Ensemble approaches for Graph Counterfactual Explanations

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Abstract

In recent years, Graph Neural Networks have reported outstanding performances in tasks like community detection, molecule classification and link prediction. However, the black-box nature of these models prevents their application in domains like health and finance, where understanding the model's decisions is essential. Explainable AI, or Explainable Machine Learning, is artificial intelligence in which humans can understand the decisions or predictions made by the AI. A special case is the Counterfactual examples which provide suggestions on the steps the system needs to take to change its decision. Historically ensemble learning and explainability have been jointly exploited to explain the decision of ensemble models. Contrarily, in this work, we focus on the ensemble mechanisms of the explainers to improve the quality of explanations. In this work, we explore, thus, which are the possible ensemble mechanism that can be adopted in several explainability scenarios. Furthermore, we introduce and discuss a new explainability problem where a single coherent counterfactual explanation must be provided for a set of input instances and their explanations.

Keywords

Explainable AI, Counterfactual Explanations, Ensemble, Machine Learning

1. Introduction

Nowadays, Machine Learning (ML) methods are fundamental to several tools in different application domains. In domains, like health or finance, understanding the decision process is of paramount importance. On the opposite, the predictions made by black-box systems, due to their nature, are hardly understandable, preventing their broad adoption. To overcome this limitation, explanation methods were developed to give insight into how the ML model has taken a specific decision for a given case/instance [1].

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Since their creation, Graph Neural Networks (GNNs) [2] have attracted the interest of the ML community because they allow leveraging the advantages of Deep Neural Networks (DNN) on graph data. However, this also means that GNNs behave as black boxes. Given the particularities of graph data, many explanation techniques have had to be developed specifically for GNNs. In particular, Graph Counterfactual Explanations (GCE) are one of the possible explanation types in the Graph Learning domain. A counterfactual explanation answers the question: *what changes should I make to the input to obtain a different output?* GCE techniques can be helpful to discover, for example, i) molecular compounds similar in specific desired properties [3] or ii) new insights into the interplay of different brain regions for certain diseases [4]. Existing works on GCE diverge mainly in the problem definition, application domain, test data, and evaluation metrics [5]. Most of them do not compare against other counterfactual explanation techniques in the literature, making it challenging to promote the advancement of this research field.

According to the works proposed in the literature, ensemble learning and explainability have been jointly exploited to explain the decision of ensemble models. Contrarily, in this work we focus on ensemble mechanisms on the explainers, thus, improving the quality of explanations. Moreover, the aggregation of the explanations produced in the ensemble might lead to new explanations encapsulating the ones before the fusion. Additionally, we extend the classic multi-instance learning explanation of several instances to multiple single-instance explanations. Here, the predictor is trained on single instances, and the explainer takes in input a set of graphs coupled with their predictions to provide a single common explanation.

Overall, multiple single-instance explanation strategies provide a final counterfactual explanation valid for all the input instances and their corresponding predictions. In this way, the produced counterfactual explanation can be used to identify substructures shared by the input graph instances. Moreover, one can pinpoint the specialized structures of the counterfactual and input graph instances that produce the predicted outcomes.

We can summarise the contributions of this work as follows:

- we provide a formal discussion of ensembles for Single-Instance Explanations;
- we provide a formal discussion of ensembles for Multiple-Instance Explanations;
- we introduce and formalise a new Multiple Single-Instance Explainability problem;
- we provide a formal discussion of ensembles for Multiple Single-Instance Explainability;

The rest of this paper is organised as follows. Section 2 briefly discusses background concepts and the related work. In Section 3, we discuss single-instance ensemble approaches and present our multiple single-instance explanations in detail. Section 4 concludes the paper.

2. Background and related work

Before delving into the details of ensembles for GCE methods, we provide the reader with a thorough discussion of the background of ensemble learning, graph neural networks (GNNs), and model interpretability via counterfactual explanations.

Ensemble learning (EL) [6] refers to algorithms that rely on the aggregation of base models to obtain more accurate prediction models. EL comes in three variants: i.e. bagging [7], boosting

[8], and stacking [9]. Briefly, bagging consists of sampling with replacement n different views of the same dataset to train n base models. The predictions of the base models get aggregated via a majority voting consensus function [10]. Boosting consists of iterative algorithms that train the next base model according to the misclassified instances from the previous model. Stacking considers heterogeneous weak learners and learns to combine them using a meta-model differently to the deterministic combination used in bagging/boosting.

