Pedagogical Rule Extraction for Learning Interpretable Models

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Abstract
Machine-learning models are ubiquitous. In some domains, for instance, in medicine, the models’ predictions must be interpretable. Decision trees, classification rules, and subgroup discovery are three broad categories of supervised machine-learning models presenting knowledge in the form of interpretable rules. The accuracy of these models learned from small datasets is usually low. Obtaining larger datasets is often hard to impossible. We propose a framework dubbed PRELIM to learn better rules from small data. It augments data using statistical models and employs it to learn a rule-based model. In our extensive experiments, we identified PRELIM configurations that outperform state-of-the-art.

Keywords: rule extraction, model explanation, density approximation, tabular data augmentation, XAI

1 Introduction
Machine learning models are an essential part of modern technology. While the internal structure of some models, e.g., artificial neural networks, is complex, other models, e.g., shallow decision trees, are relatively easy to understand for a human. We call them black-box (bb) and white-box (wb) respectively. Interpretability is a desirable feature — the user of an interpretable model can validate its logic, decide whether to trust its predictions, and ensure the absence of discrimination. To achieve interpretability, one can (1) directly learn a white-box model or (2) train a black-box model and explain it [30]. Some argue that the former option is preferable, at least for high-stakes decisions [51]. But learning an accurate white-box model tends to require large datasets that are often not available.

This paper proposes PRELIM (Pedagogical Rule Extraction for Learning Interpretable Models), a framework to improve white-box rule-based models learned from small datasets. PRELIM learns a “generator”, a model that creates new data points, and a powerful black-box model that labels them. So PRELIM creates extensive artificial data sets to train a white-box model.

Pedagogical (black-box model agnostic) rule extraction (PRE) methods have been proposed in the last decades, and Section 2 reviews them. However, it is unclear which methods improve the accuracy of which wb models. This is because experiments in the respective publications do not satisfy the following requirements.

R1: White-Box Generality. Experiments should cover different categories of rule-based models. While decision tree (DT) and classification rule (CR) learners target at accurate classification, subgroup discovery (SD) methods find individual rules covering many examples of a given class and possibly few examples of other classes [2]. Rule extraction literature has not covered all three categories simultaneously.

R2: Comparison to State-of-the-Art. To find the state-of-the-art, PRE methods should be compared. This has rarely been the case. Existing comparisons [20, 24] cover only few generators.

R3: Accuracy Increase. Our main goal is to increase the accuracy of a white-box model learned from small datasets, whereas many PRE methods exclusively aim at explaining a black-box model. In effect, PRE-related papers do not restrict the dataset size in the experiments and sometimes do not measure the accuracy [5].

R4: Significance. A conclusive result requires experimenting with many datasets. Many related papers use fewer than seven datasets.

R5: White-Box Interpretability. Models obtained with DT or CR learners can loose interpretability if they consist of many rules; rules discovered with SD methods are not interpretable if they have too many features in the antecedent [2]. Many related papers do not restrict the complexity of wb models. This has sometimes resulted in models consisting of hundreds of rules [14].

R6: Strong Baseline. Default hyperparameter values of a white-box model may cause overfitting. An overfitted model is a weak, easy-to-beat baseline. Although the importance of hyperparameter optimization has been demonstrated elsewhere [59], many PRE papers do not claim to have this feature.

We will demonstrate the practical importance of these requirements. For instance, we have found that the majority of generators proposed for PRE so far, on average, do not increase the accuracy of a white-box model when its interpretability is controlled. With PRELIM, we evaluate several generators never studied before with PRE methods and show that they can help
learning white-box models of higher quality. It turns out that these generators are also competitive for explaining black-box models. Our code is openly available\footnote{https://github.com/Arzik1987/prelim}.

Paper outline: Section 2 reviews related work. Section 3 describes PRELIM. Section 4 covers the experimental setup and says how it addresses the requirements. Section 5 features results. Section 6 describes future research. Section 7 concludes.

2 Related Work

Related work includes rule extraction, dataset augmentation, and semi-supervised learning.

