high level of knowledge has different explanation expectations than a user with less knowledge regarding the involved machine learning model.

More formally it can be reformulated as follows; explaining is a human knowledge transfer process involving an explainer (e.g., machine) E^* and an explainee \tilde{E} (e.g., user, engineer) concerning a phenomenon P (e.g., machine learning model). In order to have a profitable conversation (e.g., providing the explanation of P from E^* to \tilde{E}), both involved individuals must share a common vocabulary set. It means that shared ideas must be expressed upon a shared set of concepts by both individuals. This allows the conversation to be profitable for them. For explanation purposes, the term profitable means increasing the knowledge quantity of P of \tilde{E} thanks to E^* explanation. For explaining, those concepts are framed as atomic parts that, when carefully mixed, allow the explainer E^* to provide an explanation of P to the explainee \tilde{E} . However, those elementary bricks are chosen conditionally to both knowledge quantity of E^* and \tilde{E} that are also dependent on P . Indeed if the explainee \tilde{E} has already a solid background or culture relatively to P , basic insights allowing shallow understanding of P is already acquired by the explainee \tilde{E} . Only finer details must be provided by the explainer E^* to explainee \tilde{E} to have total understanding of P . On the contrary, an explainee \tilde{E} who has freshly begun to be interested in P must assimilate the coarsened concepts relative to P before reaching the finest ones with the explainer E^* having to adapt his vocabulary complexity in order to be understandable.

3.1 EiX-GNN

EiX-GNN (**eig**centrality explainer for **g**raph **n**eural **n**etwork) is a post-hoc local model-based explaining method suited for any GNN classifiers. In our terminology, it provides its explanations according to a set of atomic concepts. These concepts are for explanation processes what coins are for money exchanges, i.e., they are the elementary parts of the explanation process that explainers, when explaining, will build their arguments upon those atomic concepts. Those concepts must be carefully chosen by the explainer in order to match the explainee background on the explained phenomenon. With assuming that the explainer has an optimal knowledge of a phenomenon P regardless concept selection, the concept selection process depends on the background (relatively to P) of the explainee and P . EiX-GNN has been designed to integrate this social dependence on the explainee background given a phenomenon to explain. Formally, we frame the set of explainee-admissible concepts as a probability space \mathcal{C}_p where concepts are \mathcal{C}_p -valued random variable. Parameter p is the explainee concept assimilability constrain. It is bounded as $p \in [0, 1]$ and is proportional to the explainee concept assimilability given P . In the following, except for contrary mentions, we consider the phenomenon $P = (f^*, G, Y)$ where f^* is an optimized GNN classifier¹ which has been trained on a dataset \mathcal{D} which (G, Y) belongs to. In accordance with the graph formulation we have used before, we consider in the following a graph $G = (\mathbf{X}, \mathbf{A})$ has been composed of $N \in \mathbb{N}$ nodes and $M \in \mathbb{N}$ edges. We also assume that the explainee has an explainee concept assimilability constraint $p \in [0, 1]$. EiX-GNN provides its explanation based on a conditioned local and global explainee-suited concept ordering. Firstly, we introduce the concept generation procedure, then the global concept ordering process which is the common thread of the overall explaining procedure is described. Finally, the local concept ordering procedure is presented, this second step is a refining procedure that highly precise at a node level the provided explanation.

Concept generation As mentioned above, concepts are atomic elements that allow the explainer to provide its explanation. Given the explainee concept assimilability p , concept C_p is a \mathcal{C}_p -valued random variable. This variable is a subgraph of G such that $|C_p| = \lfloor |G| \times p \rfloor$. Our motivation from the signal point of view is to describe an insightful subpart of the signal evolving on a subdomain of G . Indeed in many deep-based data representation tiny but numerous low-level informations (e.g., high frequencies in the picture) are gathered along model depth to produce a unified high-level information (e.g., a probability distribution of classes that this picture belongs to). Classes probability is understandable by any person interested in deep learning approaches whereas high-frequency understanding is only doable for peoples with dedicated knowledge in image processing. We have designed our concept generation process with respect to this data representation hierarchization, from detailed expert-understandable representation to commonly understandable representation, involves in deep representation methods. Once determined the desired explanation granularity thanks to p , we need to sample those concepts from the initial graph G . We have selected sampling approaches which depend either on a prior distribution or not. Sampling concept is thus a subgraph sampling process which has a combinatorial aspect inherent of any subgraph sampling problems. Concepts are key components of our approach, they have to be carefully selected since they are providing our raw materials for conceiving explanations. From all $\binom{|G|}{|C_p|}$ possible subgraphs we can derive from G , some are more suited for providing explanation of P than others. Assuming a uniform relevance distribution for explaining P among all those subgraphs is not adapted, seamlessly, assuming that the sampling distribution is $\mathbb{U}_{\binom{|G|}{|C_p|}}$ is not adapted either. We rather consider a light importance sampling approach that quantifies the prior relevance distribution of nodes conditionally to P . For building such probability distribution, we apply a node ablation approach that assesses the importance of nodes within their neighborhood with respect to P . Formally, for a neighboring node $v_j \in \mathcal{N}_i = \{v_j | (v_i, v_j) \in E\} \subset V$