Generally, a neural network has interconnected layers of neurons that propagate information to the next layer [11]. Similarly, a *GNN* learns to transform the attributes of a specific graph G, which typically maintains its proximity characteristics.Connectivity is essential in graph structures because it induces the embedding function to map similar nodes together. To exploit the connectivity in a graph G, GNN can rely on three main strategies: i.e. random walks [12], message passing [13, 14], and graph convolutional networks (GCNs) [15].

Considering the black-box nature of deep learning systems, non-specialists are interested in understanding *what is happening under the hood.* The European AI regulation [16] suggests that interpretability creates safer and digital environments, and encourages privacy, trustworthiness, and fairness. Guidotti [17] addressed counterfactual explainability (CE). Consider an automatic systems rejecting a bank loan requests. We need to answer the question, *"what should change such that the loan request gets accepted?"*. Counterfactual examples provide suggestions on the steps to take for the system to change its decision. As a specialisation of CE, graph counterfactual explanation (GCE) methods answer the question, *"how should the input graph or its components (e.g. vertices, edges) change to obtain a different outcome?"*.

Connectivity is crucial in many graph role problems. In biochemistry, neurobiology, ecology, and engineering, graph substructures are highly related to their functionalities [18]. Additionally, the neighborhood of a specific vertex is essential to determine its classifications. Therefore, most explanation methods designed for vectors, tables, and images cannot be applied to graphs. Instead, specific strategies have been devised. Wu et al. [19] train a learnable soft-mask matrix to mask the features of vertices/edges in the input graph while keeping the same class. The unmasked features are are the counterfactual explanations. Lucic et al. [20] explore a binary perturbation matrix to sparsify the input graph's adjacency matrix. The authors generate the counterfactual example with the smallest distance according to the input graph. Wellawatte et al. [21] identify similar counterfactual molecules, by selecting a small number of these using clustering and Tanimoto similarity. Similarly, Numeroso et al. [3, 22] use reinforcement learning to generate counterfactual examples given an input molecule. Bajaj et al. [23] find decision regions for each class. Then, based on the boundaries of the regions, they produce subsets of the input graph edges as counterfactuals. Abrate [4] rely on a bidirectional search heuristic such that the resulting counterfactual has minimal changes from the original graph in brain networks.

Ensembles of counterfactual explanations have been explored in [24] to boost weak explainers and combine them into a single more robust one explaining a single input instance. To the best of our knowledge, ensembles for graph counterfactual explainability have not received any attention in the literature of eXplainable AI (XAI). Moreover, differently from what discussed in Section 3.2, the literature focuses on ensembles of single-instance explainability.

3. Ensembles in Graph Counterfactual Explanations

The discussion of diverse theories to explain a phenomenon is paramount in science. The main goal is to analyse the strengths and weaknesses of each theory explaining the phenomenon and reach a consensus on the best explanation. Likewise, the AI community has successfully used ensembles of ML models for many years. However, existing works on the intersection of EL and Explainability are mainly focused on explaining the decisions of ensemble models [25]. Conversely, in this work, we propose to use ensemble mechanisms on the explainers with the aim of improving the explanations' quality and/or providing a brand new explanation. Recall that GCE is usually a new graph or a set of actions to transform the input graph into the counterfactual graph. Let x be an explanation that belongs to an explanation space χ, $\mathcal{G}$ the set of all possible graphs, and $\mathcal{M}$ the set of all GNN predictors. Below, we formally define what an explanation is in two different explainability scenarios, namely, single-instance (see Definition 3.1) and multi-instance (see Definition 3.3).

Definition 3.1. Let C be the set of classes, $G \in \mathcal{G}$ be the input graph, $\Phi \in \mathcal{M} : \mathcal{G} \longrightarrow C$ the prediction model, and $\mathcal{E} : \mathcal{G} \times \mathcal{M} \longrightarrow \chi$ an explanation method. Then $x = \mathcal{E}(G, \Phi)$ is a *single-instance explanation* if $\Phi(x) \neq \Phi(G)$.

Definition 3.2. Let C be the set of classes, $S = \{G_1, G_2, \ldots, G_k\}$ the input set of graphs, with $G_i \in \mathcal{G}$, $\Phi \in \mathcal{M} : 2^{\mathcal{G}} \longrightarrow C$ a prediction model, and $\mathcal{E} : 2^{\mathcal{G}} \times \mathcal{M} \longrightarrow \chi$ an explanation method. Then $x = \mathcal{E}(S, \Phi)$ is considered a *multi-instance explanation* if $\Phi(x) \neq \Phi(S)$.