**Rule Extraction.** Rule Extraction refers to the task of explaining the logic of a black-box model with a rule-based model [30]. Rule extraction methods can be pedagogical or decompositional. The first group of methods treats a complex model as a black-box oracle [24], in the same way as PRELIM does. The methods from this group differ from each other, mainly regarding the generators and sometimes the white-box models they use. Table 1 reviews PRE methods and contrasts them with our work.

Related work does not satisfy the requirements listed in the introduction. In particular, only [35, 46, 71] explicitly compare their methods to another PRE algorithm. Thus, related work generally does not satisfy R2. We use various generators proposed for pedagogical rule extraction and other generators with PRELIM, hence the symbol $\infty$ in the column $R2$ in Table 1. The column “GENA” indicates PRELIM’s generator similar to the one proposed in the respective paper.

Only [2, 20, 24, 36, 37] address R3. However, [20, 24, 36, 37], do not restrict the complexity of a white-box model, so they do not comply with R5.

All papers, except for [2], do not satisfy R6. Although the work [2] complies with both R6 and R5, it covers only datasets produced in computer experiments where one knows the distribution of inputs and does not need to develop a generator approximating it.

None of the papers considers three categories of rule-based wb model learners — DT, CR, and SD. So they do not address R1. Much related work uses few datasets for experiments — it does not satisfy R4.

**Dataset Augmentation.** Rule extraction techniques are part of a larger group of knowledge distillation methods [33] where the end model is generally not interpretable. One of the generators we use in PRELIM comes from [10] that falls into this group.

Knowledge distillation techniques in turn often rely on dataset augmentation methods that create artificial data and add it to the train set. They are proven particularly effective for object or speech recognition tasks where invariant (producing objects of the same class) input transformations are apparent. For instance, such transformations are scaling or shifting images [29].

Several data augmentation techniques exist for tabular data, e.g., [23, 67]. To our knowledge, they either have not been used for training white-box models [23] or did not increase their quality [67].

**Semi-Supervised Learning.** In the presence of unlabeled data, some semi-supervised techniques use a metamodel to create pseudo-labels and augment the train set [66, 73]. Our setting is more general as we do not assume the existence of unlabeled data.

3 PRELIM

This section features our method, PRELIM. We start with notation. Let $D^{tr}$ be a train dataset:

$$D^{tr} = \left( \begin{array}{ccccc} x_{i1} & \ldots & x_{iM} & y_i \\ \vdots & \ddots & \vdots & \vdots \\ x_{iN} & \ldots & x_{NM} & y_N \end{array} \right).$$

In each row $i \in \{1, \ldots, N\}$, the first $M$ elements contain feature values $x_i = (x_{i1}, \ldots, x_{iM})$ and constitute a point in an $M$-dimensional space; the last column $(y_1, \ldots, y_N)$ contains the target class for each point. This work considers a binary classification problem with continuous features, i.e., $x_i \in \mathbb{R}^M$, $y_i \in \{0, 1\}$. We refer to the entire row $d_i = (x_i, y_i)$ as an example.

3.1 The Algorithm

Algorithm 1 is the PRELIM framework. It takes as input a dataset $D^{tr}$, a black-box model learning algorithm BBA, a white-box model learning algorithm WBA, a generator learning algorithm GENA, and the number $L$ of examples to create. It outputs a white box model wb. PRELIM works as follows.