¹see Appendix A.2 for details

of v_i . To quantify node ablation importance we define a random variable $s : V^2 \rightarrow \mathbb{R}^+$ that measures the relative disturbance effect between two nodes relatively to P (e.g., relative f^* performance alteration impact of removing v_j from \mathcal{N}_i). With assuming a uniform relevance distribution $\mathbb{U}_{|\mathcal{N}_i|}$ of nodes composing \mathcal{N}_i , we defined the prior relevance distribution α_P of the node v_i conditionally to P by:

$$\alpha_P(v_i) = \mathbb{E}_{v_j \sim \mathbb{U}_{|\mathcal{N}_i|}} [s(v_i, v_j) | v_i, P] \quad (1)$$

With a normalizing constant $F \in \mathbb{R}^*$ such that $F^{-1} \sum_{v_i \in V} \alpha_P(v_i) = 1$ we obtain a prior node importance probability distribution that allows more efficient sampling process for determining pertinent concepts with respect to P . Once such prior distribution is determined, we sample in an i.i.d manner $L \in \mathbb{N}$ realizations of C_p which we denote by $(C_i)_{i \in \{1, \dots, L\}}$ where each node composing the subgraph C_i has been sampled thanks to the prior node sampling distribution. Next, we will present the procedure for hierarchizing those L concepts relatively to P .

Global concept ordering Once concepts are sampled, we must find an ordering relationship in order to classify their relevance according to P . Thanks to the prior node importance sampling approach, we have already established such hierarchization but among all possible subgraphs of G with size $|C_p|$ which considerably reduces the research perimeter of the optimal substructure that will explain P . Instead, here we present an ordering method that hierarchizes pair-wisely concepts among the L sampled concepts. Considering these L concepts, we build an operational research tree with G as root and these L concepts as leaves. Without any further works, we do not know yet if a concept C_i is more relevant than another concept C_j for explaining P . In order to provide such ordering, we derive from the sample a complete graph K_L where each node represents a concept and edge of K_L represents the relative similarity between two concepts relatively to P . Since in this context graph are seen as signal evolving on a precise deformation, we take into account each both aspects for quantifying concept similarities pair wisely.

Relative concept domain similarity We define the domain similarity between two concepts $C_i, C_j \in (C_l)_{l \in \{1, \dots, L\}}$ as the relative edge density between C_i and C_j . The graph edge density of a concept C_i , denote $d(C_i)$ is the ratio between the actual edges composing C_i over the total number of possible edges C_i can be composed of. For a graph $G = (\mathbf{X}, \mathbf{A})$ with N nodes and M edges, it is defined as follows:

$$d(G) = \frac{(2 \times \mathbf{1}_{\{\mathbf{A}=\mathbf{A}^T\}} + \mathbf{1}_{\{\mathbf{A} \neq \mathbf{A}^T\}})M}{N(N-1)} \quad (2)$$

It measures how C_i tends to be a complete graph. We choose this measure because of the local aggregation operation involve in many GNN models. We know that complete subgraphs aggregate much more signal than sparser ones. This is due to the local invariance operation involved in any geometric deep learning models, especially GNN [Bronstein et al.(2021)Bronstein, Bruna, Cohen, and Veličković]. Admittedly, aggregating numerous neighboring signal does not imply to aggregate more relevant information of this neighboring than with more sparse structures. Nevertheless, doing so will produce in statistically a fairer estimation of the local information relevance given P than it can be done on more degenerated localities. In other terms, this approach allows yielding statistically more fidel local representations of P .

Relative concept signal similarity The concept signal similarity quantifies how similar f^* behaviors are with respect to P when the signal is propagated over a given concept subdomain and when it is propagated over another subdomain supplied by another concept. Let assume that we considered two concepts C_i and C_j , the case where C_i is similar to C_j given P means that f^* sees equivalently C_i and C_j . Considering C_i does not provide any added value than solely considering C_j itself, with respect to P . As a similarity metric between two concepts C_i and C_j we use the Kullbach-Liebler divergence of both inferred probability distributions of C_i and C_j thanks to f^* . Formally, we frame $s_{f^*}(C_i, C_j) : \mathcal{C}_p \rightarrow \mathbb{R}^+$ as the f^* behavior similarity metric concerning C_i and C_j by:

$$s_{f^*}(C_i, C_j) = D_{KL}(f^*(C_i) || f^*(C_j)) \quad (3)$$

where $D_{KL}(\cdot || \cdot)$ denotes the Kullbach-Liebler divergence. This metric is widely used in machine learning problems. It has been deeply studied in various applications, especially for deep-based classification problems. In such problems, data representation is rendered as probability laws, and Kullbach-Liebler divergence is used in this context to quantify the similarity between inferred and groundtruth probability laws.

