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# EiX-GNN : Concept-level eigencentraliity explainer for graph neural networks

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## Abstract

Explaining is a human knowledge transfer process regarding a phenomenon between an explainer and an explainee. Each word used to explain this phenomenon must be carefully selected by the explainer in accordance with the current explainee phenomenon-related knowledge level and the phenomenon itself in order to have a high understanding from the explainee of the phenomenon. Nowadays, deep models, especially graph neural networks, have a major place in daily life even in critical applications. In such context, those models need to have a human high interpretability also referred as being explainable, in order to improve usage trustability of them in sensitive cases. Explaining is also a human dependent task and methods that explain deep model behavior must include these social-related concerns for providing profitable and quality explanations. Current explaining methods often occlude such social aspect for providing their explanations and only focus on the signal aspect of the question. In this contribution we propose a reliable social-aware explaining method suited for graph neural network that includes this social feature as a modular concept generator and by both leveraging signal and graph domain aspect thanks to an eigencentraliity concept ordering approach. Besides our method takes into account the human-dependent aspect underlying any explanation process, we also reach high score regarding state-of-the-art objective metrics assessing explanation methods for graph neural networks models.

## 1 Introduction

Graphs are widely used data structures involved in many real-world problems. Graph Neural Network (GNN) [11] are artificial neural networks suited for such data structure. For graph classification, node classification or link prediction tasks, GNN models have shown impressive performances [5, 16, 21]. Artificial neural networks are more and more used in daily life task, including GNN. GNN models show impressive results in drugs design [2], web recommendations [17] or traffic forecasting [6]. A major drawback of those deep models is their occluded internal decisionnal processes. For many daily usage of such models, 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. Nonetheless, understanding and interpreting decisions remain human-relative and context-dependent notions. One of those social-related requirements is that an explainer must adapt its explanation formulation according to the relative background of the explainee regarding the phenomenon to explain. 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. 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 and provide its relevance against compared methods.

## 2 Related Work

The explaining process has been intensively numerically investigated despite the lack of common ground knowledge of what an explanation is and how to compare them. Moreover several methods have been designed according to different paradigms. XGNN [19] is a model-level approach that generates iteratively explaining graphs through a reinforcement learning procedures. During this sequential process, each graph is upgraded from the previous one, according to the learned policy. From an empty graph, nodes and related features are incorporated until a sufficient large graph sequence has been generated. The state space of this Markov Decision process can be assimilated to the cartesian product of the node space and finite feature space, which is a finite-dimensional space, under these conditions, a sufficient long graph sequence leads to an optimal solution. GNNExplainer [18] is a mask generator model based on mutual information optimization. It starts with randomly initialized nodes and node features masks jointly optimized, with mutual information, against the class label of the assessed graph. PGExplainer [10] is also based on maximizing mutual information between a class label and a highly contributing graph towards GNN prediction. Explained graphs are sampled from a probability distribution where their parameters are learned to use a multiperceptron. SubgraphX [20] derived connected subgraph sequences from the input graph, to overcome the relevant information flow breaks that may arise in PGExplainer or GNNExplainer. To address this generation problem, SubgraphX uses a Monte Carlo Tree Search and assigns the shapely value of each graph; the higher the shapely value is, the more the subgraph is pertinent concerning explainability purposes. Layer-wise Relevance Propagation (LRP) [12] is an adaptation of the original LRP implementation. For computing relevance, LRP-GNN adopts a walk-based approach, introducing the node anteriority and apply the original LRP propagation rule. 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. Besides aforementioned methods show interesting results, they often miss social-dependent parameters, a central importance in any human-related explanation process. We tackle this issue by supplying an efficient explaining method for graph neural networks that take into account such aspects.

