GRAPHSHAP: Motif-based Explanations for Black-box Graph Classifiers*

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Abstract. Most methods for explaining black-box classifiers (e.g., on tabular data, images, or time series) rely on measuring the impact that the removal/perturbation of features has on the model output. This forces the explanation language to match the classifier features space. However, when dealing with graph data, in which the basic features correspond essentially to the adjacency information describing the graph structure (i.e., the edges), this matching between features space and explanation language might not be appropriate. In this regard, we argue that (i) a good explanation method for graph classification should be fully agnostic with respect to the internal representation used by the black-box; and (ii) a good explanation language for graph classification tasks should be represented by higher-order structures, such as motifs. The need to decouple the feature space (edges) from the explanation space (motifs) is thus a major challenge towards developing actionable explanations for graph classification tasks.

In this paper we introduce GRAPHSHAP, a Shapley-based approach able to provide motif-based explanations for black-box graph classifiers, assuming no knowledge whatsoever about the model or its training data: the only requirement is that the black-box can be queried at will. For the sake of computational efficiency we explore a progressive approximation strategy and show how a simple kernel can efficiently approximate explanation scores, thus allowing GRAPHSHAP to scale on scenarios with a large explanation space (i.e., large number of motifs).

We devise a synthetic dataset generator with artificially injected motifs in order to empirically compare different masking approaches and to demonstrate that the proposed kernel is able to approximate the exact Shapley values with a computational complexity that is linear with respect to the number of explained features. Furthermore, we introduce additional auxiliary components such as a custom graph convolutional layer and algorithms for motif mining and ranking.

Finally, we test GRAPHSHAP on a real-world brain-network dataset consisting of patients affected by Autism Spectrum Disorder and a control group. Our experiments highlight how the classification provided by a black-box model can be effectively explained by few connectomics patterns.

Keywords: explainable artificial intelligence, graph classification, shapley values

1 Introduction

Model interpretability of prediction tasks is increasingly needed for accountability, trust, fairness and debugging [38,13,6,28], especially when machine learning algorithms are incorporated into decision-making that may directly affect people's lives [44]. While transparent-by-design models should be preferred for high stakes decisions [32], in an increasing number of cases black-boxes are already deployed and used as decision support-systems. Therefore, researchers in AI-intensive companies and

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academia devised model-agnostic techniques to provide local post-hoc explanations on model predictions [14,13]. While such methods mainly focus on tabular data [31,23], and have been further extended to images [35,39] and time series [4], much less attention have been devoted to provide actionable explanations for graph classification tasks.

Graphs are a powerful mathematical representation of several real-world systems and, as learning from networked-structures requires ad-hoc approaches [60,57], so do explanation techniques aimed at interpreting algorithmic decisions on graphs. Most model-agnostic explainability methods either rely on tabular data or on some form of vectorisation of the original input space: explanations are then provided by ranking the input features according to some scores [31,23,9], thus constraining the explanations to be expressed in the very same language of the training data of the black-box. Following the same approach in a graph classification task, one could embed the adjacency matrix of a graph in a d-dimensional space vector, and then feed the resulting graph dataset to a learning algorithm. When applying standard explainability methods, the explanation language for one given graph would correspond either to the whole adjacency matrix, or to the d-dimensional vector. The former option contains a high number of fine-grain features, while the latter option has limited explainability due to the not interpretable embedding transformation. Neither option is well suited for human understanding and interpretation.

Here we argue that (i) a good explanation method for graph classification should be fully agnostic w.r.t. the internal representation used by the black-box; and (ii) a good explanation language for graph classification tasks should be represented by motifs, as they are higher order structures which encode more information and are more adequate for human understanding. Thus our approach completely decouples the input space of the classifier from the explanation space.

1.1 Overview of contributions and roadmap

With the growing availability of Graph Neural Networks (GNNs) methods which can indifferently handle several different predictive tasks, such as, e.g., link predictions [7,55], node classification [16,22,12], and classification of the whole graph [56,48], the term "graph classification" is more and more used in the literature to indicate a general class of machine learning tasks on graph-structured data, typically having additional information in the form of nodes and edges features. In this paper, instead, we consider a specific type of graph classification that arises in many application domains, in which a specific node id corresponds to the same entity in all the input networks: for instance, in classification of brain networks, the same node id represents the same brain region in all the input graphs. We call this setting graph classification with node identity awareness [15,20,1]. While not every application domain requires node identity awareness, it is crucial to exploit these property whenever it occurs, as ignoring it represents an important loss of information.

More formally, we are given a database \mathcal{D} of graphs, where each graph $G \in \mathcal{D}$ is defined over the same set of nodes \mathcal{V} and it has a label in $\{0,1\}$ (for sake of simplicity we consider the binary classification case, but our approach can be easily extended to te multi-class case). Let \mathcal{G} denote the set of all possible graphs defined over \mathcal{V} , we want to learn a model that for any unseen graph $G \in \mathcal{G}$ it is able to predict whether it belongs to class 0 or 1.

In this context of graph classification with node identity awareness, we are given a "black-box" model $B: \mathcal{G} \to [0,1]$ returning, for any graph $G \in \mathcal{G}$, the probability that G is in class 1. Here "black-box" means we can not inspect B, we do not know the learning algorithm that produced B, nor its parameters, nor we have access to its training data. B might as well be an opaque executable or an exposed API. The only requirement about B is that it can be queried at will. The problem tackled in this paper is that of producing an explanation for the black-box graph classifier logic, using an explanation language (motifs) that does not coincide with the input space of the classifier (adjacency matrix).

After providing the needed background (§2) we formally state our problem (§3), and we introduce our method GRAPHSHAP (§4), a Shapley-based approach for motif-based explanations of black-box graph classifiers. One key mechanism in any Shapley-based explanation approach is the creation of

the features coalitions to query the black-box. In our setting this corresponds to the task of masking a set of motifs from a given graph. For this basic task we propose three different approaches (§4.1).

The explanation language (i.e. a set of motifs) is assumed to be given in input. This can be provided by the domain expert or mined from a dataset (when available). When the input set of motifs is too large, the exact estimation of Shapley values becomes computationally not doable. For dealing with these cases, we propose a simple approximation kernel (§4.2).

As a (non-trivial) side contribution we devise a synthetic dataset generator for graph classification (§5.1) which we use to benchmark GRAPHSHAP (§6.2), to empirically compare different masking approaches (§6.3), and to demonstrate that the proposed kernel is able to approximate the exact Shapley values with a computational complexity that is linear with respect to the number of explained features (§6.4). We also develop a algorithms for motifs mining and ranking (§5.2) and a custom graph convolutional layer able to deal with a graph dataset with node identity (§5.3).