Domain and signal relevancy unification We introduce here our process for unifying those two modalities in order to have a global concept ordering. For each modality, we have obtained real values quantifying the relative marginal relevance of each concept. Given a concept, we obtained the relative joint relevancy (i.e., the relative global concept relevancy) by multiplying each marginal value (i.e., the relative concept domain relevancy value and the relative concept signal similarity). More formally, computing the relative global ordering concept relevancy between concept C_i and C_j is the real value $a_{i,j}$ defined by:

$$a_{i,j} = \frac{d(C_i)}{d(C_j)} \times s_{f^*}(C_i, C_j), \forall i, j \in \{1, \dots, L\}^2 \quad (4)$$

From now, instead of considering $L \times L$ relative local ordering values, we want to hierarchies globally those L concepts with a global concept ordering strategy. Since the relative global concept relevancy can be seen as interactive strengths between concepts, a natural representation to render those relational interactions are graph themselves. Thereby, we consider the graph K_L composed of L nodes that represent concepts with an adjacency matrix $\mathbf{A}(K_L)$ which entries are determined by $a_{i,j}$. However, although we have obtained most L meaningful concepts thank to previous processes, we look, at global scope, for the most dissimilar concepts pairwise ordonnance. Indeed, from explanation point of view, two highly similar concepts C_i and C_j (i.e., $a_{i,j}$ is low) bring similar insights regarding the explanation. In other terms, it produces redundant information that is unnecessary and may flood and alter the user understanding of phenomenon P . Higher values in $\mathbf{A}(K_L)$ stand for those less redundant concepts (relatively) regarding the explanation of P . But what is the concept that is both relevant and less redundant among concept candidates? This question can be reformulated under graph theory by which node has the higher normalized centrality. A good approach is to compute the PageRank [Page et al.(1999)Page, Brin, Motwani, and Winograd] of each node of K_L . Once obtained it gives a total ordering relation between nodes of K_L (i.e., concepts). Formally, we consider:

$$\widehat{\mathbf{A}}(K_L) = \mathbf{\Lambda}(\mathbf{A}(K_L)\mathbf{e})^{-1}\mathbf{A}(K_L) \quad (5)$$

which is the normalized version of $\mathbf{A}(K_L)$ where \mathbf{e} the unit vector of size L and for any fixed-size vector \mathbf{x} , $\mathbf{\Lambda}(\mathbf{x})$ denotes the diagonal matrix containing \mathbf{x} in its diagonal.

$\widehat{\mathbf{A}}(K_L)^T$ is a stochastic version of $\mathbf{A}(K_L)$ that by definition always admit a right eigenvector \mathbf{r} with eigenvalue equal to 1. Under this context, this eigenvector \mathbf{r} defines a probability law and its components are *PageRank* values of each node. Regarding the explanation process, the *PageRank* centrality measures yield a global concept ordering scheme where concept candidate with highest *PageRank* value is the explicative representant that proposes the less information redundancy while being in both modalities relevant. This global concept ordering procedure allows to tremendously shrink the search space to find relevant subgraphs which is known to be a combinatorial problem. Once addressed this refinement, we can go further and we propose a less coarsening approach that assesses relevancy at G nodes scope that we framed as the local concept ordering procedures.

Local concept ordering Considering only subgraph-level as the only set of explanation arguing terms may lead to incomplete formulation of explanations. Indeed, although in underlying manner, nodes relevance is already partially encoded in concept relevance quantification processes, nodes composing these subgraphs may have themselves their own role on the global concept ordering outcomes; that given a concept; node has non-uniform contribution to this outcome. Besides that purely signal-based argue, in many real-life applications, nodes may represent atoms for molecule representations or city on a roadmap for traffic forecasting and therefore have their own semantic embeddings that may not be rendered in a single subgraph-level focus. That is why, including such node-level data have to be included in our explanation conception pipeline. To carefully quantifying the contribution of each node within a concept candidate C_i we have exploited game theory. It consists in computing the *Shapley* value [Shapley(1951)] of each node i composing C_i . The Shapley value is a conceptual solution in cooperative game theory quantifying how important the marginal role of a player has in the game outcome. Considering a coalition of $K \in \mathbb{N}$ players indexed within $Q = \{1, \dots, K\}$ playing a cooperative game with a game payoff $v : \mathcal{P}(Q) \rightarrow \mathbb{R}$ where $\mathcal{P}(Q)$ denotes all possible subsets of Q . The Shapley value of a player $i \in Q$, is defined by:

$$\gamma_Q(i) = K \mathbb{E}_{j \sim \mathbb{U}_K} \left[\mathbb{E}_{S \subset Q \setminus \{i\}} [v(S \cup \{i\}) - v(S)] \mid |S| = j \right] \quad (6)$$

We denote further $\gamma_j(i)$ the *Shapley* value of the node i of concept C_j .

Global and local concept gathering Under our context, given a node i that belongs to a concept C_j , computing the *Shapley* value of i required to consider all possible subgraphs of C_j and compute, according to them, the perturbing effects of i regarding f^* at C_j scope. Numerically, $\gamma_j(i)$ provides a precise concept relevance value of node i belonging to C_j regarding P ([Duval & Malliaros(2021)Duval and Malliaros,

Yuan et al.(2021)Yuan, Yu, Wang, Li, and Ji]). Note that this value $\gamma_j(i)$ remains dependent to C_j definition. From the computational point of view, the assessment requires $\mathcal{O}(2^{|G| \times p})$ inferences of f^* which can be intensive, even intractable in practice and is by definition dependent on the explainee concept assimilability constraint p . To overcome this issue, we can estimate each $\gamma_j(i)$ by a Monte Carlo estimation strategy with an error rate bounded. Those computations produce a set of L node-level explaining assessments $(\gamma_j)_j \subset \mathbb{R}^{|G| \times p}$ where each γ_j is normalized by its L_1 norm. We then extend each γ_j to $\gamma_j^{ext} \in \mathbb{R}^N$, such that for node i :

$$\gamma_j^{ext}[i] = \begin{cases} \gamma_j[i] & \text{if } i \in C_j \\ 0 & \text{otherwise} \end{cases}$$