Hereafter we discuss - considering a graph classification task, remarking that the provided definitions can be easily adapted to the other tasks of the GCE domain (i.e. vertex and edge classification) - the ensembles of explainers on the two aforementioned scenarios (i.e. single-instance and multi-instance) to then introducing (in Section 3.2.2) a new one that was not considered before in the literature.

3.1. Ensembles for Single-Instance Explanations

As in other Learning tasks - e.g. clustering, anomaly detection - ensembles of explainers can be successfully used to improve the performance of the explanations [24]. In Figure 1, we present a bagging ensemble pipeline for the single-instance explanations scenario. The single instance and the trained ML model are the input for several base explainers (those may vary the algorithm and/or the hyper-parameters settings). The produced explanations are then combined by an aggregation phase to output the final explanation.

According to [24], the produced counterfactual explanation are more robust than the one produced by a single explainer by increasing the stability of the method and reducing the variability of its quality. In the graph domain, the aggregation phase might leverage quantitative metrics (like Graph Edit Distance, Fidelity and Sparsity - see [5] for a more complete discussion) to drive the selection or the generation of the best counterfactual explanation. Additionally, it can adopt voting-like mechanism to promote the most common actions (i.e. adding/removing vertices/edges from the original graph) that lead towards the generation of the counterfactual graph.

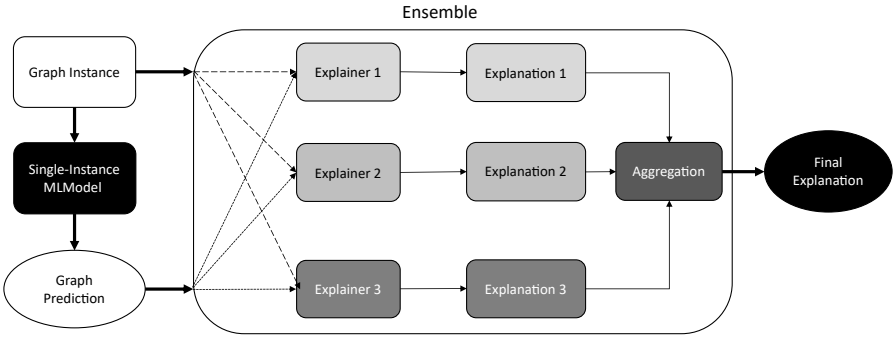
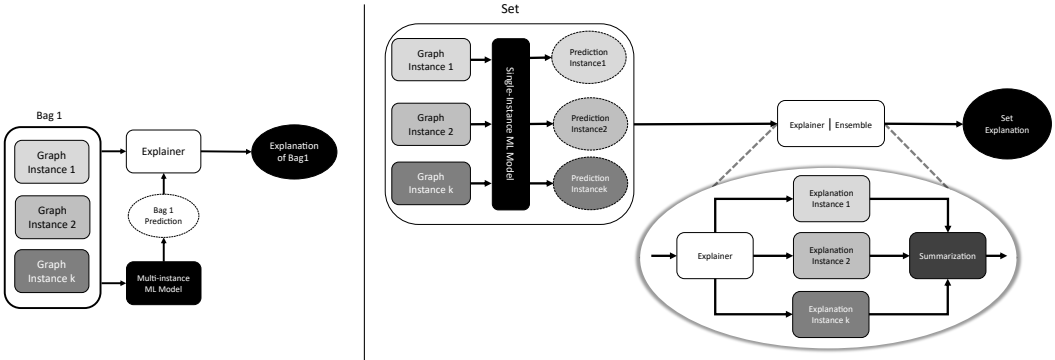


Figure 1: Pipeline of an ensemble for single-instance explanations.



(a) Classic multi-instance learning explanation of a *bag* of k instances.

(b) Multiple single-instance explanations of a *set* of k instances and their predictions. The ensemble mechanism is highlighted in the zoom.

Figure 2: Generating explanations via classic multi-instance learning (left) and ensemble of multi-instance explanations (right).

3.2. Multiple Instance Explainability vs Multiple Single-Instance Explainability

In this Section, we discuss a new explainability scenario, namely Multiple Single-Instance Explainability (MSIE). First, we introduce Multiple Instance Explainability and then delve into providing more details on MSIE. For both scenarios, we guide the reader on how to incorporate the ensemble mechanisms thereon.