## 3 Problem formulation

Explaining is a human knowledge transfer process involving an explainer  $E^*$  and an explainee  $\tilde{E}$  concerning a phenomenon  $P$ . 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  $P$  are already acquired by the explainee  $\tilde{E}$ . Only finer details must be provided by the explainer  $E^*$  for 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 coarsed 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 GNN explanation framework

**Graph Neural Network** A graph  $G = (V, E)$  is a couple of two sets. The set  $V = \{v_1, \dots, v_N\}$  of size  $N$  is the set of nodes of  $G$ . We abusively denote by  $|G|$  the size of  $G$  which is the cardinal of  $V$ . The set  $E \subset V \times V$  is the set of edges describing the topology of  $G$ . This set can be fully encoded by its adjacency matrix  $\mathbf{A}$  defined as  $\mathbf{A} \in \{0, 1\}^{|V| \times |V|}$  such that  $\mathbf{A}_{i,j} = 1$  if  $(v_i, v_j) \in E$ , 0 otherwise. A graph is said to be either undirected if  $\mathbf{A}^T = \mathbf{A}$  or directed otherwise. In the context of graph representation learning,  $G$  is rather seen as a domain which structure is determined by the topology of  $G$  (i.e. described thanks to  $\mathbf{A}$ ) and a  $\mathcal{H}$ -valued signal  $x$  with  $V$  as a support. Here  $\mathcal{H}$  denotes a  $d$ -dimensional Hilbert space. Under this paradigm, graphs are couples  $(\mathbf{X}, \mathbf{A})$  where  $\mathbf{X} = \{\mathbf{x}_i = x(v_i) | v_i \in V\}$ . One singularity of this data structure is that node ordering do not matter. Graphs are very rich mathematical objects that are widely used for representing real-world problems. There is an increasingly interest from the community to integrate such data structure in deep learning frameworks. Powerful graph signal encoder has been proposed. They leverage at the same time; deformation stability and scale separation, ubiquitous notions in modern deep learning approach; and the aforementioned permutation insensibility. Such models are named GNN. For instance, inspired by Convolutional Neural Network (CNN), Graph Convolutional Network (GCN) [8] proposes a learning module which follows a nonparametric local signal permutation-invariant aggregation scheme. This module has been extended by the Graph Attention Network (GAT) [14] module which proposes an attentional node-pairwise interaction scheme for encoding local signals. Those modules show strong results for node classification, graph classification or link prediction problems.

**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  $\theta$ . For a given architecture  $\hat{a}$ , we seek  $f^*$  such that:

$$f^* = \arg \min_{f \in \mathcal{F}_{\hat{a},\theta}} \mathbb{E}_{Z \sim \hat{\mathcal{D}}} [\mathcal{L}(f, Z)] \quad \text{with} \quad \mathbb{E}_{Z \sim \mathcal{D}} [\mathcal{L}(f, Z)] = \int_{\mathcal{D}} \mathcal{L}(f, z) d\mathbb{P}_Z(z) \quad (1)$$

where  $\hat{\mathcal{D}}$  is  $f_\theta$ -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.

**Explaining graph classification models** Like modern deep learning models, GNN model leverages signal evolving on domain localities describing elementary low-level representations which are recursively combined (producing higher-level representation) in order to englobe all those sub-representations and carefully encoding them until producing the output. At a given model depth, such subrepresentations are, in a domain aspect: subgraphs of the input graph; and in a signal aspect: sub-parts of the signal evolving on such subgraph structure. Under the aforementioned graph learning paradigm, we redefine the subgraph  $G_S$ , denoted as  $G_S \subset G$ , of a graph  $G = (\mathbf{X}, \mathbf{A})$  of size  $|G| = |\mathbf{X}| = N$ . Considering  $\mathbf{X}_S \subset \mathbf{X}$ , we define the subgraph  $G_S = (\mathbf{X}_S, \mathbf{A}_S)$  of  $G$  such that  $\mathbf{X}_S = \{\mathbf{x}_i = x(v_i), v_i \in S \subset V\}$  and  $\mathbf{A}_S$  is the adjacency matrix of  $G_S$  which is the same size as  $\mathbf{A}$  but we respect the new node adjacency distribution induced by  $\mathbf{X}_S$ . More generally, explaining methods that deal with learned signal thanks to a deep model often focus on finding relevant subdomains and associated signals that preserve model abilities (e.g. model performance, model expressivity, etc.) without taking into account the social aspect underlying any explanation procedures. The design of EiX-GNN has as key component this social-aware feature that, as far as we know, state-of-the-art methods do not consider.