And we concatenate columns wisely each γ_j^{ext} defined for a explainee concept assimilability constrain p in $\Gamma_p \in \mathbb{R}^{N \times L}$. Finally, our explanation map $\text{EiX-GNN}_{L,p}(P)$ ² of the phenomenon P with an explainee concept assimilability constrain p is algebraically defined as below:

$$\text{EiX-GNN}_{L,p}(P) = \Gamma_p \mathbf{\Lambda}(\mathbf{r}) \mathbf{e}^T \quad (7)$$

The explanation map $\text{EiX-GNN}_{L,p}(P) \in \mathbb{R}^N$ describes the relevance of each feature describing the phenomenon P with respect to p . In the context of deep graph classification, it described the normalized relevance of each node composing G regarding f^* with feature granularity of size p . Now we lead a quantitative and a qualitative study on real-world applications as well as providing an impact study regarding the explainee concept assimilability that we have introduced.

4 Results

4.1 Experimental setup

Datasets To assess our method we have used four real-world datasets that are made of human intelligible features : MNISTSuperpixels [Monti et al.(2017)Monti, Boscaini, Masci, Rodola, Svoboda, and Bronstein], PROTEINS [Borgwardt et al.(2005)Borgwardt, Ong, Schönauer, Vishwanathan, Smola, and Kriegel], MSRC [Shotton et al.(2009)Winn et al.(2005)Winn, Criminisi, and Minka], REDDIT-BINARY [Yanardag & Vishwanathan(2015)Yanardag and Vishwanathan]. These datasets are widely used in the literature for illustrating GNN explainer. We give further details regarding those datasets in Appendix A.1.

Learning procedures We have used two main GNN configurations for classifying our instances. Either based on GCN or GAT modules, astonishingly both produce similar results in terms of test accuracy. But GCN-based model is less parametrized than GAT-based one, so we have selected GCN models. Models architecture and learning setup are described in Appendix A.2.

Comparing methods For comparing our results, we have retained three state-of-the-art methods that achieve strong results for explaining GNN: GNNExplainer [Ying et al.(2019)Ying, Bourgeois, You, Zitnik, and Leskovec], SubgraphX [Yuan et al.(2021)Yuan, Yu, Wang, Li, and Ji], PGExplainer [Luo et al.(2020)Luo, Cheng, Xu, Yu, Zong, Chen, and Wang]. We give further details regarding these methods in Appendix A.3 .

Objective assessment metrics Assessing explanation quality or relevance given a phenomenon often deals with requiring a P -specialist approval. Context-free and objective method has been proposed for quantifying explanation method relevance. Two of them have been widely used in the literature [Duval & Malliaros(2021)Duval and Malliaros(2021)Pope et al.(2019)Pope, Kolouri, Rostami, Martin, and Hoffmann, Yuan et al.(2021)Yuan, Yu, Wang, Li, and Ji], namely Infidelity [Yeh et al.(2019)Yeh, Hsieh, Suggala, Inouye, and Ravikumar] and spatial sparsity [Duval & Malliaros(2021)Pope et al.(2019)Pope, Kolouri, Rostami, Martin, and Hoffmann, Yuan et al.(2021)Yuan, Yu, Wang, Li, and Ji]. We have used them to lead our quantitative study. Further details are provided in Appendix B.1.

4.2 Qualitative assessment: a real-world application

For illustrating our method we have oriented our experiment in an omniscient setup: $L = 70$ allowing drawing complex explanations with large argumentation basis and $p = 0.05$ for focusing on finest data details. We discuss afterward the marginal impact of each of these parameters in regard with the omniscient setup as a baseline. Each instance of *REDDIT-BINARY* is a discussion involving users with varying knowledge regarding the discussion topic. Some users have a serious understanding of the subject and can be seen as experts.

²Code repository will be released after reviewing process.

Explaining those discussions, in terms of user interactivity, consist in looking for those experts as mentioned in [Ying et al.(2019)Ying, Bourgeois, You, Zitnik, and Leskovec].