1. Use $D^{tr}$ with algorithms BBA and GENA to obtain a black-box model bb and generator gen (Lines 2–3):

\begin{algorithm}
\caption{PRELIM algorithm}
\begin{algorithmic}[1]
\Procedure{PRELIM}{D^{tr}, BBA, WBA, GENA, L, ...}
\State $bb = \text{BBA.fit}(D^{tr}, ...)$
\State $gen = \text{GENA.fit}(D^{tr}, ...)$
\State $D^{new} = []$
\For{$0 < i < L + 1$}
\State $x_i^{new} = \text{gen.sample}()$
\State $y_i^{new} = \text{bb.predict}(x_i^{new})$
\State $D^{new}.append(x_i^{new}, y_i^{new})$
\EndFor
\State $wb = \text{WBA.fit}(D^{tr} \cup D^{new}, ...)$
\State \textbf{return} $wb$
\EndProcedure
\end{algorithmic}
\end{algorithm}
Table 1: Related methods. Column names: BBA — bb model learner; WBA — wb model learner; R2 — compared to related work; R3 — in the paper, the method has improved the wb accuracy; #D — the number of datasets used; GENA — name of the most similar generator used in PRELIM. Values: RF — random forest; NN — artificial neural network; SVM — support vector machine; DT — boosted trees, [XX] — artificial points with algorithm WBA, [XX]e — an ensemble of models [XX]; CR/RR — classification/regression rules; DT/RT — decision/regression tree; SD — subgroup discovery; na — no information; ∞ — explained in the text.

2. create $L$ artificial points with gen and label them using $D^T \cup D^{new}$ to form a new dataset $D^{new}$.
3. use $D^T \cup D^{new}$ with algorithm WBA to get a white-box model wb.

PRELIM differs from the algorithms in Table 1 in that it does not rely on a particular generator but rather takes one as input. This renders PRELIM more flexible and allows to experiment with different generators.

Next, we describe the white-box models, the black-box models, and the generators we employ. Our experiments compare various generators and suggest promising combinations of GENA and BBA. PRELIM is easy to extend and lets its users add new components.

3.2 White-Box Models With PRELIM, we use five white-box models of three categories — decision trees, classification rules, and subgroup discovery. Decision trees and classification rules aim at maximizing accuracy. Subgroup discovery methods search for large groups of examples of the same class, they use weighted relative accuracy (WRAcc) quality measures. Section A explains the three groups in detail; [26] describes similarities and differences between these models.

We use a version of the decision tree learning algorithm, CART [8], a rule learning algorithm IREP [27], its successor RIPPER [16], subgroup discovery algorithms PRIM [25], and BI [44]. The implementations of CART, RIPPER, IREP, and BI we use allow restricting the complexity of the learned model, as we will explain.

3.3 Generators We describe two groups of generators. The first includes sampling algorithms that have been used for PRE and extensions of these algorithms we propose. The second group contains generators that have not been used with PRE methods.
Conventional Generators and Their Extensions. Literature (Table 1) uses several algorithms for PRE. We describe them below and propose extensions.

**DUMMY.** Similarly to [14, 34, 35, 37, 45, 46], this generator returns all points from D.

**UNIF.** This generator creates new points by sampling the value of each feature, i.i.d. from a continuous uniform distribution with bounds defined by minimum and maximum values of the feature in D. References [2, 19, 71, 72] do similarly.

**NORM.** As [36] does, NORM generates points by sampling the value of each feature, i.i.d. from a Gaussian distribution with mean and standard deviation estimated from the values of the feature in Dtr.

**GMM.** Gaussian mixture models represent a probability density function (pdf) as a weighted mixture of k Gaussian distributions [31]:

\[ f(x) = \sum_{i=1}^{k} \alpha_i N(\mu_i, \Sigma_i). \]

GMM uses the resulting composite pdf to generate new points. The weights \(\alpha_i\) and the elements of the covariance matrix \(\Sigma_i\) are estimated from the data. The structure of the covariance matrix and the number of components \(k\) are hyperparameters of GMM.

**GMMAL.** This generator from [5] refers to the Gaussian mixture model with the diagonal covariance matrix.

**KDEM.** Kernel density estimation [58] is another method to approximate pdfs. For this method, one has to specify a kernel function and a bandwidth parameter. For KDEM, in line with [6, 18, 70], we use a Gaussian kernel and model the distribution of each feature separately.

**KDE.** This generator extends KDEM to a multidimensional case. For KDE, one specifies a set of bandwidths rather than a single value.

**KDEB.** The ANN-DT algorithm [54] suggests to sample points uniformly at random from M-balls with a radius \(r\) and centered at points of the train data. One can see KDEB as a variant of KDE, akin to nearest-neighbor density estimation [56].