## 4 EiX-GNN

**EiX-GNN** (eigencentralality explainer for graph neural network) provides its explanations according to a set of atomic concepts. These concepts are for explanation processes that coins are for money exchanges. They are the elementary parts of the explanation process that explainers, when explaining, will build their arguments upon those 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-dependancy 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  $P$ . We define phenomenon  $P$  as being a  $\mathcal{F}(\mathcal{G}, \mathcal{Y}) \times \mathcal{G} \times \mathcal{Y}$ -valued random variable <sup>1</sup>. In the following, excepting for contrary mentions, we consider the phenomenon  $P = (f^*, G, Y)$  where  $f^*$  is an optimized GNN classifier which has been trained on a dataset  $\mathcal{D}$  which  $(G, Y)$  belongs to. We consider that graph  $G = (\mathbf{X}, \mathbf{A})$  is 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 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.

### 4.1 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  $|C_p| = \lfloor |G| \times p \rfloor$ . From a signal point of view, it describes a sub-part of the signal evolving on a subdomain of  $G$ . To generate those concepts, we have selected sampling approaches which depends 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 graphs is not adapted, thus 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  $v_j \in \mathcal{N}_i = \{v_j | (v_i, v_j) \in E\} \subset V$  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 of the node  $v_i$  conditionally to  $P$  by:

$$\alpha_P(v_i) = \mathbb{E}_{v_j \sim \mathbb{U}_{|\mathcal{N}_i|}} [s(v_i, v_j) | v_i, P] \quad (2)$$

With a normalizing constant  $F$  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 determinitating pertinent

<sup>1</sup>Note : since  $G$  is a  $\mathcal{G}$ -valued random variable, it follows that the node set  $V$  of  $G$  is a  $\mathcal{V}$ -valued random variable and the edge set  $E$  of  $G$  is a  $\mathcal{E}$ -valued random variable. The probability space  $\mathcal{G}$  can thus be seen as the product of  $\mathcal{V} \times \mathcal{E}$  which is a probability space as well.

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  $P$ . The impact of the values taken by  $p$  and  $L$  will be further investigated in supplementary part.

## 4.2 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 hierarchizing 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 pairwise.

**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

$$d(G) = \frac{(2 \times \mathbf{1}_{\{\mathbf{A}=\mathbf{A}^T\}} + \mathbf{1}_{\{\mathbf{A} \neq \mathbf{A}^T\}})M}{N(N-1)} \quad (3)$$

It measures how  $C_i$  tends to be a complete graph. We choose this measure because of the local aggregation operation (e.g. sum) involve in many GNN models. It appears that complete substructures (i.e. subdomains) aggregate much more signal information than sparser substructures. Indeed, widely used GCN-based or GAT-based GNN models aggregate node signal representation according to node neighborhoods. The completeness aspect of such a substructure does not ensure that they are more relevant than a sparser one but we empirically measure that node feature has a significant variance (i.e. signal variance) across the node set of  $G$ . From a statistical point of view, by averaging node information with many node signal representations it produces a more fidel local signal representation than with taking less node signal representation. As well as in local signal representation, when dealing with the same information aggregation strategy, the error made in the relevance attribution of a node given  $P$  is much farther from the one which has been obtained with far fewer neighboring nodes. The prior on the complete structure of  $C_i$  is thus more suited for less node importance attribution error than with a more degenerated concept  $C_i$ . With relative edge density, we favor concepts that are closer to complete substructure than those which are more degenerated.

**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 Kullback-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 two concepts  $C_i$  and  $C_j$  by :

$$s_{f^*}(C_i, C_j) = D_{KL}(f^*(C_i) || f^*(C_j)) \quad (4)$$

where  $D_{KL}(\cdot||\cdot)$  denotes the Kullback-Liebler divergence.