Finally, we test GRAPHSHAP on a real-world brain-network dataset consisting of patients affected by Autism Spectrum Disorder and a control group. Our experiments highlight how the classification provided by a black-box model can be effectively explained by few connectomics patterns (§7).

2 Background and Related Work

In this section we first discuss related literature, then we introduce the needed preliminaries about explaining machine learning models via Shapley values.

2.1 Explainable graph classification

The task of building a model able to accurately predict the target class for unseen graphs is receiving increasing attention, as witnessed by the many approaches proposed in the last few years in the literature, which are mostly based on kernels [37], embeddings [27,2,15], and deep learning [51,21,47]. As these approaches rely inherently on black-box approaches whose inner logic is hardly intelligible, some post-hoc explainability techniques have been recently proposed. A recent taxonomic survey [53] grouped the existing instance-level explanation methods for graph neural networks in few classes.

Gradients/features-based methods decompose and approximate the input importance considering the gradients or hidden feature map values [41,59,35,40]. While these approaches have been proposed for prediction tasks in the domain of images and texts, they are quite general and have been extended to the graph domain [5,29,34].

Perturbation-based methods measure the output variations in model prediction with respect to perturbed inputs. In this context, the most important features are those that lead to similar predictions once retained [24,52,33,54]. The methodology proposed in the present work belongs to this category.

Surrogate methods approximate the outputs of the complex GNN models locally, i.e. with simpler linear approximation in the neighbourhood of the instance to be explained[17,58,46]. Finally, the recently proposed GraphSVX learns a surrogate model on a perturbed input to decompose the explanations among the nodes and features of the graph [11].

Most of the above mentioned explanation methods have been devised for node classification and link prediction: these are different classification tasks from the one that we consider in this paper, i.e., classification of graphs with node identity, which has received much less attention. As they deal with explainability of different classification tasks, a direct comparison with these methods would not be meaningful. While some of them seem a promising approach also for explaining graph classification models, their use has not yet been demonstrated for classification of graphs with node identity. Moreover, they would not suitable to provide explanations by means of motifs.

In §7 we present an application of GRAPHSHAP for explaining classification of brain networks in the context of Autism Spectrum Disorder. [50] proposes a deep learning approach for explainable classification of brain network, using a node-grouping layer before the convolutional layer: such nodegrouping layer provides insight in the most predictive brain subnetworks. Also in the context of brain network classification, [20] proposes a method based on *contrast subgraphs*, i.e., a subgraphs which are dense in one class of graphs and sparse in the other. This way, the resulting classifiers are simple and self-explanatory.

2.2 Explanations with Shapley values

A common perturbation-based approach to provide post-hoc explanations of a classifier is through local linear explanations (LLE). Let x be a F-dimensional data point of a dataset X, that is fed to a black-box model B. For the sake of generality, no assumption on the details of B are made, but some explainers require knowledge about the distribution of features of X [31] or access to the model B [39,23]. In general, the prediction B(x) is explained with a linear function of the input variables by building an interpretable classifier g that mimics B around x, in the form:

$$g(x) = \varphi_0 + \sum_{i=1}^{F} \varphi_i \cdot x_i$$

In the equation above g assigns to each feature i a weight φ_i , in order to approximate the behaviour of B in the local neighbourhood of x. The absolute value φ_i provide the importance of feature i in explaining the prediction B(x).

SHAP [23] derives local explanations leveraging the concept of Shapley values from cooperative game theory [36,26,42]. In this context, the input features of a classifier are akin to players cooperating to win a game (the model prediction). The more important is a player to the cooperation, the higher is its Shapley value. Features are grouped into coalitional sets, corresponding to the power set of the set of features F. A coalitional game is a function $v: 2^{|F|} \to \mathbb{R}$ that maps a coalitional set S to a gain value. It follows that, for a feature $f_i \in F$, its Shapley value $\varphi(i)$ is defined as follows:

$$\varphi(i) = \sum_{S \subseteq F \setminus \{i\}} \frac{\binom{|F|+1}{|S|}^{-1}}{|F|+1} (v(S \cup \{i\}) - v(S))$$
(1)

where v(S) is the gain value of a coalitional set and the sum extends over all subsets S of F not containing feature i. SHAP attributes importance φ_i to each feature $i \in F$. Importance is determined w.r.t. one (or more) background values, which are typically chosen as the centroids of the dataset X. A feature is important if its deviation from the background value produces a large variation in the model output. Since the exact evaluation of Shapley values requires to compute $2^{|F|}$ marginalizations that can result in a computationally infeasible process, several approaches were proposed to provide estimates of φ_i by sampling only a fraction of the entire possible space of S [23,43,25]. However, when two or more features F are not independent, convergence towards the exact Shapley values can require to sample a higher number of configurations [8].

3 Problem Statement

We are given a graph $G = (\mathcal{V}, \mathcal{E})$ with nodes $i, j \in \mathcal{V}$, edges $(i, j) \in \mathcal{E}$. We let \mathcal{G} denote the set of all possible graphs defined over a fixed set of nodes \mathcal{V} . We are also given a black-box graph classification model B, that is, we can not inspect B, we do not know the learning algorithm that produced B, nor its parameters, nor we have access to its training data. The only requirement about B is that it can be queried at will. Without loss of generality we assume a binary classification with class labels $\{0,1\}$; in particular we model the black-box as a function $B:\mathcal{G}\to[0,1]$ returning, for any graph $G\in\mathcal{G}$, the probability that G is in class 1.

For the scope of this paper, we consider G to be a simple, undirected, unweighted graph. In this context a motif M is any *connected* subgraph defined over any subset of \mathcal{V} . Formally, the set of all possible motifs is defined as

$$\mathcal{M} = \{ M_i = (\mathcal{V}_i, \mathcal{E}_i) | \mathcal{V}_i \subseteq \mathcal{V} \land \mathcal{E}_i \subseteq V_i \times V_i \land M_i \text{ is connected} \}.$$

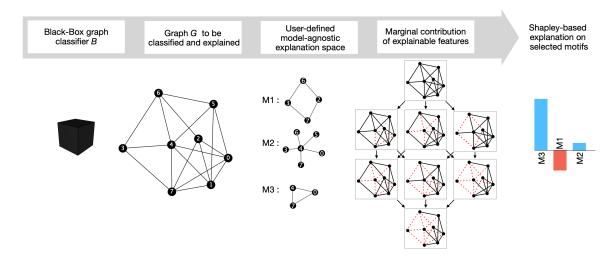


Fig. 1: GRAPHSHAP framework. The inputs are a black-box graph classifier, a graph whose classification by the black- box is to be explained, and an arbitrary set of motifs as an explanation language. GRAPHSHAP leverages a lattice-based process of maskings and marginalisations to compute the explanation score of each motif. A visual explanation is finally presented to the user.