**CMM.** The CMM method [20] uses an opaque model, C4.5-rules ensemble, to generate artificial points and to label them. It creates new points by sampling from the area defined by each rule in the ensemble uniformly at random. The number of artificial points is proportional to the number of points in train data covered with the respective rule. We use a similar approach, CMM, with a random forest instead of a C4.5-rules ensemble.

**RE-RX.** The RE-RX method [57] uses a subset of train examples where bb predictions match true labels.

**VVA.** The ALPA algorithm [24] creates new points that are (a) not very different from points in train data and (b) lie near the decision boundary of a bb to be explained. Section B describes this generator. [41] proposes a generator doing almost the opposite; we do not use it due to an unclear description.

Other generators. To deal with the imbalanced classification problem, one sometimes creates artificial examples of the minority class. To use such methods with PRELIM, we create a set of points \(P_{new}\) with the UNIF generator and construct an artificial classification problem where points from D belong to the minority class and ones from \(P_{new}\) to the majority class. We adapted the SMOTE and ADASYN generators in this way.

**SMOTE.** SMOTE [13] (Synthetic Minority Over-sampling Technique) takes the train data belonging to the minority class and creates new data for each point \(x\) as follows. First, it finds the \(k\) nearest neighbors of \(x\) belonging to the minority class and selects one of them, \(x'\). It then creates a new point \(p_{new}\) with coordinates \(x'_{new} = gap_i \cdot x_i + (1 - gap_i)x'_i\), where \(gap_i\) is a random number between 0 and 1, new for each point, coordinate and iteration. SMOTE stops after creating a new dataset of the required size. The number of nearest neighbors \(k\) is a hyperparameter of SMOTE; SMOTE is the corresponding PRELIM generator.

**ADASYN.** ADASYN [32] creates more synthetic points than SMOTE for the minority class points densely surrounded by the majority class examples. The respective PRELIM generator is ADASYN.

**MUNGE.** The authors of [10] replace an ensemble of artificial neural networks with a shallow neural network. We use their algorithm MUNGE to generate new points. For each point \(x\) in train, it finds its nearest neighbor \(x'\). Then MUNGE creates a new point by changing each coordinate \(x_i\) of \(x, i = 1, \ldots, M\) with a predefined probability \(P\) to a random value sampled from the Gaussian distribution \(N(\mu, |x - x'|/s)\), \(s\) is hyperparameter of MUNGE. One can see MUNGE as a random-bandwidth variant of KDE, similar to nearest neighbor density estimation [56]. MUNGE is also similar to SMOTE with \(k = 1\).

**SSL.** To test PRELIM in a semi-supervised learning setting, we introduce the SSL generator; it returns some existing points without their labels.

3.4 Black-Box Models. We use random forests (RF) [7] and boosted trees (BT) [15] as black-box learners (BBA) since they perform well in classification tasks [65] and for rule extraction [2]. Beyond label predictions, both models can output continuous probability scores that are essential for the VVA generator; we also use the scores in the experiments with subgroup discovery.
4 Experimental Setup

This section presents our experimental setup and explains how it satisfies the requirements R1–R6. Section C provides further details on implementation details, datasets characteristics, and hyperparameter values for BBA algorithms and generators.

4.1 Datasets We use 30 datasets from the UCI [21], PMLB [50] and OpenML [63] repositories. We removed categorical features, features taking fewer than 20 unique values, and rows with missing values. We denote each resulting dataset with $D$, $|D| = N^*$. Using many datasets allows us to satisfy R4: Significance.

4.2 Design of Experiments A single experiment has the following steps

1. Split a dataset into $D^{tr}$ with $|D^{tr}| = N$ and $D^{test}$;  
2. normalize features in $D^{tr}$, transform $D^{test}$ correspondingly;  
3. obtain $wb = \text{PRELIM}(D^{tr}, \text{BBA}, \text{WBA}, \text{GENA}, L, \ldots)$;  
4. evaluate quality of the resulting model $wb$ on $D^{test}$.

We experiment with the generators, black-box model and white-box model learners listed in Section 3. For each dataset, we experiment with $N = |D^{tr}| \in \{100, 400\}$. To average random effects, we do $K = 25$ splits into $D^{tr}$ and $D^{test}$, sets $D^{tr}$ resulting from different splits overlap as little as possible.