Computing in a pairwise manner relative concept domain and signal similarity of the  $L$  concepts, we obtain a pairwise concept ordering between those  $L$  concepts. Indeed, with considering two concepts  $C_i$  and  $C_j$  such that  $i \neq j$ ,  $a_{i,j} = \frac{d(C_i)}{d(C_j)} \times s_{f^*}(C_i, C_j)$  quantifies how much  $C_i$  and  $C_j$  are similar in both, domain and signals, aspects at the same time. This quantity provides a relational measurement of two given concepts. It becomes natural to consider  $a_{i,j}$  as being the entries of the adjacency matrix of  $K_L$  that we denote now by  $\mathbf{A}(K_L)$  that is not symmetric. In terms of both concepts signal and domain dissimilarity, the concept that has to be considered the most is the one identified has been the highest dissimilar concepts within  $L$  concepts relatively to  $P$ . Under the terms of graph theory, such a concept is the one which has the highest eigencentality value among concepts of  $K_L$ . With considering:

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

as the normalized version of  $\mathbf{A}(K_L)$  with  $\mathbf{e}$  the unit-vector of size  $L$ , we have that the eigencentality vector of  $K_L$  is the right eigenvector  $\mathbf{r}^2$  of  $\widehat{\mathbf{A}(K_L)}^T$  which has 1 as eigenvalue. Formally  $\mathbf{r}$  satisfies the following equation :

$$\mathbf{r} = \widehat{\mathbf{A}(K_L)}^T \mathbf{r} \quad (6)$$

Thereby, components of  $\mathbf{r} = (r_i)_{i \in \{1, \dots, L\}}$  provide a natural ordering between  $L$  sampled concepts given  $P$ .

### 4.3 Local concept ordering

For each of the  $L$  concepts, the global concept ordering phase assigns a global score  $r_i$  to each concept  $C_i$ . It means that nodes composing  $C_i$  have a uniform contribution in explaining  $P$  proportional to  $r_i$ . Nonetheless, we know that in any graph learning problems, each node provides a varying contribution towards the learning task as mentioned in section [number]. Previously, we took the same approach for getting some trends concerning prior node relevance distribution, this compute has a complexity  $\mathcal{O}(N^2)$  where  $N$  is the number of nodes composing  $G$ . Here we consider subgraphs of  $G$  which have a fixed size  $\lfloor Np \rfloor \leq N$  for all  $p \in [0, 1]$ . Since we deal with smaller graphs (i.e. concepts), we investigate a more precise strategy for quantifying node relevance distribution. Given a concept  $C_i$ , it deals with computing the Shapley value of each node  $v_j$  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 measurable function  $v : \mathcal{P}(Q) \rightarrow \mathbb{R}$  where  $\mathcal{P}(Q)$  denotes all subsets of  $Q$ . With supplying counting measure  $\mu$  to  $\mathcal{P}(Q)$ , the Shapley value of a player  $i \in Q$ , is defined by

$$\nu(i) = K \mathbb{E}_{j \sim \mathbb{U}_K} \left[ \mathbb{E}_{S \subset Q \setminus \{i\}} [v(S \cup \{i\}) - v(S) | \mu(S) = j] \right] \quad (7)$$

Computing such value has a complexity of  $\mathcal{O}(2^K)$  which is far more than the previous shallow node relevance computing procedure. Under our context, we want to provide at a node level a precise concept relevance value regarding  $P$ . With being consistent with the approach described in [section] (i.e. quantifying  $f^*$  behavior changing when removing some nodes). For a given node  $v_j$  belonging to a concept  $C_i$ , computing the Shapley value of  $v_j$  required to consider all possible subgraphs of  $C_i$  and compute the perturbing effect value of  $v_j$  over  $f^*$ . As mentioned, this computes is intensive. If we assume that a  $f^*$  call take  $t \sim \mathcal{O}(1)$  then it requires an amount of time surrounding  $\mathcal{O}(2^{\lfloor Np \rfloor})$  which is dependent on the explaine concept assimilability constraint. We can adopt a Monte Carlo sampling strategy for computing the Shapley value of  $v_j$  in order to have a reasonable time computation for any level of explaine concept assimilability constraint with a quantifiable error on the approximation made.