Given a graph $G \in \mathcal{G}$, a black-box $B : \mathcal{G} \to [0,1]$ and a set of motifs \mathcal{M} , the problem tackled in this paper is that of assigning an explanation score $\xi(G, B, M_i) \in [-1, 1]$ to each motif $M_i \in \mathcal{M}$, quantifying the impact of the motif in explaining the label B(G): a value close to -1 means that M_i is important in explaining B(G) = 0, a value close to 1 means that M_i is important for B(G) = 1.

Moreover, when dealing with a large explanation language where exact Shapley values calculation is not doable for computational reasons, we tackle the problem of approximating the feature importance attribution by drastically shrinking the number of Shapley marginalizations, without compromising the correct estimation of the features importance.

4 GRAPHSHAP

As previously stated, our approach is rooted in the computation of Shapley values as in [23], with the key difference that the explanation space does not need to correspond to the features F (the input space of B); conversely, we base our explanations on the arbitrarily defined set of motifs \mathcal{M} . Mapping this approach and Equation 1 to our setting, we obtain the single-motif explanation score:

$$\xi(G, B, M_i) = \sum_{S \subseteq \mathcal{M} \setminus \{M_i\}} \frac{\binom{|\mathcal{M}|+1}{|S|}^{-1}}{|\mathcal{M}|+1} (B(G_S) - B(G_{S \cup \{M_i\}}))$$

The overall structure of the Shapley formula is preserved, with $v(\cdot)$ being replaced by $B(\cdot)$, as the coalitional value is provided by querying the black-box on a masked G_S , i.e., the graph G from which the motifs in S are "masked". G_S is the graph-equivalent of the feature removal concept upon which the Shapley theory is based. In our setting we call this operation $motif\ masking$ (discussed in detail in §4.1). The subtraction operation is specular with respect to the original Shapley formulation because in our setting we are masking motifs rather than adding features: that is, if in standard Shapley the information about a feature i is added by transitioning from S to $S \cup \{i\}$, in our setting we obtain the same by transitioning from $G_{S \cup \{M_i\}}$ to G_S , by un-masking M_i .

Figure 1 summarizes our framework: given a graph G, a black-box classifier B, and a set of motifs \mathcal{M} , GRAPHSHAP provides a motifs-based explanation $\xi(G, B, \mathcal{M})$. The set of motifs \mathcal{M} might be directly provided by the domain expert as hypotheses to be tested or, in the case a dataset of graphs defined over the same \mathcal{V} is available, interesting motifs (e.g., frequent or discriminative) can be mined.

Algorithm 1: GRAPHSHAP

```
Input: graph G, black-box B, set of motifs \mathcal{M}, masking strategy ms
     Result: explanation \xi(G, B, \mathcal{M})
 1 for S \subseteq \mathcal{M} do
           Compute B(G_S) according to ms
 3 end
 4 \xi(G, B, \mathcal{M}) \leftarrow \emptyset
 5 for M_i \in \mathcal{M} do
           \xi(G, B, M_i) \leftarrow 0
 6
           for S \subseteq \mathcal{M} \setminus \{M_i\} do
                val \leftarrow B(G_S) - B(G_{S \cup \{M_i\}})
  8
                coef \leftarrow \binom{|\mathcal{M}|+1}{|S|}
 9
                \xi(G, B, M_i) \leftarrow \xi(G, B, M_i) + coef * val
10
11
           \xi(G, B, \mathcal{M}) \leftarrow \xi(G, B, \mathcal{M}) \cup \xi(G, B, M_i)
12
13 end
14 return \xi(G, B, \mathcal{M})
```

As for other Shapley-based approaches, GRAPHSHAP (whose pseudocode is provided in Algorithm 1) requires to visit the powerset of the set features (which in our case is the set of motifs \mathcal{M}). This operation can be implemented by means of a lattice data structure. The first step (line 2) materializes all possible partial maskings G_S of G by visiting the lattice and queries the black-box for every such partial masking. The second step (line 8) involves computing the difference between scalar values of subsets of \mathcal{M} which differ only by one motif; this difference quantifies the answer to the question how would my classification score change if that specific motif was masked? Finally, in lines 9,10 we compute the marginal contributions of each motif by weighting the values obtained in line 8 with binomial coefficients, in order to account for the different number of edges across lattice layers. We then sum together all weighted values corresponding to the same motif, obtaining $\xi(G, B, M_i)$ for all motifs M_i . We denote GRAPHSHAP's \mathcal{M} -based explanation for the label assigned by B to G as $\xi(G, B, \mathcal{M}) = \{\xi(G, B, M_i), \forall M_i \in \mathcal{M}\}$.

4.1 Motif masking

Shapley values assess the relevance of a player by measuring the difference in gain between each coalition with/without that player: in the machine learning setting, this corresponds to feature masking. As most of the classifiers cannot be trained on a dataset with a given number of features and then be queried over data-points with a different number of features, the common workaround is to replace each feature to be masked with its so-called background value, typically corresponding to the mean/median value for that feature in the dataset. For instance, instead of truly removing the feature age from a data-point corresponding to a patient, SHAP might replace it with the background value of 50 (i.e. average age of patients in the training set), thus maintaining the number of features of the data-point.

In our context we do not need to substitute features with their background value: we can always query the black-box classifier with any graph G, as far as it is defined over the same set of nodes \mathcal{V} . As features are motifs, we can mask motifs from a graph, obtaining another graph that can be fed to

the black-box. In the following we propose three simple motif masking approaches that we will later compare empirically in §6.3.

Remove. The first motif masking approach simply removes from $G = (\mathcal{V}, \mathcal{E})$ all edges occurring in any motif in S. Formally, we define the resulting masked graph $G_{\mathcal{M}}$ as

$$G_{\mathcal{M}} = (\mathcal{V}, \{e \in \mathcal{E} \mid e \notin \mathcal{E}_i \ \forall \ M_i = (\mathcal{V}, \mathcal{E}_i) \in \mathcal{M}\}).$$

Average. The second strategy is inspired by the background value approach of SHAP. In this masking strategy, all edges e appearing in motifs to be masked in G are assigned a weight w(G, e) corresponding to their average weight in the dataset which, in the case of unweighted graphs, corresponds to the frequency of e in G.

