Post-hoc Explanation using a Mimic Rule for Numerical Data

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Abstract: We propose a novel rule-based explanation method for an arbitrary pre-trained machine learning model. Generally, machine learning models make black-box decisions that are not easy to explain the logical reasons to derive them. Therefore, it is important to develop a tool that gives reasons for the model's decision. Some studies have tackled the solution of this problem by approximating an explained model with an interpretable model. Although these methods provide logical reasons for a model's decision, a wrong explanation sometimes occurs. To resolve the issue, we define a rule model for the explanation, called a mimic rule, which behaves similarly in the model in its region. We obtain a mimic rule that can explain the large area of the numerical input space by maximizing the region. Through experimentation, we compare our method to earlier methods. Then we show that our method often improves local fidelity.

1 INTRODUCTION

Recently, machine learning models produce highly accurate predictions that are applied to various tasks. Because these models tend to be complex and lacking transparency, humans might have difficulty interpreting their decisions. Interpretability and transparency issues present urgent difficulties to be resolved in the machine learning field. Especially, it presents severe difficulty when applied to sensitive fields such as credit risks(Rudin and Shaposhnik, 2019), educations(Lakkaraju et al., 2015), and health care(Caruana et al., 2015).

Many studies have been conducted recently to improve machine learning model transparency(Guidotti et al., 2018b). Among the approaches are methods that build another explanatory model approximating a pre-trained model ex-post. Such methods are called post-hoc explanations. Such methods are preferably model-agnostic, meaning that they are applicable to any machine learning model without knowing model details. Because of these properties, post-hoc explanation can be widely applicable to tabular data(Guidotti et al., 2018a), image(Ribeiro et al., 2016; Ribeiro et al., 2018), and sentiment prediction(Ribeiro et al., 2016).

Although post-hoc explanations are a useful and applicable framework, several issues must be resolved for further improvement. First, to exploit the internal decision rule of a black-box model, this method approximates a black-box model using other interpretable machine learning such as a linear model(Ribeiro et al., 2016; Lundberg and Lee, 2017) or a decision tree(Guidotti et al., 2018a). The approximation model sometimes has insufficient accuracy; it can lead to an incorrect explanation(Rudin, 2019). Moreover, although the explanatory model approximates a black-box model locally, the applicable scope is unclear. Therefore, the explanatory model cannot be used globally. It is therefore necessary to develop a more accurate and globally applicable post-hoc explanation method.To resolve these issues, we propose a novel rule-based explanation method: Mimic Rule Explanation (MRE). The MRE explanation consists of a rule that mimics the black-box model we call a mimic rule. Users can readily derive the decision using only a mimic rule because a mimic rule is an interpretable rule model representing the region with the same decision. Because of the mimic rule property, the MRE explanation shows higher correctness than the previous rule-based explanation method. The contributions of our study are the following.

1. We formulate a novel rule-based explanation method using a mimic rule and propose an algorithm to construct the explanation.
2. We show parameter-dependence and comparison of earlier methods with illustrative results.
3. Our method generates a more accurate explanatory rule than the earlier rule-based explanation method.

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2 RELATED WORK

One approach to enhancing interpretability is building globally interpretable and highly accurate machine learning models such as those of rule lists (Wang and Rudin, 2015; Angelino et al., 2017), and rule sets (Lakkaraju et al., 2016; Wang, 2018; Dash et al., 2018). Users can clearly comprehend model behaviors and explanations of any decision. Especially, rule models give users simple logic based on `If-Then` statements. They are often applied in interpretable/explainable machine learning. These models become simple to interpret. Therefore, they present difficulty when performing highly accurate analyses of problems with a complex input domain.

Lakkaraju et al. (Lakkaraju et al., 2016) demonstrated through a user study that disjoint rule sets provide high interpretability to users. As a method of explaining any machine learning model, Ribeiro et al. (Ribeiro et al., 2016; Lundberg and Lee, 2017) proposed a locally interpretable model-agnostic explanation framework. It uses an explanatory model to exhibit the behavior of black-box models to users. In fact, it locally approximates a black-box model using a sparse linear model. Then users can understand the model behavior using explanatory model weights. Ribeiro et al. (Ribeiro et al., 2018) also proposed another local model-agnostic explanation system called Anchor , which uses an important feature set as an explanatory model.