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<sup>2</sup>Since  $\widehat{\mathbf{A}(K_L)}^T$  is a stochastic matrix it always admits an eigenvalue equal to 1. Analogously, we can see  $(C_l)_{l \in \{1, \dots, L\}}$  as a  $C_p$ -valued irreducible and recurrent Markov chain which admits its stationary law  $\mathbf{r}$ .

Once achieving global and local concepts ordering, we concatenate node relevance distribution described under the node set of  $G$  that we denote by  $\bar{\mathbf{X}} \in \mathbb{R}^{N \times L}$ . Then, we provide our explanation mapping  $\xi_p$ <sup>3</sup> of  $P$  through

$$\xi_p(P) = \text{diag}(\mathbf{r})\bar{\mathbf{X}}^T \quad (8)$$

## 5 Experiments

We first introduce datasets we used to provide our explanation through EiX-GNN. We then provide the training conditions and setup of each of our GNN classifier. Finally, we provide a quantitative objective assessment of EiX-GNN according to objective metrics that are widely used in the literature.

### 5.1 Datasets

In order to provide meaningful results, we chose real-world datasets that incorporate human intelligible features. Each of the following datasets is suited for graph classification problems. (a) MNISTSuperpixels [4] is a dataset composed of 60000 graphs, that each represents a superpixel version of the well-known handwritten digit MNIST [9] dataset. Each MNISTSuperpixels instance is a graph representation of the original MNIST instance. Two vertices are linked according to their spatial proximity. (b) PROTEINS [3] 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. (c) MSRC [13, 15] 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.

### 5.2 Objective assessment metrics

Assessing explanation quality or relevance given a phenomenon often deals with requiring a  $P$ -experted approval. Acquiring such expert validation is not always practically obtainable. Context-free and objective method has been proposed for quantifying explanation method relevance. Explaining method quality is driven by quantifying the infidelity of the explaining method, measuring in which manner input masked by relevance features keep the deep model performances; and the sparsity, measuring the relative size of the relevant subdomain with respect to the whole domain size. Those metrics focus on explained signal itself rather than considering it with its structure particularity. In the context of graph deep models,  $\xi$ -explained graph signal  $\mathbf{X}$  is denoted by  $\xi(\mathbf{X})$ .

**Infidelity** [1] quantifies in which manner the explanation maps provided by the explainer changes in average when the input signal is perturbed by a random variable  $\mathbf{I} \in \mathbb{R}^d$  following a law  $\lambda$ . For a  $\xi$ -explained graph  $G = (\mathbf{X}, \mathbf{A})$ , and a deep model  $f^*$ , the infidelity is defined as

$$\text{Infid}(\xi, f^*, G) = \mathbb{E}_{\mathbf{I} \sim \lambda} \left[ (\mathbf{I}^T \xi(\mathbf{X}) - (f^*(G) - f^*(\hat{G})))^2 \right] \quad (9)$$

with  $\hat{G} = (\mathbf{X} - \mathbf{I}, \mathbf{A})$ .

In this study, we consider unit-reduced Gaussian noisy perturbation that we further respectfully refer as Gaussian perturbation and as unit-tensor perturbation that we refer to unit perturbation

**Entropy** is the Shannon entropy of the normalized node relevance map  $\bar{\mathbf{X}} \in \mathbb{R}^d$ . The entropy of a probability distribution encodes the uncertainty amount induced in this probability distribution. It can be seen as a sparsity metric since the more certain (i.e. lower entropy) the distribution is, the

<sup>3</sup>We project this relevance map to  $V$  by considering  $\xi_p(P)^T \mathbf{e} \in \mathbb{R}^N$ .



more the relevance is spatially concentrated and the explanation arguments clearly identified. On the contrary, the more the entropy is important, the more unclear the relevance attribution process is. It is defined as

$$H(\xi(\mathbf{X})) = - \sum_{i=1}^d \xi(\overline{\mathbf{X}}_i) \log(\xi(\overline{\mathbf{X}}_i)) \quad (10)$$