Toggle. In the last strategy, each edge belonging to a motif to be masked is removed from G if occurring, and added otherwise. This masking strategy can be computed by symmetric difference:

$$G_{\mathcal{M}} = (\mathcal{V}, \mathcal{E} \triangle \ (\bigcup_{\mathcal{M}_i = (\mathcal{V}, \mathcal{E}_i) \in \mathcal{M}} \mathcal{E}_i))$$

This is the only masking strategy that equally captures the information conveyed by the presence or absence of a link.

4.2 Approximation kernel

GRAPHSHAP is based on the computation of Shapley values - a process with intrinsic exponential time and space complexity with respect to the number of features, as described in §2. It is worth mentioning that, due to the decoupling of the black-box input space and the desired explanation space, in our setting we are free to arbitrarily define the latter. However, to obtain explanations in larger feature spaces, kernels for approximating Shapley values are necessary to overcome the computational bottleneck. In order to explain the rationale between the approximation strategy, we refer to Figure 2, depicting a classical Shapley lattice.

Each node label represents which of the features A, B, C, D, E are to be masked, each edge represents a marginalisation with respect to a given feature, and the Shapley value of a feature is the weighted sum of all marginalisations associated to that feature. Another important concept is the depth of a layer of edges - that is, the distance from the closed terminal node of the lattice. Figure 2 shows an example of Shapley lattice, with depth-1/2/3 edges colored in red, blue and grey respectively. Intuitively, depth-1 edges measure the independent impact of each feature, depth-2 edges measure the impact of pairs of feature, and so on.

Approximations do not necessarily reproduce the exact values and might produce a rescaled score; however, for the sake of interpreting the results, only the ranking and the relative importance of the features are needed. The approximation can be performed by random sampling the lattice nodes [42], but visiting nodes in a layered fashion with increasing depth has been shown to create better approximations [23]. We follow this last approach and compute approximations by summing marginalisations up to a given depth. For instance, a depth-2 approximation in Figure 2 would only consider the red and blue coloured edges in the lattice. We show experimentally that in our setting, i.e. when the explanation space differs from the input space, this approach provides a good estimate of the feature importance even when the motifs are not independent. In the real world examples reported in §7, we will rely on depth-1 approximation, that allows to drastically reduce the operations from order $2^{|F|}$ to 2*|F|.

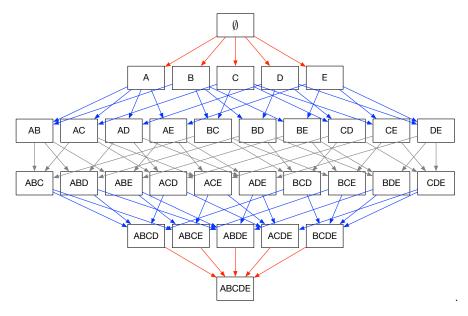


Fig. 2: Shapley lattice and depth of layers for the case of 5 input features to explain. The number of nodes in the lattice grows exponentially with the number of input features, while the number of layers grows linearly.

5 Implementation

A non-trivial part of our contribution resides in the practical deployment of GRAPHSHAP, together with a number of auxiliary utilities that we have developed to test our framework.

The complete GRAPHSHAP package includes:

- A synthetic graph generation algorithm (described in §5.1);
- Algorithms for mining and ranking motifs from a graph dataset (described in §5.2);
- A custom graph convolutional layer and network (§5.3);
- The core GRAPHSHAP algorithm (§4);
- A kernel to approximate the explanation scores ($\S4.2$).

The source code is available at https://github.com/notnotalan/GraphShap

5.1 Synthetic dataset generation

Our goal is to produce synthetic graph datasets with controlled motifs injection, in such a way that we can know, *ex ante*, which motifs are more discriminative, and thus should have higher explanation score.

In particular, our method (pseudocode in Algorithm 2) produces a set of synthetic graphs \mathcal{G} and a class labeling $\tau: \mathcal{G} \to \{0,1\}$. Through a construction parameter $\rho(k)$, we can control how much each injected motif M_k is predictive of the mapping τ , as follows.

Given $n \in \mathbb{N}$, we consider a fixed set of nodes $\mathcal{V} = \{1, ..., n\}$. We also consider a set \mathcal{M} of n_m motifs defined over \mathcal{V} , such that each motif $M_k \in \mathcal{M}$ is predictive of class 0 if k is even and of class 1 otherwise. A correlation matrix $\mathbf{C} \in [0, 1]^{n_m \times n_m}$ is given as input to control if motifs are added independently or not: $c_{i,j}$ represents the probability that motif j is added to a graph, given that motif i was added. We create a dataset with n_g Erdős–Rényi (ER) graphs having density d_g and mapping function $\tau(G_i) = 0$ if i is even and $\tau(G_i) = 1$ otherwise. Then, for each graph-motif pair (G_i, M_k) , with a perturbation probability proportional to $\rho(k)$ we add the motif to the graph if motif and graph belong to the same class, and remove it otherwise.

Algorithm 2: Synthetic Graphs Generation

```
Input: n: number of nodes, n_g: number of graphs,
                 d_g: graph density,
                 \mathcal{M}: set of n_m motifs.
                 \rho(k), \forall k \in [n_m]: motif probabilities,
                 \mathbf{C} \in [0,1]^{n_m \times n_m}: motif correlation matrix
     Result: Labelled graph dataset (\mathcal{G}, \tau)
 1 \mathcal{G} \leftarrow \emptyset
 2 Initialize \mathbf{R} \in [0,1]^{n_g \times n_m} with random values
 3 for j in 0..n_g - 1 do
           G \leftarrow \text{ER}(\mathcal{V} = \{1..n\}, d_g)
           for k \ in \ 0..n_m - 1 \ do
 5
                if \mathbf{C}_k \cdot \mathbf{R}_i^{\mathsf{T}} \leq \rho(k) then
 6
                      if (j \mod 2) \equiv (k \mod 2) then
  7
                           add edges of motif \mathcal{M}_k to G
  8
  9
                      else
                           remove edges of motif \mathcal{M}_k from G
10
                      end
11
                \mathbf{end}
12
13
           \tau(G) \leftarrow j \mod 2
14
           \mathcal{G} \leftarrow \mathcal{G} \cup \{G\}
15
16 end
17 return (\mathcal{G}, \tau)
```

5.2 Motif mining and ranking

We envision GRAPHSHAP as a tool for discovering the importance of candidate subgraphs in a graph classification ML task. Ideally, these subgraphs might be provided from domain experts or inferred from domain-specific literature. However, it might also be interesting to automatically generate potential subgraph candidates, so that GRAPHSHAP can compute explanation scores for previously unexplored motifs.

