Clustering-Based Approaches for Symbolic Knowledge Extraction

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Abstract. Opaque models belonging to the machine learning world are ever more exploited in the most different application areas. These models, acting as black boxes (BB) from the human perspective, cannot be entirely trusted if the application is critical unless there exists a method to extract symbolic and human-readable knowledge out of them. In this paper we analyse a recurrent design adopted by symbolic knowledge extractors for BB regressors—that is, the creation of rules associated with hypercubic input space regions. We argue that this kind of partitioning may lead to suboptimal solutions when the data set at hand is high-dimensional or does not satisfy symmetric constraints. We then propose a (deep) clustering-based approach to be performed before symbolic knowledge extraction to achieve better performance with data sets of any kind.

Keywords: explainable AI · symbolic knowledge extraction · clustering

1 Introduction

Machine learning (ML) models in general – and (deep) artificial neural networks in particular – are nowadays exploited to draw predictions in almost every application area [7]. However, when facing critical domains – e.g., involving human health or wealth – ML models behaving as opaque predictors are not an acceptable choice. The opaque nature of these models makes them unintelligible for humans and this is the reason why they are called black boxes (BBs). Nonetheless, explainability can be obtained from BBs via several strategies [4]. For instance, one can rely uniquely on interpretable models [8], or build explanations by applying reverse engineering to the BB behaviour [6]. This latter approach allows users to combine the impressive predictive capabilities of opaque models with the human readability proper of symbolic models.

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The literature offers a wide variety of procedures explicitly designed to extract symbolic knowledge from opaque ML models, especially for classifiers—e.g., Rule-extraction-as-learning [2] and TREPAN [3]—, but also for BB regressors—e.g., ITER [5], GridEx [12], GridREx [9] and REFA NN [14].

Unfortunately, any method is subject to drawbacks and limitations. In the following we focus on the issues deriving from the extraction of rules from BB regressors. In particular, we observe that a typical design choice adopted for extractors applicable to opaque regressors is to find hypercubic regions in the input feature space having similar instances and then to associate symbolic knowledge to each region, for instance in the form of first-order logic rules [5,9,12]. We agree that rules associated with hypercubic regions are the best choice from the human-readability perspective, since they enable the description of an input space region in terms of constraints on single dimensions (e.g., \(0.3 < X < 0.6, 0.5 < Y < 0.75\) for a hypercube in a 2-dimensional space having features \(X\) and \(Y\)). However, this solution may lead to the creation of suboptimal clusters, especially if the partitioning into hypercubes is performed following some sort of symmetric procedure (on asymmetric data sets). In this paper we suggest to exploit clustering techniques on the data set used to train the BB before extracting knowledge from it, in order to preemptively find and distinguish relevant input regions with the corresponding boundaries. This theoretically allows extractors to: (i) automatically tune the number of output rules w.r.t. the number of relevant regions found; (ii) give priority to more relevant regions, for instance those containing more input instances or having the largest volume; (iii) avoid unsupervised partitioning of the input feature space, otherwise leading to suboptimal solutions in terms of readability and/or fidelity.

2 Related Works

A predictive model can be defined as interpretable if human users are able to easily understand its behaviour and outputs [1]. Since the majority of modern ML predictors store the knowledge acquired during their training phase in a sub-symbolic way, they behave and appear to the human perspective as unintelligible black boxes. The XAI community has proposed a variety of methods to enrich BB predictions with corresponding interpretations/explanations without renouncing their superior predictive performance. Usually, the proposed methods consist of creating an interpretable, mimicking model by inspecting the underlying BB in terms of internal behaviour and/or input/output relationships. For instance, REFA NN analyses the architecture of neural network regressors with one hidden layer to obtain information about the internal parameters and thus build human-readable if-then rules having a linear combination of the input features as postconditions. This kind of technique is called decompositional. On the other hand, when the internal structure of the BB is not considered to build explanations, the algorithms are classified as pedagogical. In the following we focus on three pedagogical techniques for BB regressors—namely, ITER, GridEx and GridREx.
ITER The ITER algorithm [5] is a pedagogical technique to extract symbolic knowledge from BB regressors. It follows a bottom-up strategy, starting from the creation of infinitesimally small hypercubes in the input feature space and iteratively expanding them until the whole space is covered or it is not possible to add or expand further the existing cubes. All the hypercubes are non-overlapping and they do not exceed the input feature space. After the expansion step, ITER associates an if-then rule to each cube, selecting as action the mean output value of all the instances contained in the cube. The algorithm’s main advantage is to be capable of constructing hypercubes having different dimensions. However, especially when dealing with high-dimensional data sets, it may present several criticalities related to the hypercube expansion. In particular, at each iteration it is necessary to build temporary cubes around the existing cubes, two per input dimension (as shown in the bidimensional example reported in Figure 1), but only one temporary cube of a single existing cube is chosen as actual expansion. This may lead to an enormous waste of computational time and resources due to the repetition of (the same) useless calculations, other than the possibility to exceed the maximum allowed iterations without having convergence. The absence of convergence results in a non-exhaustive partitioning of the input feature space, which in turn implies the inability to predict output values of data samples belonging to regions that are not covered by a hypercube (i.e., there are no human-interpretable predictive rules associated with uncovered regions). Conversely, the coverage of the whole input feature space enables to draw predictions for any input instance.