4.3 Quality Measures The main goal of PRELIM is to increase the accuracy of decision trees and classification rules or the weighted relative accuracy of subgroups. Measuring accuracy and comparing it to the baseline (Step 3 in Section 4.2) satisfies R3: Accuracy Increase. For decision trees and classification rules, we also evaluate how well PRELIM explains a black-box model. The respective measure is fidelity, the accuracy of a white-box model over black-box model predictions rather than true labels [54]. We count the number of leaves in decision trees, the number of rules in decision lists of RIPPER and IREP, and the number of features in the rule antecedent in subgroups. These are conventional proxies of white-box interpretability [24].

4.4 Hyperparameters We use grid search hyperparameter optimization with 5-fold cross-validation unless otherwise specified. Using various white-box models and generators satisfies R1: White-Box Generality and R2: Comparison to State-of-the-Art.

Varying hyperparameters of white boxes lets our experiments comply with R5: White-Box Interpretabiliy and R6: Strong Baseline. We optimize hyperparameters of white-box learners using $D^{tr}$.

**White-Box Models.** We experiment with three parametrizations of the decision tree learning algorithm: DTcomp, DTcv, and DT. For DTcomp, we limit the number of leaves in the tree to eight; DTcv thus complies with R5. DTcv obeys R6, we optimize the number of leaves, choosing it from $2^{\{1,2,3,4,5,6,7\}}$. For a DTcv model obtained with PRELIM, we ensure that it does not have more leaves than DTcv learned from $D^*$, so that the accuracy comparison is fair. To limit the depth of $DT$ somewhat, we restrict the number of samples reaching non-leaf nodes to be greater than 10. Note that we use DT to show the importance of R5 and R6, as DT does not satisfy them.

For IREP and RIPPER, we limit the number of rules they output to eight, to comply with R5.

In preliminary experiments, we have found PRELIM with subgroup discovery methods to work better if a black-box model assigns class probabilities rather than class labels to examples in $D^{tr} \cup D^{new}$; we set up PRELIM accordingly. Next, we adjust BI and PRIM to find precisely one subgroup; this simplifies the analysis and does not reduce generality of the result [2].

We limit the number of features in the rule antecedent for BI to 15 and select it from $\{Z - j\lceil Z/5 \rceil, j > 0, j\lceil Z/5 \rceil < Z, Z = \min(15, M)\}$. We ensure that the BI algorithm with PRELIM is not exposed to more features than BI applied solely to $D^{tr}$. BI satisfies R5 and R6. We have also optimized a hyperparameter of PRIM (cf. Section C), so PRIM complies with R6.

**PRELIM.** Some generators automatically determine the size $L$ of the generated sample. In particular, DUMMY creates a sample of size $L = N$, in RE-RX $L \leq N$, VVA internally optimizes the ratio $L/N$, cf. Section B. For SSL, we keep at least half of $D^{test}$ for testing, and set $L = \min(10^4 - N, \lfloor (N^* - N)/2 \rfloor)$. For other generators, $L = 10^4 - N$ if the WBA is a decision tree learner and $L = 10^4 - N$ otherwise. Large $L$ values tend to be better [2]. We limit $L$ to keep the runtime reasonable.

5 Results

We present the results separately for decision trees, classification rules, and subgroup discovery. We draw a heat map for each white-box model, dataset size $N$,
5.1 Decision Tree. Accuracy does not only depend on the quality of model predictions but also on the class imbalance in the dataset. For instance, the accuracy estimate averaged across 30 × k experiments for each black-box model (columns) and generator (rows) combination. Grouped columns refer to different k, class in [1,2] is overrepresented. To mitigate the influence of class imbalance, we report the relative accuracy increase, i.e., the difference between the accuracy of the model and of the naive classifier.

Figure 1: Decision tree. Average quality change for N = 100 (top panel) and N = 400 (bottom panel)
some generators can only improve the model if it consists of many rules.

PRELIM with KDE, KDEB, MUNGE, SMOTE improves accuracy and fidelity of \(\text{DTcomp}, \text{Dtcv}\) and yields models with almost the same number of leaves. From these generators, only KDEB has been proposed for rule extraction; we have now shown its ability to increase the accuracy of decision trees, which has not been done before.