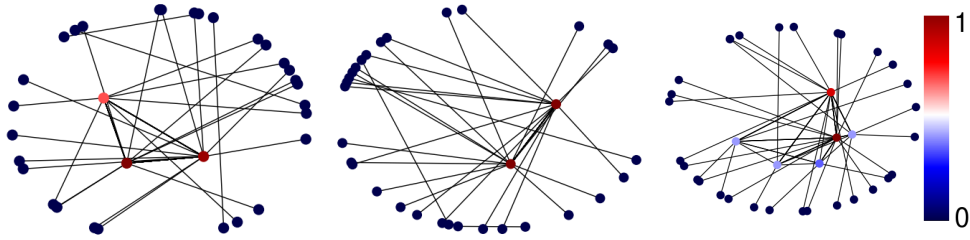


Figure 1: Threads explanation with EiX-GNN

It turns out that expert is actually users that are responding the most to all other users. In graph theory terminology, those experts are represented by node with highest relative degree. Under the omniscient setup, EiX-GNN highlights those expert users and it locates them in a graph with low attribution to users with low interactivity (low knowledge) and high attribution to users with high interactivity (high knowledge), i.e., experts (Figure 1). Those results are in accordance with those obtained in [Ying et al.(2019)Ying, Bourgeois, You, Zitnik, and Leskovec]. Now we measure the marginal impact of each of p and L on some thread explanations and we compared such explanations with the omniscient baseline which is seen as the practically upper bound of quality explanations that required both high understanding and high knowledge (i.e., retrieving only most relevant information, localizing carefully thread experts). From the social point of view, we seek to qualify the marginal impact of these two parameters on the social expressiveness of EiX-GNN explanations. What we expect to get is to have uncomplete explanation with an uncomplete concept basis (i.e low L) and coarsed explanation with a large explainee concept assimilability constraint p , all in regard with a complete and finest explanation through the omniscient baseline.

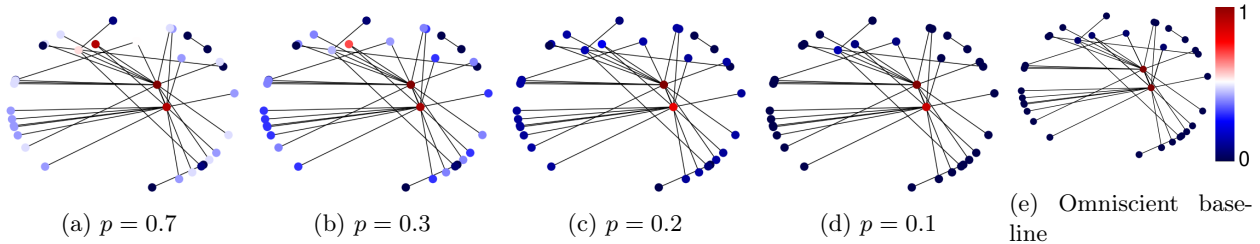


Figure 2: Social expressiveness: explainee concept assimilability constraint variation

Explainee concept assimilability constraint: qualitative impact In this sequence of explanations of the same thread, we have made an explainee concept assimilability constraint variation and we have fixed the concept basis width. Low value of p stands for low explainee concepts assimilability constraint meaning that the explainee is able to reach finest understanding of the phenomenon. Here, it signifies to be able to precisely recognize thread expert which is the most relevant information in the context of *REDDIT-BINARY* classification. The opposite scheme appears with high value explainee concept assimilability constraint. We observe that as long as we raise the constraint penalty (p decreases), we gain insights (Figures 2c, 2d) with respect to explanation precision and we incrementally increase the knowledge quantity until reaching the omniscient regime (Figure 2e).

- $p = 0.7$: explanation is based on large concepts providing coarse knowledge, single interactivity users have quite important role in the explanation and experts have higher explaining value. This explanation is not the finest one but allow explainee to have an imprecise but global view of the thread. For low knowledge requirements, this explanation is suitable (Figure 2a).
- $p = 0.3$: we observe here that specialist-level information is far more emphasized than previously. We have experts recognizing and less insightful information are much discarded (single interaction users that are not specialists) (Figure 2b).
- $p = 0.2$: the previous tendency has been accelerated, specialist knowledge is far more mentioned than the poor knowledge (Figure 2c).
- $p = 0.1$: we have almost reached the omniscient regime and we have gained an understanding comparable to specialist one (Figure 2d).

Globally we observe that this explainee concept assimilability constraint behaves as a social-aware explanation fine tuner. High constraint provides general-trended information, this information is general but imprecise. It provides a global idea about the underlying phenomenon. It thus allows non-specialist individuals to handle those explanation of the phenomenon. As long as the constraint is raised, we tend to reach expert understanding of the explained phenomenon by including only finest details and discarding entities that only are able to supply generalities that are only dedicated to non-specialist peoples.

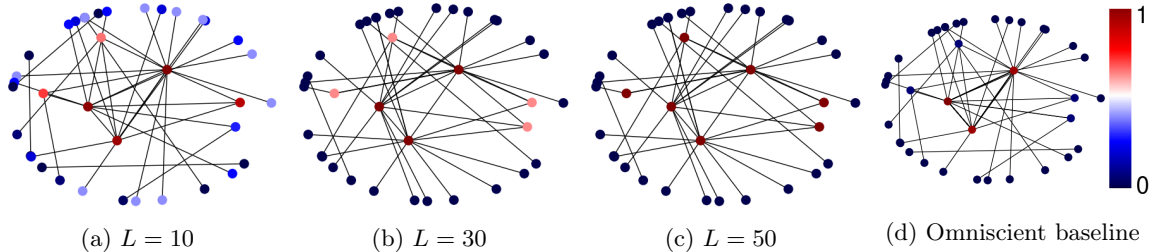


Figure 3: Social expressiveness: concept basis variation

Number of concepts: qualitative impact We observe that as long as the number of concepts L increases from low width (Figure 3a) to high-width (Figure 3c) the explainer is able to furnish more and more precise explanations. So, as much as the concept basis width increases, we are getting closer to the omniscient baseline (Figure 3d). Actually, this behavior can be expected since if the explainer is able to provide explanation based on large arguments basis, we obtain precise and meaningful explanations ³.