### 5.3 Experimental setup

**Training** For the datasets PROTEINS, MSRC-9, MSRC-21, we train a GCN<sup>4</sup>-based classifier composed of two chained GCN modules. We choose Relu fonction as activation function. A global pooling layer is then added, combined with a dense layer, allowing to classifying graphs according given classes of these datasets. For the MNISTSuperpixels dataset, we use four chained GCN modules, tanh activation functions and a concatenation of the output of global mean pooling and global maximum polling layers linked to a dense layer for achieving the classification task. Both model approach and their datasets produce accurate classifiers that we can rely on to apply our explaining method over. Accuracy of those deep models are provided in Supplementary. Those different implementations all use the Adam [7] version of the stochastic gradient descend 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 trainings.

**Explaining** Providing explanations of graph neural networks often deal with combinatorial problems (e.g. finding relevant subgraphs). It thus requires high amount of computes to obtain explanation method outcomes. Among state-of-the-art methods and for a given instance of data and computing machine, only GNNExplainer provides their explanation in a realistic amount of time (i.e. few seconds) whereas PGExplainer and SubgraphX provide their explanation respectfully in ten minutes and three hours in the same experimental setup. Consequently, we only consider for this study GNNExplainer as a baseline method. For benchmarking purpose we have fixed our concepts number to  $L = 15$  and our explaineer concept assimibility to  $p = 0.2$ . Considering the average number of nodes contained in each graphs of considered datasets, these parameters set up allow low probability of concept redundancy when they are sampled and provide fine-coarsed explanations.

### 5.4 Results

The objectives metric benchmark is summarized in Table 1. The impact of key parameter  $L$  on EiX-GNN objective assessments is described in Figure 1. Regarding objective metrics, EiX-GNN achieve stronger results on both infidelity approaches than GNNExplainer. EiX-GNN also provides explanation map with lower entropy than GNNExplainer. It means that explanation map produced through EiX-GNN are more specified than those proposed by GNNExplainer. Regarding the impact of key parameter  $L$  of EiX-GNN on its ability to provide non-infidel explanation map and specified ones, it appears that the greater  $L$  is the lower the infidel level of EiX-GNN is (in both settings). Regarding the entropy of explanation map provided by EiX-GNN, it also appears that the greater  $L$  is, the lower the explanation map entropy is. Meaning that explanation map specification increases with the number of concepts considered for building explanation upon. These results show that the more the argument basis is dense (i.e. considering a larger set of concepts that cover a larger span of explaining arguments) the more EiX-GNN is able to supply specific and phenomenon-closed explanation map. Since  $p$  has an higher impact in terms of amount of computations for providing explanation maps, its impact on objective metrics will be further discussed in Supplementary.

In this part, we supply additional work relative to the variation of the explaineer concept assimibility. Although, it is a impacting computationnal parameter as well as  $L$ , it is the only parameter that is truly

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<sup>4</sup>We discard the GAT usage since it achieve similar results on both classification accuracy and explanation-related metrics

Code repository will be released.