Some studies(Laugel et al., 2019; Aivodji et al., 2019; Rudin, 2019) have specifically examined the danger of post-hoc explanations. Post-hoc explainers(Ribeiro et al., 2016; Ribeiro et al., 2018; Guidotti et al., 2018a) sometimes provide an incorrect explanation. That is, they cannot capture the behavior of the black-box model because of approximation. Our explanatory method does not approximate the black-box model with another interpretable machine learning model. It improves the descriptions of the model by constructing the explanatory rule with geometric consideration. Moreover, we surmise that the post-hoc explanation still has an important aspect because users cannot necessarily use the information of a machine learning model like the training data of the pre-trained machine learning data in practical terms.

3 PRELIMINARIES

We show the notations and definitions and show previous rule-based explanation methods: Anchor (Ribeiro et al., 2018) and LORE (Guidotti et al., 2018a).

3.1 Notations and Definition

We denote the indicator function by $\mathbb{I}(c)$ where $\mathbb{I}(c)$ returns 1 if a condition c is satisfies, and otherwise 0. We also denote a set of features by $[d] = \{1, \ldots, d\}$. For a set A, $|A|$ is a cardinality of A.

We denote notations of a classification problem using a tabular dataset. A black box classifier is $f : \mathbb{R}^d \to \mathcal{C}$, where, the domain of f is d-dimensional numeric features and $\mathcal{C}$ is a target space and set of classes. Consequently, for any instance x, $y = f(x)$ is the label assigned by the model f to x.

Because we consider post-hoc explanations, we do not assume f and internal information of f. For example, if the model is a neural network, then information such as network construction or weighting is not used.

A rule-based explanation $\mathcal{E}$ is formulated as a tuple of a rule R and a label y:

$$\mathcal{E} = (R, y). \tag{1}$$

This definition is similar to an association rule. Therefore, if it satisfies $x \in R$, it is expected that $f(x) = y$. A rule is a subspace of input space $R \subset \mathbb{R}^d$ and is represented as a Cartesian product of each feature's interval.

$$R = \prod_{i=1}^{d} R_i = \prod_{i=1}^{d} [a_i, b_i]. \tag{2}$$

It is a readable model. Users can understand the behavior of the black-box model using the rule.

3.2 Previous Methods

3.2.1 Anchor

The explanations of Anchor consist of a set of discretized features. In the anchor algorithm, the input space is converted to discretized space called an interpretable representation(Ribeiro et al., 2018; Lundberg and Lee, 2017). It is expected to assign the corresponding label by the black-box model with high probability if instances that contain the feature set.Anchor generates the interpretable feature set with the beam-search and KL-LUCB algorithm(Kaufmann and Kalyanakrishnan, 2013) for a multi-armed bandit problem.

When Anchor applies data having a continuous feature, the feature is converted to categorical features by splitting. This process lacks ordering of a continuous feature. Because the feature set is formulated in the interpretable feature space and because this space has a gap separating the input space, the explanation might not be accurate in the input space. Anchor sometimes fails to show an explanation when applied to an imbalanced labeled dataset.

3.2.2 LORE

LORE uses a decision tree model(Guidotti et al., 2018a) as the explanatory rule. The decision tree locally approximates the black-box model near an explained instance x. The decision tree is trained with the data that is generated by a genetic algorithm(Tsai et al., 2013). Using an appropriate evaluation function for a genetic algorithm, it can generate data that have good properties: neighborhood of x and balanced labels.

The LORE's explanation is local approximation with a decision tree, thereby the possibility exists that the rule includes the incorrect region: $\{z \in R : f(z) \neq f(x)\}$. A rule of a decision tree would consist of infinite intervals: ($a_i = -\infty$ or $b_i = +\infty$ in eq. (2)). Moreover, it causes low accuracy of the explanatory rule. Genetic algorithms often cannot generate appropriate training data. For example, if an explained instance is far from the decision boundary, then a genetic algorithm might be able to generate balanced labeled data.