Table 2 reports the average relative accuracy increase of black box models and wins/draws/losses of PRELIM with KDE and decision tree over the baseline for different \(N\) and black box models. For \(\text{DTcomp}\) and \(\text{Dtcv}\), \(N \in \{100, 400\}\), PRELIM with KDE allows retaining 17–41% of accuracy difference between black-box model and white box model trained solely on \(D^{tr}\).

### 5.2 Classification Rules

For small \(N\), IREP and RIPPER learn few rules of low accuracy. To make a comparison between PRELIM and the baseline (generator

\[
\begin{array}{cccc|c|c}
\text{BBA} & \text{N} & \text{IREP} & \text{RIPPER} \\
\hline
\text{BT} & 100 & 594/0/154 & 550/4/194 \\
\text{BT} & 400 & 554/2/194 & 513/5/232 \\
\text{RF} & 100 & 597/2/149 & 542/3/203 \\
\text{RF} & 400 & 535/0/215 & 490/2/258 \\
\end{array}
\]

Table 3: CR accuracy. PRELIM with kde versus NO

\[
\begin{array}{cccc|c|c}
\text{BBA} & \text{N} & \text{BI} & \text{PRIM} \\
\hline
\text{BT} & 100 & 482/34/232 & 562/2/184 \\
\text{BT} & 400 & 504/34/212 & 511/4/235 \\
\text{RF} & 100 & 469/8/271 & 522/0/226 \\
\text{RF} & 400 & 468/7/275 & 452/4/294 \\
\end{array}
\]

Table 4: SD WRAcc. PRELIM with KDE versus NO

\(\text{NO}\) on the plots) more insightful, we force IREP or RIPPER to discover more rules by amplifying dataset \(D^{tr}\) (i.e., duplicating it and joining to itself multiple times) to form \(D', |D'| \approx L\), and use rules learned by from \(D'\). In our experiments, the quality of rules learned from the original dataset \(D^{tr}\) are similar to that of PRELIM with the \(\text{RE-RX}\) generator and random forest.

Figure 2 presents the results for classification rules. PRELIM with KDE, KDEB, MUNGE, and SMOTE generators increases the accuracy of the rules from IREP and RIPPER. The results for fidelity (Section D) are similar.

Table 2 lists IREP and RIPPER wins/draws/losses of PRELIM with KDE over the baseline regarding the relative increase in accuracy. Note that, while boosted trees perform better than random forests on average, the relative accuracy increases more for PRELIM with a random forest at \(N = 100\).

### 5.3 Subgroup Discovery

Figure 3 lists the results for subgroup discovery. As with decision trees, PRELIM with KDE, KDEB, MUNGE, and SMOTE generators on average increases the quality of the discovered subgroups while retaining their comprehensibility. As before, the quality increase is more prominent for smaller datasets \(D^{tr}\). Although the WRAcc improvement from 8.9% to 9.1% for KDE and \(N = 400\) may seem moderate, it is even more significant than that for \(N = 100\). This is visible from Table 4 that reports wins/draws/losses of PRELIM with the KDE generator over the baseline for different \(N\) and black-box models concerning WRAcc.

### 5.4 Semi-Supervised Learning

The SSL generator emulates a semi-supervised setting where unlabeled data is available. By design, the number of points SSL outputs in our experiments never exceeds \(L\) in other generators except for \(\text{DUMMY, RE-RX, and VVA}\). However,
white-box models obtained with SSL tend to be more accurate than those learned by PRELIM with KDE. This shows that PRELIM is a viable semi-supervised algorithm for learning interpretable ML models and illustrates the importance of a PRELIM’s generator to model joint feature distributions accurately.

5.5 Additional Remark Sometimes one cannot share actual data due to privacy restrictions. One possibility is to share an artificial dataset with similar properties. One measure of the quality of the resulting dataset is the accuracy of a decision tree learned from this dataset [67]. Thus, one can see PRELIM as a method that can preserve privacy by creating artificial data ($D_{new}$, cf. Algorithm 1) of high quality.