In order to do so, we developed custom algorithms for mining motifs from a graph dataset and selecting a subset through ranking. Despite the task not being novel, we preferred to develop a novel algorithm for practical reasons. First of all, many subgraph mining algorithms are based on computationally-intensive procedures of subgraph- and graph isomorphism [49], but the node identity property makes these steps unnecessary, as they can be replaced by the much easier task of matching node IDs. Another family of well-established similar algorithms is frequent-itemset mining [18]. However, we are interested in mining motifs, which are connected subsets of edges, and frequent-itemset mining algorithms do not check for connectivity. One option could be use these algorithms to mine edge subsets and then filter them in order to keep only the subsets corresponding to motifs, but this is a clearly disadvantageous approach, as it temporarily produces a large amount of candidates that will be subsequently filtered out. Finally, we wanted to develop our algorithm in Python, so that it could be used within the GRAPHSHAP suite more naturally.

We therefore developed a custom motif mining algorithm, whose high-level pseudocode is described in Algorithm 3). We rely on the concept of support, and exploit the function $supp(m, \mathcal{G})$ to indicate the number of graphs in \mathcal{G} that m is a subgraph of. We use twoplets (two-edges motifs) as building blocks and we iteratively build increasingly bigger motifs, as long as their support over the dataset is above a given threshold.

Once a set of motifs is mined, our aim is to extract motifs which are promising for their discriminative potential, for being particularly frequent in one class and not-so-frequent in the other class. More in details, given a mined set of motifs \mathcal{M} , we select a subset of motifs according to a greedy

Algorithm 3: Motif Mining

```
Input: \mathcal{G}: set of graphs defined over nodes V, s: support threshold
     Result: \mathcal{M}: set of motifs with support s over \mathcal{G}
  1 \mathcal{E} \leftarrow \{e \equiv (v_i, v_j) : \{v_i, v_j\} \subseteq V, supp(e, \mathcal{G}) \geq s\}
  \mathbf{2} \ \mathcal{T} \leftarrow \{\{e_1, e_2\} : \{e_1, e_2\} \subseteq \mathcal{E}, connected(e_1, e_2), supp((e_1, e_2), \mathcal{G}) \geq s\}
  3 \mathcal{M} \leftarrow \mathcal{T}
  4 for goal \leftarrow 3 to |V| do
            foreach m \in \mathcal{M}, t \in \mathcal{T} do
  5
                  if |m \cup t| \equiv goal \ and \ supp(m \cup t, \mathcal{G}) \geq s \ \mathbf{then}
  6
                         \mathcal{M} \leftarrow \mathcal{M} \cup t
  7
  8
                   end
            end
  9
10 end
11 return \mathcal{M}
```

ranking-and-filtering procedure. Given our labelled graph dataset \mathcal{G} , let \mathcal{G}_0 and \mathcal{G}_1 be the two sets of graphs in \mathcal{G} with label 0 and 1 respectively. For each motif $m_i \in \mathcal{M}$ we can compute the support over the two sets \mathcal{G}_0 and \mathcal{G}_1 combine these two values values to compute a *cross-support* score CS:

$$CS_i = abs(log_2(\frac{supp(m_i, \mathcal{G}_0) + 1}{supp(m_i, \mathcal{G}_1) + 1}))$$

We use the CS score to rank the motifs and greedily select those having a size over a minimum number of edges and a Jaccard distance of edges from the already selected motifs larger than a given threshold. The process is summarized in is described in Algorithm 4.

Algorithm 4: Motif Ranking

```
Input: \mathcal{G}: set of graphs, \mathcal{M}: set of motifs, dt: distance threshold, st: size threshold, k: output size Result: \hat{\mathcal{M}}: selected motifs

1 Compute CS_i for all m_i \in \mathcal{M}

2 Rank \mathcal{M} for decreasing CS-score

3 \hat{\mathcal{M}} \leftarrow \emptyset

4 while |\hat{\mathcal{M}}| \leq k and |\mathcal{M}| > 0 do

5 |m_i \leftarrow pop(\mathcal{M})|

6 |mindist \leftarrow min(\{Jaccard(m_i, m_j) \ \forall m_j \in \hat{\mathcal{M}}\})

7 |if \ mindist \geq dt \ and \ |m_i| \geq st \ then

8 |\hat{\mathcal{M}} \leftarrow \hat{\mathcal{M}} \cup \{m_i\}

9 |end

10 end

11 return \hat{\mathcal{M}}
```

5.3 Graph Convolution with node identity

Despite not being the focus of this paper, an efficient black-box for graph classification is needed to validate GRAPHSHAP, with graph convolutional neural networks being our method of choice. Several existing frameworks and libraries allow to create and train such models, but – to the best of our knowledge – there is no Python-based library for graph convolutional layers able to exploit the node identity property. Without node identity, all nodes in different graphs have to be considered as different

entities, and therefore when dealing with batches of graph data-points, their adjacency matrices have to be composed as shown in Figure 3 (left). This operation requires to align all adjacency matrices along the diagonal of a batch-adjacency matrix which is created on the fly, and renaming all nodes in all graphs so that the same ID are not reused. Conversely, in the node identity setting, all adjacency matrices of different graphs share the same shape, and nodes with the same ID represent the same entity across all graphs. In short, the correct way to represent a batch of graph data-points is to stack the single adjacency matrices along a third axis, as shown in Figure 3 (right).

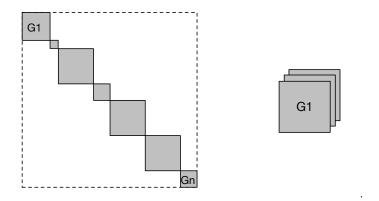


Fig. 3: Composition of a batch of adjacency matrices in the case of a graph convolution without node identity (left) and in the case of a graph convolution with node identity (right).