3.2.1. Multiple Instance Explainability

As introduced in [26], Multiple Instance Learning (MIL) generalizes the traditional data representation allowing individual data samples $\mathcal{B}_1, \mathcal{B}_2, \cdots$ (called bags) to be represented as a set of multiple d-dimensional feature vectors $\mathcal{B} = \{x_1, x_2, \cdots\}$ s.t. $x_i \in \mathbb{R}^d$ (called instances). In supervised classification, each bag is associated with a single value (e.g. $y \in \{-1, +1\}$ in the binary classification case). Thus, the derived MIL Explainability field must be seen as a special case of a single-instance explainability where the input is a bag of graphs with a corresponding

class (or classes in the multi-label setting) for the entire *bag*. Thus, the main difference with the single-instance scenario resides in how the predictor is trained, and in the characteristics of the explainer.

Figure 2a clarifies the explainability of multi-instance learning as proposed in the literature. Notice that the *bag* of k graphs is passed as input to the explainer and the prediction model. The prediction model, in this scenario, is trained to predict the class of the entire bag. Finally, the explainer produces an explanation of the whole bag considering its prediction.

The literature has attempted to tackle the multi-instance factual explanation problem in [27] by identifying instances responsible for positive bag prediction. In general, the problem has received less attention than the single-instance explanation problem. Besides, generating multi-instance counterfactual explanations still remains a completely unexplored field, especially in the graph domain. Therefore, being an extension of single-instance explainability, MIL can exploit ensembles to produce several explanations for the bag and, afterwards, combine them into a single one, as shown in Section 3.1.

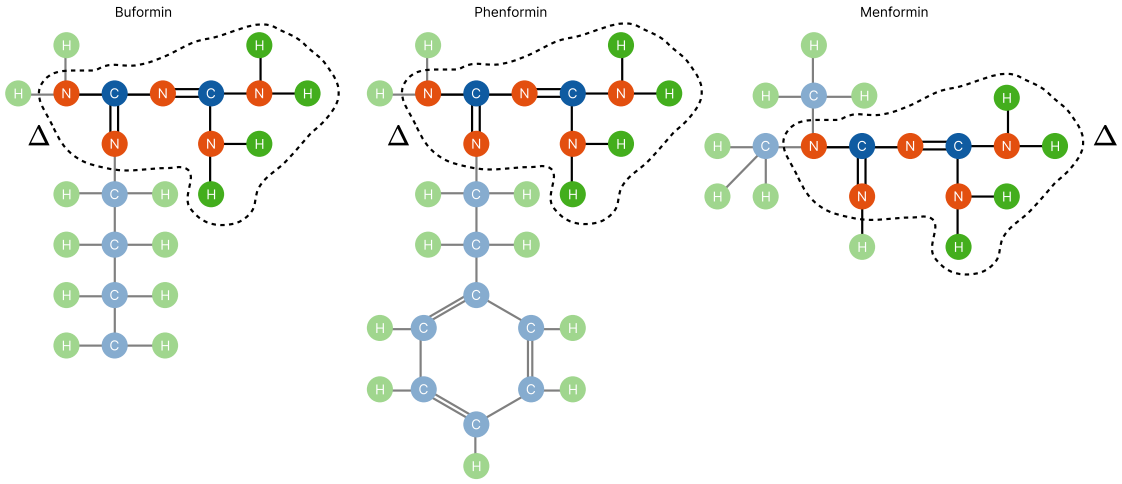


Figure 3: Example of three different drugs (i.e. buformin, phenformin, and menformin). All three drugs inhibit the growth and development of cancer, but they can also treat other complications. Buformin is a metabolic antiviral that inhibits the mTOR pathway used by influenza. Phenformin improves glycemic control by regulating insulin sensitivity to treat diabetes. Menformin can treat polycystic ovary syndrome.

3.2.2. Multiple Single-Instance Explainability

Keeping in mind the MIL scenario, we notice that a new explainability problem can be identified, namely multiple single-instances explainability. In the multiple single-instances explainability scenario the predictor is trained on single-instances (unlike how it happens in the MIL). Additionally, the explainer takes as input a set of graphs coupled with their predictions to provide a common explanation. Multiple single-instance explanation strategies can be used as an example in the chemical domain. Considering the following setting: we have two different drugs $D_1 = (V_1, E_1)$ and $D_2 = (V_2, E_2)$ that cure disease γ_1 and γ_2, respectively. Suppose that