6 Future Research

While PRELIM already is quite general, we intend to broaden its scope further, as follows. PRELIM with subgroup discovery has benefited from using class probability scores instead of class predictions; hence we plan to extend the PRELIM methodology to use class probabilities with decision trees and classification rules. We also plan to test PRELIM with regression and multiclass classification tasks. In the future, we want to extend our framework such that it can handle categorical data and data with mixed features. We also plan to enrich PRELIM with other ways to generate new data (e.g., [42, 47]) and experiment with different approaches to set the hyperparameter values of generators [69].

According to our experiments, PRELIM with the KDE generator is the state-of-the-art pedagogical rule extraction method. We plan to compare PRELIM with decompositional rule extraction techniques, cf. [3, 52].

7 Conclusions

Interpretable white-box models underpin many high-stakes decisions. In this paper, we deal with the problem of learning accurate white-box models from small datasets. We formulate requirements on methods and their evaluation and show that existing literature does not sufficiently address them. We propose a framework, PRELIM, to improve learning white-box models from small datasets. It trains a configurable set of statistical models and uses them to create an augmented dataset used in turn to learn interpretable models. Our experiments, which take the requirements into account, show that most existing methods do not consistently improve the accuracy of interpretable models. We propose several configurations of PRELIM that in turn achieve a consistently higher accuracy of white-box models and explain complex models better than the competitors.

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A White-Box Models

Decision Trees. A decision tree is a classification model in the form of a directed graph consisting of nodes and arcs. Nodes with no direct successors are leaves, the node with no direct predecessor is the root, all others are internal nodes. In the usual case of a binary tree, each node except root has exactly one direct predecessor, and each non-leaf node has two direct successors. Non-leaf nodes contain a test on a feature value, and arcs show the next node to consider depending on if the test is passed or not. Leaf nodes contain the class predicted for the examples reaching it. Decision tree learning algorithms differ in heuristics used to learn tests for non-leaf nodes and to prune a tree. We use a version of a popular decision tree learning algorithm, CART [8].

Classification Rules. A classification rule model consists of if-then rules. The part between if and then is the antecedent of a rule and contains conjunction of tests on different features. The part after then is the rule consequent; it contains a predicted class label. In contrast to decision trees that produce mutually exclusive rules, classification rules can overlap. Usually, rules are ordered to form a so-called decision list [26], i.e., if-then-else rules. To predict a class label with a decision list, one uses the first rule that fires. If no rule fires, the model assigns a “default” class. With PRELIM, we use a popular rule learning algorithm, IREP [27], and its successor RIPPER [16]. The main differences between RIPPER and IREP are in stopping criterion, pruning heuristic, and optimization technique of the latter; see [26] for details.

Subgroup Discovery. In contrast to classification rules, subgroup discovery methods focus on the properties of individual rules [26]. Weighted relative accuracy (WRAcc) commonly measures individual rule quality.

\[ WRAcc = \frac{n}{N} \left( \frac{n^+}{n} - \frac{N^+}{N} \right). \]

Here \( n, n^+ \) are the total number of examples satisfying conditions in the rule antecedent and the sum of their \( y \) values, respectively; \( N, N^+ \) are the corresponding values for the whole dataset. In PRELIM, we use BI [44] and PRIM [25] subgroup discovery algorithms that can work with continuous features. PRIM starts with defining a target function (WRAcc in this paper). It then finds a rule by cutting off a small share \( \alpha \) of examples to maximize WRAcc considering one feature at a time [2].

B Valley-Valley Approximation Generator

The vva generator creates new points as follows.

1. Take \( N_v \) train data points with the most uncertain predictions of \( \text{bb} \);
2. for each point, find its nearest neighbor with a different predicted class;
3. sort the resulting pairs of nearest neighbors according to distances between them, starting from smaller distances;
4. for each pair of points, generate a new point on the line connecting them;
5. repeat the previous step several times to obtain \( L \) new points.

The ratios \( N_v/N \) and \( L/N \) are hyperparameters of vva.