We therefore used a custom graph convolution layer for the node identity setting; its implementation is as follows:

```
class GConvNodeID(tf.keras.layers.Layer):
    def __init__(self,num_feat,num_out,activation):
        super(GConvNodeID,self).__init__()
        self.W = tf.Variable(GlorotUniform(seed=None)(shape=(num_feat,num_out)))
        self.activation = activation
    def call(self,A,X):
        XW = tf.einsum('bij,jk->bik',X,self.W)
        AXW = tf.einsum('bij,bjk->bik',A,XW)
        return self.activation(AXW)
```

The call() method implements, in batch mode, the definition of a standard graph convolution:

$$\mathbf{X}' = \mathbf{\hat{D}}^{-1/2} \mathbf{\hat{A}} \mathbf{\hat{D}}^{-1/2} \mathbf{X} \mathbf{W}$$

where $\hat{\mathbf{A}} = \mathbf{A} + \mathbf{I}$ denotes the adjacency matrix with inserted self-loops and $\hat{\mathbf{D}}_{ii} = \sum_{j=0} \hat{\mathbf{A}}_{ij}$ its diagonal degree matrix.

This graph convolution layer is used as a building block in the graph convolutional neural network that we used as a black-box throughout all the experiments described in the following section. The final architecture is inspired on the Deep Graph CNN model proposed in [56]: the input graphs with node identity are first passed through multiple graph convolution layers where node information is propagated between neighbors. The SortPooling layer is replaced by a conventional concatenation layer, in order to keep the node identities, and then passed to traditional CNN structures to learn a predictive model.

6 Experiments

In this section we first show some properties of the synthetic datasets introduced in 5.1; we then use synthetic datasets to to validate GRAPHSHAP (§6.2) and different masking strategies (§6.3). Finally, we explore the quality of depth-based approximations and their impact on the overall pipeline complexity.

6.1 Synthetic dataset validation

To validate the synthetic graph generation we test class separability for different configurations. In particular we generate datasets with 100 graphs per class, number of nodes $n = |\mathcal{V}| = 100$, graph density 0.2, and a range of parameter configurations regarding motif number and size and perturbation probability. For these experiments we did not enforce any kind of correlation within motifs (referring to the notation in 2, \mathbf{C} is an identity matrix).

Class separability is measured as the two-sample Kolmogorov–Smirnov test on the distributions of intra- and inter-class distances, where we use the Jaccard distance $J(G_i, G_j)$ for intra-class $(\tau(G_i) = \tau(G_j))$ and inter-class $(\tau(G_i) \neq \tau(G_j))$ distances. For each parameter setting we repeat the experiments 30 times, obtaining the results shown in Figure 4: each curve corresponds to a different configuration, with the solid line representing the average result and the shadow area the error range.

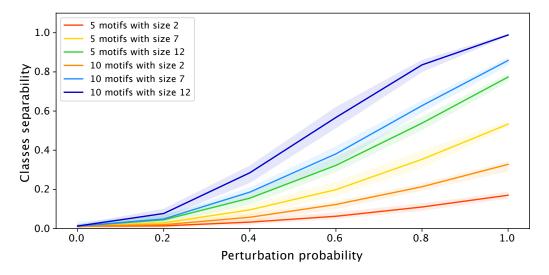


Fig. 4: Class separability on different synthetic graphs.

As expected, for all configurations higher perturbation probability induces higher class separability. Moreover, class separability is larger for larger number of injected motifs and larger size of these motifs (expressed as number of edges).

6.2 GRAPHSHAP validation

The next experiment is aimed at validating GRAPHSHAP. The idea is to exploit artificially injected motifs, checking whether the perturbation probabilities of the motifs corresponds to the explanation scores given by GRAPHSHAP.

For this purpose we build a synthetic dataset (\mathcal{G}, τ) with 100 graphs per class defined over $|\mathcal{V}| = 100$ nodes, with density $d_g = .2$ and with 6 injected motifs all containing 10 edges. The 6 motifs have

increasing perturbation probability values 0, 0.2, 0.4, 0.6, 0.8, 1, spanning from M_0 being a random control motif, to M_5 having being injected in all graphs of class 1 and removed from all graphs of class 0. As explained in §5.1, M_i is predictive of class 0 if i is odd, and of class 1 otherwise. The correlation matrix between the motifs is set to the identity, meaning that the motifs are chosen independently.

On this dataset we train a variant of a single-layer graph-convolutional neural network as our blackbox B. The first layer transforms the adjacency matrix \mathbf{A}_{G_i} of G_i using a rectifier linear unit, i.e., relu $(\mathbf{A}_{G_i} \cdot \mathbf{W})$ where $\mathbf{W} \in \mathbb{R}^{|\mathcal{V}|,32}$. We then apply an average pooling pooling and a fully connected layer. We minimize the cross-entropy between $\tau(G_i)$ and the model output, obtaining a validation accuracy of 0.84 in a 75-25 train-validation split.

Table 1 reports for each of the 6 motifs M_i , its perturbation probability and the average $\xi(G, B, M_i)$ over all graphs $G \in \mathcal{G}$, assigned by GRAPHSHAP (using remove masking strategy). The alternation

	M_0	M_1	M_2	M_3	M_4	M_5
ρ		.2		-	_	1
ξ	-0.006	0.014	-0.031	0.066	-0.067	0.095

Table 1: Perturbation probabilities and average explanation score.

between positive and negative values mirrors the parity-based criterion we used to assign motifs to classes: odd-indexed motifs have positive explanation scores, and the even-indexed ones have negative explanation scores.

Furthermore, since these motifs were injected with increasing probabilities, this is mirrored by the monotonically increasing absolute values of our explanations scores.

Due to the additivity properties of Shapley values, it holds that $-1 \leq \sum_{M_i \in \mathcal{M}} \xi(G, B, M_i) \leq 1, \forall G$ (recall that $B(\cdot) \in [0, 1]$). This also means that GRAPHSHAP scores are not independent, as the scores assigned to the motifs to explain the same graph G must not cumulatively exceed 1. This is why the average explanation scores are lower than their corresponding perturbation probabilities.

6.3 Comparing motif-masking strategies

Using the same experimental setting of §6.2 we next compare the three different motif-masking strategies remove, average, toggle. In Figure 5 we show the distribution of ξ scores (y-axis) for different values of expected explanation score (x-axis, defined next). Expected explanation scores are obtained by considering the following: (1) motifs that are injected in graphs of class 1 should have positive score, while motifs that are removed should have negative score; (2) a motif that is neither injected or removed from G should have low absolute score value; (3) the absolute score value is proportional to how much predictive is the motif for the blackbox, thus it should be proportional to the probability of injection ρ . Therefore the expected explanation score is defined as $I(G_i, M_j) \cdot C_{M_j} \cdot \rho(M_j)$, where $I(G_i, M_j)$ is 1 if M_j was injected in G_i , -1 if M_j was removed from G_i , 0 otherwise, and C_{M_j} is 1 if the class associated to motif M_i is 1, -1 otherwise. Figure 5 shows that all strategies produce explanation scores that display an increasing trend matching the explanation score, and in particular toggle is the motif-masking strategy that best correlates (Spearman coefficient of 0.91) with the expected explanation given these assumptions.