4.3 Quantitative assessment on real-world data

Objectives metrics overall benchmarking As a global view regarding state-of-the-art methods, we have compared objective metrics between each dataset and each method. For EiX-GNN, we have used the omniscient setup presented above. We find out that our method proposes numerically fewer infidel explanations with at least a factor 10^2 on MNISTSuperpixel and REDDIT-BINARY and MSRC-21 and a factor 10 on PROTEINS and MSRC-9. As well, our method outperforms other compared methods regarding the sparsity of explanation maps by at least a factor 10^3 on MNISTSuperpixel and REDDIT-BINARY, a factor 10^4 on MSRC-9, a factor 10^2 on MSRC-21 and a factor 10 on PROTEINS. We provide in Appendix B.1 a summarizing table (Table 1) with a detailed version of these measurements.

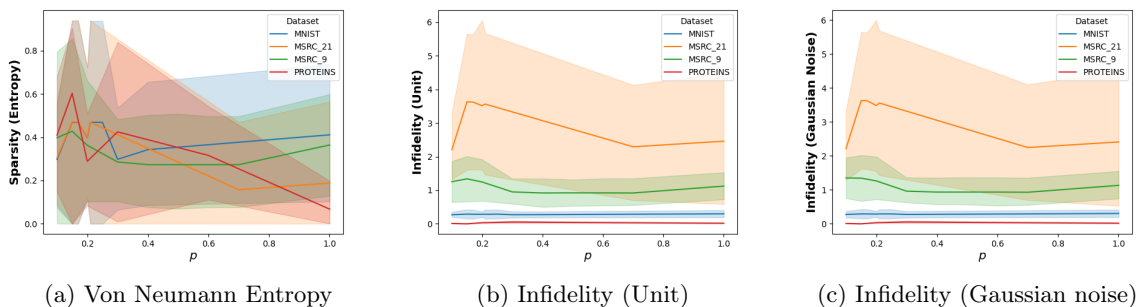


Figure 4: Impact of p regarding objective metrics

Explainee concept assimilability constraint: quantitative impact Regarding the explainee concept assimilability constraint, we find out that in average it does not have an impact on the infidelity of the explanation toward the classifier has shown in Figure 4. Moreover, specialist-level explanation is more concise so inherently sparser as shown by Figures 2d, 3c. It means that the value of p does not impact the explanation quality provided by EiX-GNN and that EiX-GNN still provides relevant explanation regardless the explainee knowledge for a given phenomenon.

³An analogous vision can be made with the neural network complexity that, if adapted to the learning task, allows to have powerful model.

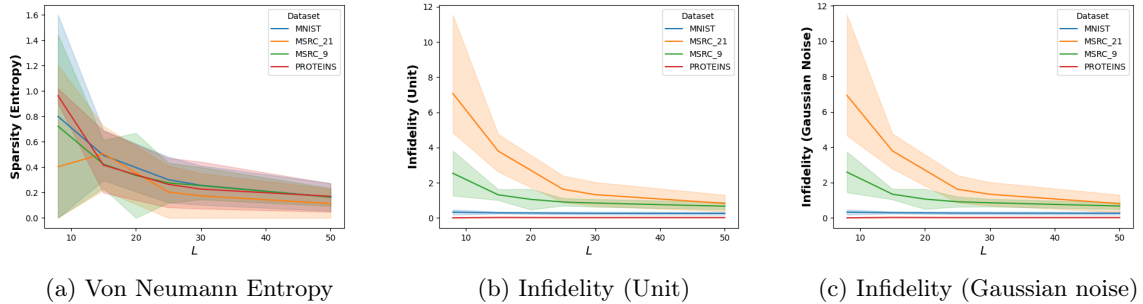


Figure 5: Impact of L regarding objective metrics

Number of concepts: quantitative impact For the concept basis width, we recover numerically our statement regarding the fact that large argument basis favors to produce expressive explanations which are prone to be on one hand less infidel and, on the other hand, more concise as shown in Figure 5.

5 Conclusion

It is common to encounter deep learning models and especially GNN for tackling academic and industrial problems notably in sensitive contexts such as healthcare, autonomous driving, etc. Their powerfulness is often at the expense of having humanly unintelligible decision processes that these models design. It raises serious issues for a safety deployment of these models in our society. We need to explain their inner working in order to gain insights and rendering them trustworthy. Nonetheless, explaining processes are profitable only and only if explanations are suited to the explainee. State-of-the-art methods often provide absolute explanation regardless explainee background or expectation and fail to include such explainee dependency although widely discussed in the literature. In this study, we address this concern with EiX-GNN, a new approach that fully integrates this ubiquitous dependency with defining the explainee concept assimilability notion allowing to adapt the explanation process to the explainee. We lead a qualitative study in regards with this social aspect over real-world data and we compared, with respect to objective metrics used in literature, the fairness and compactness properties in comparison with relevant state-of-the-art methods. In both settings, we provide meaningful results by, addressing the explainee-dependency issue and, outperforming state-of-the-art methods according to widely used objective metrics.