4 PROPOSED METHOD

We propose a novel explanation method, Mimic rule explanation (MRE), that approximates a black box model more strictly than previous rule-based explanation methods. First, we define the explanatory rule, which we designate as a mimic rule. To solve a mimic rule, we introduce an approximated formulation. The algorithm for mimic rules is summarized at the end of the section.

4.1 Definition of a Mimic Rule

We define a mimic rule as a cartesian product of each features' finite intervals. A mimic rule also follows eq. (2) and is denoted by R_M.

$$R_M = \prod_{i=1}^{d} R_{M,i} = \prod_{i=1}^{d} [a_i, b_i] \ (a_i, b_i \in \mathbb{R}). \tag{3}$$

By defining with a cartesian product of finite intervals, it prevents an explanatory rule including an incorrect region. Moreover, we require that a mimic rule satisfy the following two properties.

- Correctness: For any instance x in a mimic rule R_M, it is assigned a label y by f. Consequently, the following is satisfied:

$$\forall z \in R_M, f(z) = y. \tag{4}$$

  The mimic rule behaves similarly to model f if this is satisfied. Consequently, the mimic rule does not include an incorrect region. It is useful as an alternative to the model.

- Maximality: A mimic rule is a maximal rule. If a mimic rule is expanded, then the property (4) is not satisfied. By presenting a maximal rule, the explanation covers a large part of the input space. It is therefore more preferred as an explanation.

Innumerable mimic rules can satisfy correctness and maximality properties because the input space is continuous. Nevertheless, we presume that MRE presents a mimic rule as an explanatory rule in this study. Fig. 1a shows an intuitive illustration of a mimic rule in the input space.

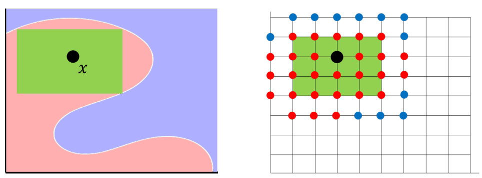
Since it is difficult to find a mimic rule in the continuous input space, we discretize the input space and consider a mimic rule in the discretized space.

Fig. 1b portrays a mimic rule in the discretized input space. It is noteworthy that multiple mimic rules can exist in the discretized space. However, the number of rules is countable. Although discretization of a continuous feature is used in many related works(Ribeiro et al., 2018; Angelino et al., 2017; Rudin and Shaposhnik, 2019), these studies handle a discretized feature as a categorical feature and deprive the ordering of the feature. By handling discretized points as prototypes of the feature, ordering of a feature is maintained. We denote the prototypes of i-th feature ($i \in [d]$) as S_i

$$S_i = \left\{x_{i,-m_-}, \ldots, x_{i,-1}, x_{i,0}, x_{i_1}, \ldots, x_{i,m_+}\right\}. \tag{5}$$

where $x_{i,0} = x_i$, and m_-, m_+ are a natural number that controls a number of quantiles. For the sake of simplicity, we assume $m = m_- = m_+$ and $x_{i,j} - x_{i,j-1} = \varepsilon$ $(-m < j \leq m)$ with a constant ε. Hence the discretized space S can be define with S_i as bellow:

$$S = \prod_{i=1}^{d} S_i. \tag{6}$$



(a) The input space (b) The discretized space

Figure 1: Illustration of a mimic rule in the input space (a) and the discretized space (b).

4.2 Algorithm for a Mimic Rule

We propose an algorithm that presents a mimic rule in discretized input space. It satisfies correctness and maximality properties. Note that a mimic rule in the discretized input might not satisfy the properties in the original input space. We summarize the algorithm as 1.

First, we simplify the problem with parameters to solve a mimic rule in practical computational time. The algorithm constructs a mimic rule by expanding a region of the rule from the explained instance. Instances in space S might be evaluated by model f in the algorithm. Here, if all instances in the space S are evaluated by f, we can get an ideal mimic rule in S.