C Experimental Setup. Additional Details

C.1 Datasets Table 5 lists the datasets together with their characteristics after the pre-processing and corresponding references. Here \( N^+ \) is the number of rows, \( M \) is the number of features, “Pos_class” — our criterion to assign the class label “1” in datasets for multi-class classification or regression, \( N^{**} \) — the number of rows belonging to class “1”.

C.2 Implementation Details We implement the experiments in Python [62]. For decision trees and random forests, we rely on scikit-learn [49]. Boosted trees are from XGBoost [15]. Classification rules are from the “wittgenstein” repository⁴; we fixed several bugs in it. We implemented subgroup discovery methods according to [2], and generators according to the descriptions in respective papers.

C.3 Hyperparameters Used in Experiments

PRIM For PRIM, we optimize \( \alpha \) (cf. Section A) by choosing its value from the set \( \{0.03, 0.05, 0.07, 0.1, 0.13, 0.16, 0.2\} \).

Black-Box Models For random forest, we select max_features from \( \{2, \sqrt{M}, M\} \). For boosted trees, we do random search in the following hyperparameter space: n_estimators is integer from the range \( \{10, 990\} \), learning_rate \( \in [0.0001, 0.2] \), gamma \( \in [0, 0.4] \), max_depth = 6, subsample \( \in [0.5, 1] \), the other hyperparameters are equal to their default values as provided in implementation. This is similar to what [48] does.

Generators For the GMM generator, we adjust hyperparameters using the Bayesian information criterion [55]. We optimize the covariance matrix structure.

³https://scikit-learn.org/stable/modules/tree.html
⁴https://github.com/imoscovitz/wittgenstein
by choosing it from all possible structures offered by the implementation and the number of components \( k \) — from \( \{1, \ldots, 29\} \). With \texttt{GMMAL}, we proceed similarly, except the covariance structure is restricted to diagonal. To set the bandwidth of \texttt{KDEM}, we use Silverman’s rule of thumb [58]:

\[
h_X = \frac{0.9 A}{N^{1/5}}, \quad A = \min\left(\sqrt{\text{Var}(X)}, \frac{\text{IQR}(X)}{1.349}\right).
\]

Here \( N \) is the number of observations, as before; \( \text{Var}(X) \) is the sample variance estimate of the feature \( X \), \( \text{IQR}(X) \) is the feature’s interquartile range. For \texttt{KDE} (multidimensional version density estimate), we set the bandwidth matrix to

\[
H = \frac{I_M}{M} \sum_{i=1}^{M} h_{X_i}.
\]

Here \( M \) is the number of features; \( I_M \) — the \( M \times M \) identity matrix; \( h_{X_i} \) — the bandwidth calculated for the feature \( X_i \) with (C.3). In line with [54], we set \( r \) in \texttt{KDEB} equal to the average distance of points in \( D^{tr} \) to their 10-th nearest neighbors. For the \texttt{CMG} generator, we use the same random forest model as the one used as \texttt{bb} in the respective \texttt{PRELIM} instantiation. Following the suggestions from [24], for \texttt{VVA}, we set \( N_v/N = 0.2 \) and select \( L/N \) from \([0, 2.5]\) via cross-validation.

For \texttt{SMOTE} and \texttt{ADASYN} generators, we use the default hyperparameters from their implementations. Specifically, we set the number of nearest neighbors \( k = 5 \). \texttt{ADASYN} fails in case of the absence of points from \( P_{\text{new}} \) in the \( k \)-neighborhood of a point from \( D^{tr} \). In this case, we try to increase \( k \) for \texttt{ADASYN} gradually; if it does not help, we use \texttt{SMOTE} instead of \texttt{ADASYN} in the respective experiment.

The work [10] does not recommend particular values.
Figure 4: Classification rules. Relative fidelity increase.

for hyperparameters $P$ and $s$ for MUNGE. After preliminary experiments, we set their values to $P = 0.5$ and $s = 5$. SSL returns $L$ points from $D_{text}$ and leaves only the remaining examples for testing.

**D Classification Rules Fidelity**

Figure 4 presents relative fidelity increase for experiments with classification rule learning algorithms.