D_1 and D_2 share a common substructure Δ (that we highlight here for the discussion but that it is not part of the input of the problem). Now, say that we want to get an overall counterfactual explanation for both D_1, D_2 and γ_1, γ_2. Thus, the counterfactual example D_3 might be a drug which shares the same substructure Δ, although it cures disease γ_3. In particular, Figure 3 illustrates three different drugs[1] of the same class (i.e. bigunaide). Here, D_1 is the compound corresponding to buformin which is a metabolic antiviral that inhibits the mTOR pathway used by influenza [28] and and Middle East respiratory syndrome-related coronavirus [29]. D_2 corresponds to phenformin[2] that helped improve glycemic control by regulating insulin sensitivity aiding in treating diabetes. Lastly, D_3 corresponds to menformin which is applicable to polycystic ovary syndrome treatments [30]. Notice that the highlighted substructure Δ is shared among the three drugs described above. Hence, the counterfactual explanation D_3 is useful for a pharmacologist/chemist to identify the chemical bonds that specialize the three drugs D_1, D_2, and D_3 in being effective when treating the previously stated complications. Moreover, notice that metaformin has the least amount of changes w.r.t. buformin and phenformin when considering the core substructure Δ. The common substructure Δ, in this scenario, represents the biguanide class that encapsulates D_1, D_2, and D_3 as oral antihyperglycemic drugs used for diabetes mellitus or prediabetes. The other attached chemical structures in each drug create additional curative properties and characterising side effects.

Figure 2b summarizes the explaining task for multiple single-instance where each input graph and its prediction are color-coded to convey their coupling. There, the single-instance predictor takes each graph to produce a different prediction. The entire set of graphs, their predictions, and the used model, are the input of a multiple single-instance explainer. The main idea is that the explainer needs to provide a counterfactual explanation which is *valid* for all the instances and their predictions. Intuitively, a counterfactual explanation, in this task, is a graph similar to the input graphs while having a different prediction regarding the ones of the input set. Formally:

Definition 3.3. Let C be the set of classes, $S = \{G_1, G_2, \ldots, G_k\}$ the input set of graphs, with $G_i \in \mathcal{G}$, $\Phi \in \mathcal{M} : \mathcal{G} \longrightarrow C$ the prediction model, and $\mathcal{E} : 2^{\mathcal{G}} \times \mathcal{M} \longrightarrow \chi$ the explanation method. Then $x = \mathcal{E}(S, \Phi)$ is considered a *multiple single-instance explanation* if $\Phi(x) \notin f(\{\Phi(G_i) \mid G_i \in S\})$ where $f : 2^{\mathcal{C}} \longrightarrow 2^{\mathcal{C}}$.

The definition above does not provide a specific implementation of the function f that can be customised according to the application domain, and the "strictness" of counterfactuality one needs to have. For example, f can be the identity function of the original set of predictions. In this way, $\Phi(x)$ needs to be different to all the predicted classes ($\{\Phi(G_i) \mid G_i \in S\}$).

Similarly to what discussed for MIL, multiple single-instance explainability can rely on ensembles to engender explanations for the graphs in S. As shown in Figure 2b, we want to have an explanation of all the instances considered singularly and not as a group, as it happens in MIL. In this regard, in the ensemble we might have at least the same number (k) of explanations as the number of elements in S. These explanations then need to be *summarized* together to

[1]We, hereby, declare that the description of these drugs is entirely for illustration purposes, and we do not claim to be experts in pharmacology.

[2]This drug is currently out of market production due to recurrent side effects of lactic acidosis in human trials.

produce a single one that clarifies the entire set S as shown before. Notice that the ensemble mechanism might also follow a multi-level fashion where several summarization phases take part between two consecutive levels as in [31].

4. Conclusion

Counterfactual explanation techniques can suffer from issues such as a lack of stability of the results, with respect to the input, and undesired variance in the results. Ensembles of counterfactual explainers have been proposed to tackle these problems [17]. However, no similar approach has been used for counterfactual explanations in the graph domain. In this work, we proposed to use ensembles of GCEs to provide new types of explanations and improve existing ones.

We provided a generic pipeline for producing single-instance GCEs using an ensemble of explainers. In addition to the classic voting approach, for selecting the best base explainer, we introduced the idea of using an aggregation function that combines multiple base GCEs into a final one. Furthermore, we analyzed the multi-instance GCE problem for the first time. There, we devised two approaches: Multi-instance explainability and Multiple Single-Instance explainability. Moreover, we proposed an ensemble-based pipeline to implement the second approach and tackle the multi-instance GCE problem.

In general, our position is that GCE ensembles can be used to solve many of the issues faced by the existing explanation methods. In future works, we will develop and test ensemble-based GCE methods to tackle the different problems presented in this work. Furthermore, we will analyze in more detail the more convenient way of designing the aggregation functions presented in our proposed pipelines.

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