However, large amounts of computation time must be used because of the number of instances: $|S|$ exist in combinatorial order. For example, even in case of $\forall i \in [d],\ |S_i| = 2$, the number of instances in S is 2^d. To avoid this issue, we introduce parameter $P \in \mathbb{N},\ 1 \leq P \leq d$ that controls the search space size. We consider instances that are combinatorially perturbed up to P. The neighbor instances $X_q(S)$, which are perturbed features in a set $q \in 2^{[d]}$, are denoted as presented below.

$$X_q(S) = \prod_{i=1}^{d} X_{q,i}(S), \tag{7}$$

$$X_{q,i}(S) = \begin{cases} S_i \setminus \{x_i\} & (i \in q) \\ \{x_i\} & \text{otherwise} \end{cases}. \tag{8}$$

Therefore, the set of instances which might be evaluated is

$$\bigcup_{q \in 2^{[d]}: |q| \leq P} X_q(S). \tag{9}$$

When the cardinality of q is large, $|X_q(S)|$ exists in exponential order with respect to the number of prototypes. Thereby, the cardinality eq. (9) would be huge. To constrain the number of evaluated instances, we introduce a parameter $N \in \mathbb{N}$ and evaluate N instances sampled from $X_q(S)$.

This algorithm repeats evaluation of neighbor instances and shrinking the search space. For evaluation, N neighbor instances are sampled from $X_q(S)$; Z denotes the set of sampled instances. Here the i-th features ($i \in q$) of the instances is perturbed. Next, we evaluate the instances $z \in Z$ with given model f. The set of instances assigned the different label from $f(x)$ is denoted as Z_-. Because a mimic rule does not include negative instances inside itself, the search space is shrunk to exclude the instances in Z_- with a function `ShrinkSearchSpace` in Algorithm 1. Such evaluation is repeated until p reaches P. It returns the mimic rule as:

$$R_M = \prod_{i=1}^{d} [\min\{S_i\}, \max\{S_i\}] \tag{10}$$

at the end of the algorithm.

In the shrinking part of the algorithm, we use set $V \subseteq S$, which is a region that has no negative instances inside of itself. At the initial step of this process, V only consists of the explained instance x. The shrinking process continues until there are no instances to expand the sum of $|S_i \setminus V_i|$ for $i \in q$ of zero. Region V_i is expanded with a prototype $x_{i,j}$ that is the nearest from the edge of V_i. The region is updated if the expanded region does not include negative instances. Otherwise, the prototypes that are outside of $x_{i,j}$ are removed from S_i.

In the implementation, every S_i is represented with a list structure. Every element is sorted in ascending order based on the absolute value of the index. We consider a `Pop`(L) method that returns the left edge element of the list L.

Algorithm 1: Construction algorithm for a mimic rule.

Require: Classifier f, explained instance x, search space S, parameters P, N
Ensure: Mimic rule R_M
  for all $p \in \{1, \ldots, P\}$ **do**
    for all $q \in \left\{Q \in 2^{[d]}: |Q| = p\right\}$ **do**
      $Z \leftarrow$ sample N instances from $X_q(S)$
      $Z_- \leftarrow \{z \in Z: f(z) \neq f(x)\}$
      $S \leftarrow$ ShrinkSearchSpace(S, Z_-, q)
    end for
  end for
  for all $i \in \{1, \ldots, d\}$ **do**
    $R_{M,i} \leftarrow [\min\{S_i\}, \max\{S_i\}]$
  end for
  return R_M

  function ShrinkSearchSpace(S, Z_-, q)
    $V \leftarrow \prod_{i=1}^{d} [x_i, x_i]$
    while $\sum_{i \in q} |S_i \setminus V_i| > 0$ **do**
      $i \leftarrow$ pick from q that satisfies $|S_i \setminus V_i| > 0$
      $x_{i,j} \leftarrow$ `Pop`$(S_i \setminus V_i)$
      $R' \leftarrow$ expand V_i with $x_{i,j}$
      if $\forall z \in Z_-, z \in V'$ **then**
        remove outside elements of $x_{i,j}$ from S_i
      else
        $V \leftarrow V'$
      end if
    end while
    return S
  end function

5 EXPERIMENTS

We next evaluate our explanation method. We present two experiments: qualitative evaluation with an illustrative example and quantitative evaluation of explanations' fidelity.

We implemented MRE (Algorithm 1), LORE and scripts for all experiments in Python 3.7. For implementation, we use an open source machine learning library scikit-learn[1], Ribeiro's anchor implementation[2]. All experiments are run with a Linux machine with 3.40 GHz Intel Core-i7 CPU and 8.0GB of RAM.