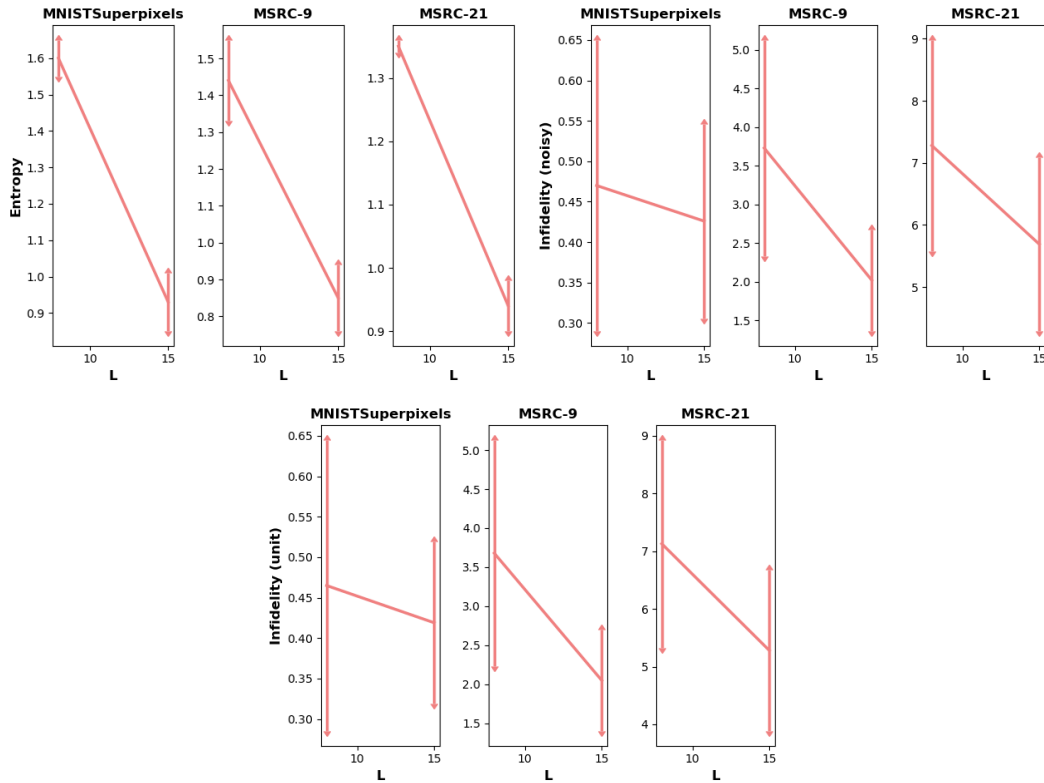


Figure 1: Impact of parameter  $L$  (i.e. number of concepts) over infidelity and entropy quality measures for a selection of datasets

Dataset	Explainer	Entropy	Infidelity (Gaussian)	Infidelity (unit)
MNISTSuperpixels	EiX-GNN	<b>9.41E-01</b> ( $\pm 3.6E-03$ )	<b>5.69E+00</b> ( $\pm 1.8E-01$ )	<b>5.69E+00</b> ( $\pm 1.8E-01$ )
	GNNEExplainer	1.30E+03 ( $\pm 1.8E+00$ )	2.43E+05 ( $\pm 2.6E+02$ )	2.44E+05 ( $\pm 1.5E+03$ )
PROTEINS	EiX-GNN	<b>9.37E-01</b> ( $\pm 1.0E-03$ )	<b>2.38E-01</b> ( $\pm 1.1E-03$ )	<b>2.78E-01</b> ( $\pm 1.2E-03$ )
	GNNEExplainer	5.21E+01 ( $\pm 1.0E+04$ )	3.36E+02 ( $\pm 3.8E+01$ )	3.47E+02 ( $\pm 3.9E+02$ )
MSRC-9	EiX-GNN	<b>9.02E-01</b> ( $\pm 4.0E-04$ )	<b>2.29E-05</b> ( $\pm 6.6E-01$ )	<b>9.68E-08</b> ( $\pm 6.1E-01$ )
	GNNEExplainer	7.84E+01 ( $\pm 1.3E+03$ )	1.14E+03 ( $\pm 6.9E+03$ )	1.12E+03 ( $\pm 1.1E+03$ )
MSRC-21	EiX-GNN	<b>8.54E-01</b> ( $\pm 4.9E-04$ )	<b>2.02E+00</b> ( $\pm 1.4E+00$ )	<b>2.05E+00</b> ( $\pm 1.5E+00$ )
	GNNEExplainer	2.79E+02 ( $\pm 4.2E+03$ )	1.03E+04 ( $\pm 6.8E+03$ )	1.04E+04 ( $\pm 7.2E+03$ )

Table 1: Comparison between EiX-GNN and GNNEExplainer over three objective quality assessment measures for a selection of datasets

dependent on the explainee. Without regarding the explainee background relative to a phenomenon  $P$ , an explainer must always provides the same explanation quality of the considered phenomenon. We provide here additionnal results that highlights that explanation quality, supplied by EiX-GNN, does not depend on the explainee concept assimilability constraint.