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A Experimental setup details

A.1 Datasets details

In order to provide meaningful results, we chose real-world datasets that incorporate human intelligible features. These datasets are often used [Baldassarre & Azizpour(2019)Baldassarre and Azizpour, Duval & Malliaros(2021)Duval and Malliaros, Huang et al.(2022)Huang, Yamada, Tian, Singh, and Chang, Lucic et al.(2022)Lucic, Hoeve, Tolomei, Rijke, and Silvestri, Pope et al.(2019)Pope, Kolouri, Rostami, Martin, and Hoffmann, Schnake et al.(2021)Schnake, Eberle, Lederer, Nakajima, and Ying et al.(2019)Ying, Bourgeois, You, Zitnik, and Leskovec, Yuan et al.(2020)Yuan, Tang, Hu, and Ji, Yuan et al.(2021)Yuan et al.] to illustrate explaining methods for GNN-based classifiers. Each of the following datasets is suited for graph classification problems. Note that REDDIT-BINARY does not need any prior knowledge to assess any explanation map and groundtruth explanation is easy to consider as mentioned in [Ying et al.(2019)Ying, Bourgeois, You, Zitnik, and Leskovec] on the contrary to PROTEINS which require chemical knowledge. In the following, we found details regarding used datasets:

MNISTSuperpixel [Monti et al.(2017)Monti, Boscaini, Masci, Rodola, Svoboda, and Bronstein] is a dataset composed of 60000 graphs, that each represents a superpixel version of the well-known handwritten digit MNIST [Lecun et al.(1998)Lecun, Bottou, Bengio, and Haffner] dataset. Each MNISTSuperpixels instance is a graph representation of the original MNIST instance. Two vertices are linked according to their spatial proximity.

PROTEINS [Borgwardt et al.(2005)Borgwardt, Ong, Schönauer, Vishwanathan, Smola, and Kriegel] is a dataset counting 1113 labeled graphs. Each graph represents a protein that is classified as enzymes or non-enzymes. Nodes represent the amino acids and two nodes are connected if they also share the same spatial locality.

MSRC [Shotton et al.(2009)Shotton, Winn, Rother, and Criminisi, Winn et al.(2005)Winn, Criminisi, and Minka] datasets are used in image semantic segmentation problems. Each image is converted into a semantic superpixel version of it. In MSRC-9, which is composed of 221 labeled graphs, semantics labels are distributed among 8 semantic labels. In the MSRC-21 version, composed of 563 labeled graphs, extends the number of possible semantic labels to 21.

REDDIT-BINARY [Yanardag & Vishwanathan(2015)Yanardag and Vishwanathan] is a dataset composed of 2000 graphs where each of them represents a question/answer-based thread of Reddit, namely *r/IAmA* and *r/AskReddit*. In these graphs, nodes represent users and there is a link between two users if one has answered the other.

A.2 Classifier details

Here the general framework of graph classification problems under the view of GNN models.

A.2.1 Supervised graph classification problems

For \mathcal{G}, \mathcal{Y} two measurable spaces, we define $\mathcal{F}(\mathcal{G}, \mathcal{Y})$ the set of measurable functions going from \mathcal{G} to \mathcal{Y} . Given an i.i.d sampled finite dataset $\mathcal{D} \subset \mathcal{G} \times \mathcal{Y}$ where each element $Z_i = (G_i, Y_i)$ is a graph G_i and its label Y_i representing the class it belongs to. A loss function is mapping $\mathcal{L} : \mathcal{F}(\mathcal{G}, \mathcal{Y}) \times \mathcal{D} \rightarrow \mathbb{R}$ quantifying how well a learning mapping $f \in \mathcal{F}_{a, \theta} \subset \mathcal{F}(\mathcal{G}, \mathcal{Y})$ associated G_i to its true label Y_i conditioned by a neural network architecture a and a learning parameter θ . For a given architecture \hat{a} , we seek f^* such that:

$$f^* = \arg \min_{f \in \mathcal{F}_{\hat{a}, \theta}} \mathbb{E}_{Z \sim \hat{\mathcal{D}}} [\mathcal{L}(f, Z)] \quad \text{with} \quad \mathbb{E}_{Z \sim \mathcal{D}} [\mathcal{L}(f, Z)] = \int_{\hat{\mathcal{D}}} \mathcal{L}(f, z) d\mathbb{P}_Z(z) \quad (8)$$

where $\hat{\mathcal{D}}$ is f_θ -unseen data and $Z = (G, Y)$ where G is a \mathcal{G} -valued random variable, Y is a \mathcal{Y} -valued random variable and \mathbb{P}_Z is the image probability measure of Z in $\hat{\mathcal{D}}$. In the context of graph classification, f is a GNN model and \mathcal{L} is the cross-entropy loss between the inferred label conditional probability law and its ground truth-conditional probability law.

A.2.2 Learning details

Except for the classification task on MNISTSuperpixel, we have trained two GNN models : one based on GCN [Kipf & Welling(2017)Kipf and Welling] and the other based on GAT [Veličković et al.(2018)Veličković, Cucurull, Casanova, et al.] that we name here generically as the descriptor module of the classifier. We chained two descriptor modules then we feed outputs to a global average pooling layer, a linear module is then used to classify with softmax function. In between layers, we use Relu function as activation function. For the MNISTSuperpixels dataset,

we use four chained descriptor modules and tanh as an activation function. All these different implementations use the ADAM [Kingma & Ba(2017)Kingma and Ba] version of the stochastic gradient descent approach with the same learning parameter equals to 10^{-4} . We use an Intel © Xeon Silver 4208 and Nvidia © Tesla A100 40 GB GPU for our training during 100 epochs. Under this consideration, we have obtained for each dataset an accurate classifier as accurate as those used in comparing method experiments.