5.1 Illustrative Examples

To present insights about characteristics of our method and dependency of parameters, we used a two-dimensional half-moon dataset. As a classifier, we use the SVC that trains with default hyperparameters of scikit-learn library. Fig. 2 shows the mimic rules under each conditions. The left image of Fig. 2 presents a mimic rule applied under numerous quantiles ($m = 25$) and all samples in search space S. Actually, MRE can present an almost ideal mimic rule in such a condition. Given a low number of quantiles ($m = 4$) in the center image of Fig. 2, a mimic rule might not satisfy the maximality. This issue arises because the distance between search points is large and because the adjacent search point crosses the decision boundary of the model. The condition under which a low number of samples N might lose the correctness property (right image of Fig. 2) occurs because the negative samples in the search space $\{z \in X_q(S) : f(z) \neq y\}$ are not sampled. Consequently, the rule expands improperly because of the low number of samples.

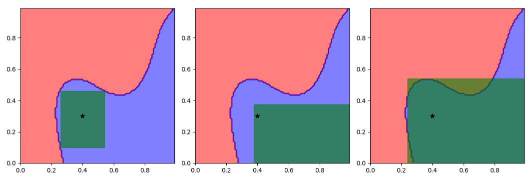


Figure 2: Illustrative result of a mimic rule (green area) with a half-moon dataset. Left: $m = 25$, $N = |X_q(S)|$, Center: $m = 5$, $N = |X_q(S)|$, Right: $m = 25$, $N = 10$.

We show the difference between Anchor, LORE, and our method in Fig. 3. Our method uses computation with numerous quantiles ($m = 25$) and a large number of samples. In this condition, our method can generate a maximal and correct mimic rule (left image of Fig. 3). The center image of Fig. 3 shows the rule of Anchor. Although Anchor's explanatory rule is correct, i.e. rule does not include incorrect region, the rule is not maximal. Moreover, LORE's explanatory rule is not correct: it includes an incorrect region (blue area), meaning that LORE presents a wrong explanation for instances in incorrect regions.

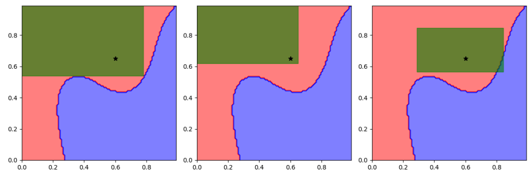


Figure 3: Comparison with the explanatory rules (green area). Left: MRE, Center: Anchor, Right: LORE

5.2 Evaluation of Fidelity

We measure the reliability of the explanatory rule with the iris dataset and breast-cancer (BC) dataset, which are opened in the UCI machine learning repository[3]. Table 1 presents details of the datasets. We used 80% of datasets as training data and the rest of 20% as test data. As black-box models, we trained a SVC and multilayer perceptron with default hyperparameters of the scikit-learn library. We set the parameters of Anchor and LORE as the same original parameters in their paper(Ribeiro et al., 2018; Guidotti et al., 2018a). Regarding the parameters of MRE, we discretized the $[0, 1]$ scaled input space with $m = 11$ and $\varepsilon = 0.05$. Then we set $N = 10$ and $P = 4$ for MRE parameters.

Table 1: Details of datasets: #, d denote the number of whole instances, the number of dimension, respectively.

datasets	#	d
Iris	150	4
BC	569	30

We use metrics for reliability: correctness and coverage, and eq. (11) and eq. (12) present their definitions. The correctness is measured using the probability of $f(x) = f(z)$, where z are sampled uniformly from the explanatory rule, and the instances z for coverage are sampled uniformly from the whole input domain. Each metric shows the value between 0 to 1 and a higher score means better. High correctness means that the explanatory rule does not include an incorrect region as $\{z \in R : f(z) \neq f(x)\}$, where high

[1]https://scikit-learn.org/

[2]https://github.com/marcotcr/anchor

[3]https://archive.ics.uci.edu/ml/index.php

coverage means that the explanatory rule covers large space over the input domain. Both of these metrics are measured using 1 million samples.