**Explainee concept assimilability quality impact study** The explainee concept assimilability  $p$  is a key component of EiX-GNN. This parameter is dependent on the explainee background regarding  $P$ . The explainee concept assimilability variation should not alter the explanation quality provided by the explainer. We have isolated (i.e.  $L = 20$ ) the impact of  $p$  shifting regarding objectives assessment metrics we have considered before. We summarized our results in Figure 5.4.

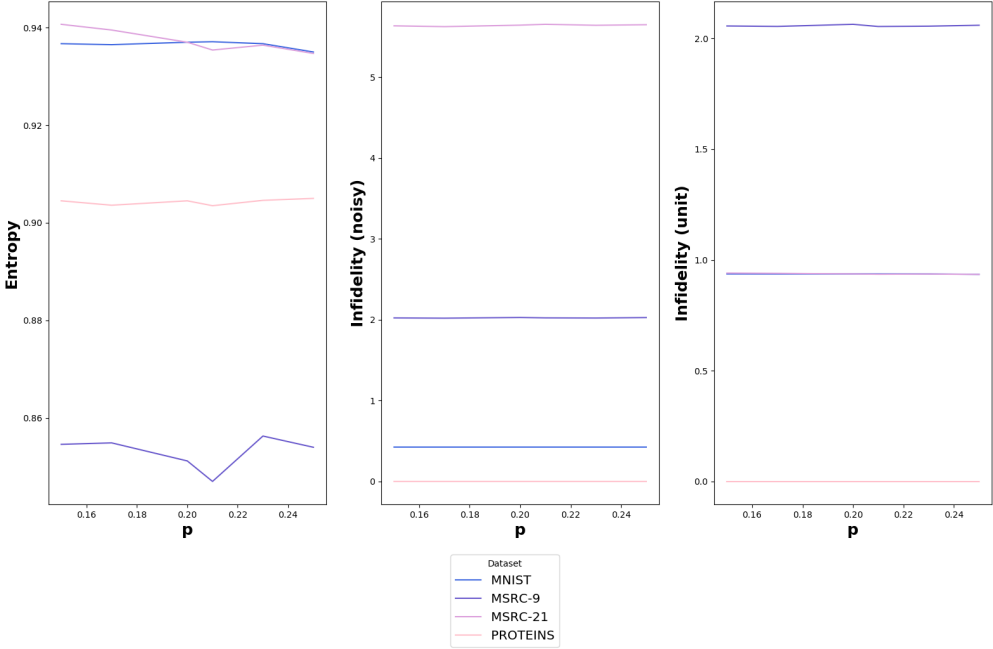


Figure 2: Impact of  $p$  with concept number  $L = 15$

We observe that entropy, Infidelity with Gaussian noise and Infidelity with unit baseline are respectfully constant with respect to  $p$ . It means that the value of  $p$  does not impact the explanation quality provided by EiX-GNN and that EiX-GNN can be suited for providing explanation regarding a phenomenon to a large public with high knowledge variability concerning this phenomenon.

## 6 Conclusion

Deep learning models, especially graph neural networks, are more and more considered for solving academic and industrial contemporary problems. When such models are used in a sensitive context (healthcare, law, etc.) their powerfulness for tackling the problem are often at the expense of having unintelligible internal that raises important concerns for safety broad deploying. It is thus important to explain such internal (i.e. signal propagation). But providing an explanation of any phenomenon is also a social-dependent task and more specifically when we want highly profitable explanations. Explaining a phenomenon is a knowledge transfer between an explainer (higher knowledge) and explainee (lower knowledge) regarding this phenomenon. State-of-the-art explaining methods suited for graph neural networks only focus on the signal aspect and do not include any social aspect in their

explanations. In this contribution, we propose a modular concept-based approach that integrates such social aspect underlying any explanation processes. This approach highlights the social dependency of the explanation process by showing that considering richer argument basis supply more specified and less infidel explanation regarding a phenomenon. Our method also provides substantial improvement of explanation quality by providing better results than state of the art methods with respect to widely used objective assessment metrics.

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