A.3 Comparing method details

As comparing methods, we have used three black-box model-based local post-hoc methods that have achieved strong results in the literature. We give here additional details regarding these methods.

GNNExplainer [Ying et al.(2019)Ying, Bourgeois, You, Zitnik, and Leskovec] is a local post-hoc model-based explaining method suited for GNN. It looks after which subgraphs, derived from the input graph, contain the highest mutual information with the this one. This method has achieved strong results on many explanations problems.

SubgraphX [Yuan et al.(2021)Yuan, Yu, Wang, Li, and Ji] is also a local post-hoc model-based explaining method suited for GNN. From the input graph, it uses a Monte Carlo Tree Search method to find heuristically relevant substructures for explanations purposes.

PGExplainer [Luo et al.(2020)Luo, Cheng, Xu, Yu, Zong, Chen, and Zhang] share the same idea as GNExplainer but is rather concentrated on which edges in the input graph is important to conserve the classifier expressivity.

B Objective assessment metric details

Explaining internal decision processes involved in classification problems are often linked with the necessity to assess obtained saliency maps meaningfulness. Thus it requires task-related expert assessment which is subjective and consequently biased. Literature has proposed several objective metrics that are expert independent to evaluate quantitatively the quality of explanation maps.

Infidelity [Yeh et al.(2019)Yeh, Hsieh, Suggala, Inouye, and Ravikumar] quantifies in which manner the explanation maps provided by an explanation mapping ϕ of predictions made by an optimized classifier f^* change when an input \mathbf{X} is perturbed by a random variable \mathbf{I} following a perturbation density B . It is defined by:

$$\text{Infid}(\phi, f^*, \mathbf{X}) = \mathbb{E}_{\mathbf{I} \sim B} [(\mathbf{I}^T \phi(\mathbf{X}, f^*) - (f^*(\mathbf{X}) - f^*(\mathbf{X} - \mathbf{I})))^2] \quad (9)$$

The perturbing distribution B is used to be a standard normal distribution, as mentioned in [Yeh et al.(2019)Yeh, Hsieh, Suggala, Inouye, and Ravikumar].

Sparsity Generally speaking, concise explanations are preferred than wide explanations that drown pertinent information. This statement does not dependent on the context of the explanations, so it is an objective statement. The Von Neumann entropy appears to be a good candidate for measuring such sparsity [Hurley & Rickard(2009)Hurley and Rickard]. The Von Neumann entropy of a probability distribution encodes the uncertainty amount induced in this probability distribution. It can be seen as a sparsity metric since if the distribution mass is spatially concentrated on the domain (i.e., lower entropy) it induced that explanation arguments are clearly identified. On the contrary, if the entropy is important, it means that explicative elements are blurry diffused and scattered on the domain which is less insightful for the user. For a probability distribution $\pi \in [0, 1]^d$ it is defined as :

$$H(\pi) = -\mathbb{E}_{\pi} [\ln(\pi)] \quad (10)$$

B.1 Summarized quantitative results

Here we have summarized quantitative results we have obtained when we have benchmarked our methods with comparing methods over real-world datasets. As mentioned by the \downarrow symbol, the lower the better.

Dataset	Explainer	Entropy (\downarrow)	Infidelity (Gaussian) (\downarrow)	Infidelity (Unit) (\downarrow)
MNISTSuperpixels	EiX-GNN	9.41E-01	5.69E+00	5.69E+00
	GNExplainer	1.30E+03	2.43E+05	2.44E+05
	PGExplainer	1.21E+03	1.80E+04	1.80E+04
	SubgraphX	1.70E+02	1.31E+03	1.31E+04
PROTEINS	EiX-GNN	9.37E-01	2.38E-01	2.78E-01
	GNExplainer	5.21E+01	3.36E+02	3.47E+02
	PGExplainer	7.02E+01	8.23E+00	8.21E+00
	SubgraphX	1.40E+01	4.56E+01	4.56E+01
MSRC-9	EiX-GNN	9.02E-01	2.29E-05	9.68E-05
	GNExplainer	7.84E+01	1.14E+03	1.12E+03
	PGExplainer	8.69E+01	2.31E+03	2.29E+03
	SubgraphX	4.45E+01	2.69E+03	2.70E+03
REDDIT-BINARY	EiX-GNN	4.02E-01	2.64E-02	4.63E-01
	GNExplainer	6.71E+01	5.17E+03	5.14E+03
	PGExplainer	5.61E+01	2.35E+02	2.36E+02
	SubgraphX	3.95E+01	1.11E+03	1.110E+03
MSRC-21	EiX-GNN	8.54E-01	2.02E+00	2.05E+00
	GNExplainer	2.79E+02	1.03E+04	1.04E+04
	PGExplainer	1.90E+05	8.74E+02	8.74E+02
	SubgraphX	4.82E+03	3.67E+04	3.67E+04

Table 1: Comparison between EiX-GNN and compared method over three objective quality assessment measures for benchmarked datasets