GridEx and GridREx The GridEx algorithm [12] is a different pedagogical technique to extract symbolic knowledge from BB regressors. It is applicable under the same conditions of ITER and outputs the same kind of knowledge, but they differ in the strategy adopted during the input space partitioning. GridEx is not a bottom-up algorithm; conversely, it follows a top-down strategy, starting from the whole input space and recursively partitioning it into smaller hypercubic regions, according to a user-defined threshold acting as a trade-off criterion between readability (in terms of the number of extracted rules) and fidelity of the output model (intended as its ability to mimic the underlying BB). Amongst the advantages of GridEx there is its ability to automatically refine the found regions according to the provided threshold, as well as to perform a merging step
Fig. 2: Example of GridEx partitioning (without merging step) when performing 2, 3 or 4 slices per input dimension. The first panel shows the input feature space. Cyan and yellow dots in the other panels represent small and large clustering errors, respectively.

after each split, when possible. In particular, the merging step consists of the pairwise unification of adjacent hypercubes to reduce the number of output rules and it is based on the similarity between the samples included in each cube, to avoid a predictive performance worsening. It is useful since a split may create an excessive amount of disjoint regions. The main disadvantage of GridEx is that, even if it can perform an arbitrary amount of slices along each dimension at each iteration, all the partitions created in a dimension in a given iteration have the same size. An example is reported in Figure 2, showing that a cube may include portions of separated input regions, thus leading to a drop in the predictive performance.

The GridREx algorithm [9] is an extension of GridEx achieving better predictive performance by providing as output linear combinations of the input variables instead of constant values. However, it performs the same grid partitioning than GridEx. As a consequence, it is susceptible to the same partitioning-related drawbacks.

3 A Clustering-Based Approach

The example in Figure 2 shows a data set described by 2 input features (x and y) and an output continuous feature (represented by the colour). The data set can be divided into three clusters of instances. Inside each cluster, the output feature is represented by a different linear combination of the input features. An optimal extraction technique should be able to identify these clusters in a fast and flawless way, since in the example they are linearly separable and, furthermore, three hypercubes can enclose them without overlaps. A bottom-up strategy like the one adopted by ITER may be suitable for the task, but in the general case – in the n-dimensional domain – convergence may result too slow. It is possible to fasten the ITER convergence by acting on the algorithm parameters, but at the expense of a coarser partitioning. This latter inconvenience is the same encountered by using GridEx, which induces an equally spaced grid. If a grid cell contains no instances belonging to different clusters, the predictive error will be small. Otherwise, it will be less or more large depending on the amount of
contamination of each cell (reported in the Figure as cyan and yellow dots if it is small or large, respectively).

An optimal and fast partitioning can be obtained by: (i) applying a clustering technique to the data set to identify the different relevant regions; (ii) constructing minimal hypercubes to include the found regions, since they will be associated with human-readable rules; (iii) exploiting an extraction technique able to describe each hypercube in terms of input features. Extraction techniques may surely benefit from cluster-aware partitioning methods. Accuracy in the selection of different clusters and in the construction of enclosing hypercubes may enable the achievement of the following desiderata: extracting the minimum number of different predictive rules (one per cluster) having the lowest possible predictive error. A number of challenges arise from the aforementioned workflow. (i) How to fix the correct number of clusters to identify? (ii) How to handle outliers in the construction of hypercubes around the found regions? (iii) How to build hypercubes around separable clusters associated with overlapping hypercubic regions?

We believe that powerful strategies to describe non-trivial clusters may exploit difference cubes – e.g., regions of the input feature space having a non-cubic shape and described by the subtraction of cubic areas – and hierarchical clusters. We stress that the importance of adopting hypercubes to describe input regions depends on the possibility to define a hypercube in terms of single variables belonging to specific intervals, in a highly human-comprehensible form. This is not true when dealing with other representations—e.g., oblique rules, m-of-n rules.

4 Conclusions

In this paper we propose a (deep) clustering-based workflow to enhance the symbolic knowledge extraction procedures from BB regressors in terms of computational complexity, fidelity and predictive performance. Our method can be exploited to build hypercubic regions associated with human-readable logic rules in presence of linearly separable clusters of input instances. In our future works we plan to implement and include in the PSyKE framework [10,11,13] different knowledge extractors adhering to the presented concepts and capable of handling more complex situations—e.g., outliers, clusters with more challenging shapes, non-linearly separable clusters.

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