6.4 Depth-based approximation

As mentioned in §4.2, the computation of Shapley-based explanation scores is an intrinsically exponential process, and it is therefore common to employ approximation strategies in order to lower the computational time. In order to text our depth-based approximation strategy, we generated different

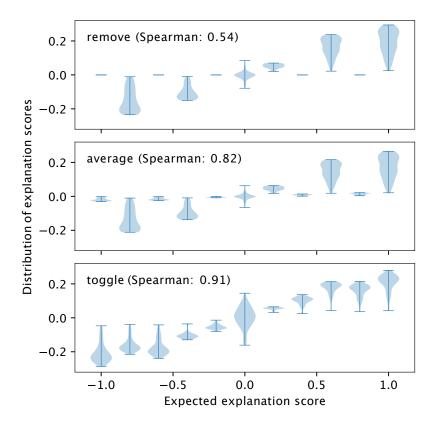


Fig. 5: Distribution of explanation scores $\xi(G, B, M_i)$ produced by GRAPHSHAP, given an expected explanation score.

datasets, computed approximations at all depths, and compared the approximated results with the exact explanation scores for all cases.

We created an initial dataset with 10,000+1,000 (train/test) graphs, 100 nodes per graph, initial graph density of 0.2, 8 motifs, perturbation probability of 0.25, and no forced correlations between motifs. We then forced partial and total correlation between a couple of same-class motifs (\mathcal{M}_0 and \mathcal{M}_2) by inserting the values of 0.5 and 1 in the correlation matrix - so that, for instance, partial correlations was obtained by setting $\mathbf{C}_{0,2} = \mathbf{C}_{2,0} = 0.5$, where 0 and 2 are the indexes of the two selected motifs. We also repeated the same process with a triplet of same-class motifs $\mathbf{C}_{0,2} = \mathbf{C}_{2,0} = \mathbf{C}_{0,4} = \mathbf{C}_{4,0} = \mathbf{C}_{2,4} = \mathbf{C}_{4,2} = 0.5$ (or = 1 for strong correlation).

As mentioned above, for all five datasets we run the whole GRAPHSHAP pipeline, training a graph convolutional neural network as black-box and building a marginalisation lattice. We then computed all depth-based approximations: with 8 motifs, the approximation depth spans from 1 to 4, included. We also remark that a depth-4 approximation takes into account all edges and therefore trivially corresponds to the exact explanation scores. We compared each approximation with the exact explanation scores by means of Pearson correlation to measure how much approximations can portray the relative importance of the exact explanation scores.

The results of this experiment are reported in Figure 6. Each boxplot represents the distribution of Pearson correlation scores over the test set of 1,000 graphs, for a given approximation depth and feature correlation level. As expected, the higher the approximation depth, the better the explanation values are approximated to the exact values. While within the datasets we observe some fluctuations, with graphs whose explanation rankings are exactly the same even when calculated on depth=1, while

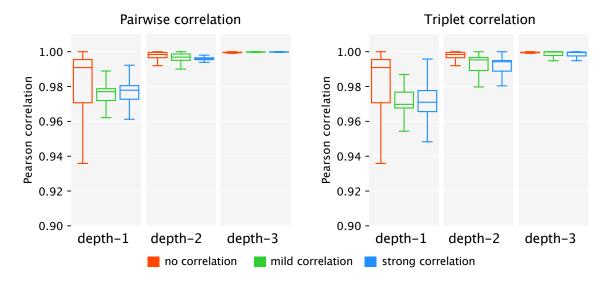


Fig. 6: Pearson correlation between exact and approximated explanation scores. Each boxplot represents the distribution of Pearson correlation coefficients when explanation scores are approximated by using only lattice layers up to a depth from 1 to 3, being depth 4 the complete lattice (the boxes extend from the lower to upper quartile values of the data, with a line at the median). Explanation scores were approximated in datasets with no correlation (red), partial correlation (green) or strong correlation (blue), with pairwise motif correlation (left) or with correlation among a triplet of motifs (right).

others have explanations ranking with some mismatches. Besides the within-dataset fluctuations, we also observe that datasets with stronger correlation among motifs converge slower to the exact ranking. However, we observe that in all scenarios three quarters of the correlation scores are above 0.95, meaning that depth-1 approximated explanation scores already achieve a very good approximation to the exact feature importance. This is remarkable, given that depth-1 approximation requires two marginalisations per feature, while the computation of exact explanation scores requires to perform an exponential number of marginalisations.

7 GRAPHSHAP on brain data

In this section we apply GRAPHSHAP on a brain network dataset to show how a black-box for the diagnosis of Autism Spectrum Disorder can be explained with a custom set of motifs.

Dataset and black-box classifier. We use the publicly-available eyesclosed dataset released by the Autism Brain Imagine Data Exchange (ABIDE) project [10]. The dataset contains neuroimaging data of 294 different patients, 158 Typically Developed (TD, class 0) and 136 suffering from Autism Spectrum Disorder (ASD, class 1). We parcel the brain area in 116 Regions of Interest (ROIs) according to the Automated Anatomical Labeling (AAL) [45] and pre-process the neuroimaging raw data as in [20]. In the end each patient is represented by an undirected unweighted graph G_i defined over the 116 nodes corresponding to the ROIs. As black-box B we adopt the same architecture as described in § 6.2 obtaining a validation accuracy of 0.783 in a 75-25 train-validation split.

Interesting motifs generation. In this experiment we extract a set \mathcal{M} of interesting motifs from the dataset (as discussed in §4, motifs could be provided by a domain expert or be generated in any other way). We use our motif miner introduced in Algorithm 3 with minimum support of 25, minimum lengthh of 3 edges, thus mining 92834 motifs. We then exploit Algorithm 4 to rank motifs

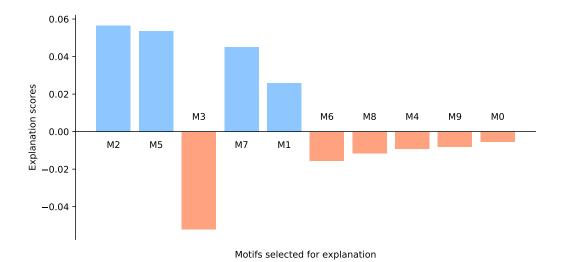


Fig. 7: GRAPHSHAP: local explanation for a single patient.

by cross-support and greedily select them (with a Jaccard-distance threshold of .85), selecting 10 top motifs.