$$correctness = \mathbb{E}_{z\sim\mathcal{U}(R)}[\mathbb{I}(f(x)=f(z))] \quad (11)$$

$$coverage = \mathbb{E}_{z\sim\mathcal{U}(X)}[\mathbb{I}(f(x)=f(z))] \quad (12)$$

Comparison with correctness is presented in Table 2. MRE shows higher correctness than Anchor and LORE in every conditions. This fact indicates that a mimic rule satisfies the required condition: correctness. Actually, LORE works better than Anchor for the Iris dataset. Although approximation with a decision tree has good accuracy for low-dimensional data, it does not work well with high-dimensional data.Some possible causes include the number of training data for a decision tree. The correctness of Anchor is lower in all conditions. Anchor presents the feature set that captures the model well. However, it is precise in the binarized input space, not in the original space(Ribeiro et al., 2018). Consequently, binarization and lack of numeric ordering might cause a low-quality explanation. MRE performs high correctness by keeping the numeric ordering and by not approximating using another model. In the result with BC dataset and SVC, MRE shows lower correctness than that of other conditions. The decision boundary of SVC sometimes contains a small region that does not include training data(Laugel et al., 2019). It leads to incorrect explanations. Because of the discretization of the input space, it might miss such regions and tend to show low correctness. Consequently, explanations of MRE are more reliable because the explanatory rule has high correctness.

Table 2: Comparison of MRE, Anchor and, LORE with the correctness.

		MRE	Anchor	LORE
Iris	SVC	1.000	0.440	0.761
	MLP	1.000	0.440	0.656
BC	SVC	0.741	0.360	0.351
	MLP	0.991	0.388	0.377

Comparison with the coverage is presented in Table 3. The coverage of MRE tends to be lower than that of the earlier method.Anchor and LORE show higher coverage, meaning that their explanatory rule covers a large area of the input space. The rule of Anchor and LORE consists of a few conditions of features and it improves its coverage. However, a mimic rule consists of many conditions. It causes low coverage. We consider that there is a trade-off between correctness and coverage. The high-coverage rule might be easy to interpret for users. However, it gives users a misunderstanding of the black-box model. The high-correctness rule covers a small region. Therefore, the user cannot apply the rule widely, but the rule behaves similarly to the model: users can use the rule as a surrogate model.

Table 3: Comparison of MRE, Anchor and, LORE with the coverage.

		MRE	Anchor	LORE
Iris	SVC	0.021	0.828	0.182
	MLP	0.026	0.813	0.125
BC	SVC	0.220	0.603	0.801
	MLP	0.085	0.445	0.446

Table 4 presents the correctness with time expended. MRE finds the explanatory rule faster than other methods in a low-dimensional dataset. The computation time of Algorithm 1 increases exponentially with the number of dimensions. Therefore, it takes much time in the BC dataset. However, by introducing the discretization and by constraining the search space with parameter P, it can compute in practical time. Anchor presents the explanatory feature set with beam search(Ribeiro et al., 2018). For that reason, the computation time increases with the number of binarized dimensions. The computation time of LORE is almost constant because LORE trains a decision tree using a constant number of training data. It is noteworthy that we generate 5000 samples in this experiment.

Table 4: Comparison of MRE, Anchor and, LORE with the computation time in second.

		MRE	Anchor	LORE
Iris	SVC	0.005	0.107	0.250
	MLP	0.007	0.250	0.252
BC	SVC	16.42	3.457	0.374
	MLP	17.45	5.294	0.811

6 CONCLUSIONS

We proposed MRE: a novel local explanation method using a mimic rule. We defined the mimic rule as showing an internal decision rule of a black-box model. To compute a mimic rule effectively, we introduce some approximations and propose the algorithm. In the experiment with tabular datasets, our method showed higher fidelity than the previous rule-based explanation: Anchor and Lore. We showed a tradeoff between fidelity and coverage experimentally. Moreover, MRE is solved in practical computation time. It indicates that our method is widely applicable.

Our method supports only numerical input. Therefore to improve the range of application, it must be extended to the mixed data input: numerical and categorical data. Although our method shows high fidelity in the experiment, coverage is still lower than those of earlier methods so that improving coverage is an important task.It remains a global explanation of a black-box model.

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