Motifs selected in \mathcal{M} are thus quite different from one another, so to avoid providing explanations by mean of similar structures that might be redundant. We then use those 10 mined motifs as our first explanation language of choice.

Producing local explanations. We next apply GRAPHSHAP (with *toggle* masking) to produce explanations based on \mathcal{M} for the classifications produced by B.

Figure 7 shows an example of \mathcal{M} -based GRAPHSHAP explanation for a TD patient. The patient was correctly classified as non-ASD, so it is not surprising that the most important of the selected motifs correspond to positive explanation scores. For instance, M_2 is the strongest driver for the correct classification of our patient, M_5 is in second place, and so on. Conversely M_3 , due to its negative explanation score, acts as the strongest arguments in favour of classifying the patient as ASD. It is worth noting that positive and negative explanation scores are to be interpreted as positive and negative correlation of the motif with the classification as TD, and not with any actual value of the feature within the data-point: for instance, M_3 does not occur in the graph, so its absence concurs to cause the TD classification.

Producing and approximating global feature rankings. GRAPHSHAP produces *local*, data-point-level explanations; it is therefore possible to collect explanation scores across the whole dataset and aggregate them to obtain a *global* feature ranking.

In §6.4 we observed how, for our synthetic datasets, a depth-1 approximation yielded high Pearson correlation scores with respect to the exact values. We run the same experiments for the brain dataset (for the 10 mined motifs of the previous section), obtaining analogous results: depth-1 approximations are extremely good proxies for the exact explanation scores (median Pearson's correlation coefficient across the test set is 0.997 and lower/upper quartile values are 0.994 and 0.999 respectively). In Figure 8 we show how the depth-1 approximations strongly correlate with the exact scores.

Exploiting this result, we then extend the set of motifs, from the top-10 to the top-100 emerging from the ranking process, and compute their depth-1 approximated explanation scores. We remark that this process has linear computational cost with respect to the number of features, and therefore requires only 10x time with respect to the previous 10-features explanations. It is worth stressing that our approach allows to save 10^{26} operations, making features attribution feasible in such a large space.

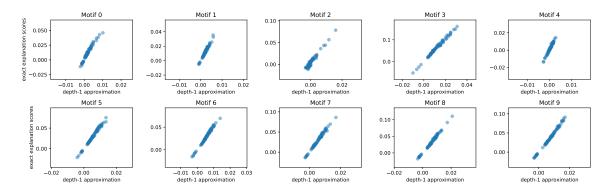


Fig. 8: Depth-1 approximation versus exact values for the explanation scores on the brain dataset.

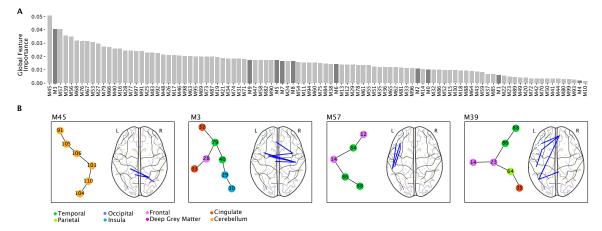


Fig. 9: (A) Top 100 motifs by global relevance, darker bars correspond motifs in the top 10 according to cross-support. (B) Four top motifs depicted as graphs and superposed to brain regions; the node IDs in the figure correspond to the ROI identifiers in the AAL atlas [45].

In Figure 9(A) we report, for each motif in \mathcal{M} , the average absolute value of the explanation scores across all graphs in \mathcal{G} . In Figure 9(B) we report the four top-scoring motifs, both as graphs and as mapped on the corresponding ROIs.

We observe that M_3 , one of the high-scoring motifs for the local explanation of Figure 7, appears to be highly relevant across the whole dataset, while the other top10 motifs are globally less relevant. It is also worth mentioning that the most globally-relevant motif, M45, is located in the *cerebellum area*, which is implicated in social cognition and has often been linked with ASD in neuroscience. literature [19].

On the other hand, considering only motifs from 0 to 9, although they are selected for their high CS, would have hidden the effects of more important motifs for explaining the black-box predictions. Thus, when a classifier is not inspected by a domain expert to validate existing hypothesis (i.e. asking explanations considering a small set of plausible motifs), the proposed kernel can be used to scale massively the number of explanations to generate novel hypothesis.

8 Discussion and Future Work

While machine learning models aimed at classifying entire networked structures might have impactful applications, suitable approaches for explaining decisions of such models are still missing. Here, we have

presented GRAPHSHAP, a novel approach for explaining black-box models for graph classification by means of expressive and understandable network motifs, regardless of the internal graph representation used by the classifier. Our method can use an explanation language (motifs) that does not coincide with the input space of the classifier (adjacency matrix): this is the main element of novelty of our work when compared to the related literature on Shapley-based methods for black-box models explainability. By devising a novel approach to generate synthetic data, we were able to test the ability of GRAPHSHAP of correctly identify the structures that are most predictive of each class.

One of the main issues when presenting novel explainability techniques is the one related to benchmarking and comparison with existing methodologies. While there are few approaches aimed at quantitatively compare different explanations techniques on specific settings [30,3], most proposed explanation generation techniques evaluate their methods by visual inspection. At the the time of writing, we are not able to perform a fair comparison of GRAPHSHAP with other methods because i) the lack of explanability techniques targeting graph classification tasks with node identity; ii) the lack of explanations techniques based on network motifs; iii) the lack of an explanation ground truth or a quantitative measure of goodness-of-explanation that is usually very context-dependent. Future work will be devoted to define a proper setting for performing fair comparison accross different techniques spanning multiple prediction tasks.

Although GRAPHSHAP builds explanations based on motifs, the approach can be expanded so that the explanation language includes additional network features, such as, e.g., nodes centrality, dense subgraphs, or higher-order structures. This a promising avenue for future investigation. Finally, ongoing collaboration with neuroscientists will both validate the usability of GRAPHSHAP and its capability in increasing trust in machine learning models by domain experts and in validating neuroscience hypotheses connecting brain network structures and neurodegenerative diseases.

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