

Paper ID 735

We deeply appreciate all the reviewers who made sharp and valuable comments on our paper and gave us the opportunity to submit a revised version. We have done our best for the revision according to their comments as shown below. We also thank in advance all the reviewers for reconsidering our revised paper’s suitability for the conference.

Summary of revisions

We appreciate all the reviewers for their clear and insightful comments. We have improved our paper based on their comments. The major revision points are listed as follows:

- We mentioned the names of other existing methods in section 2.
- We added discussion about parameter selection in section 5.3.
- We conducted qualitative and quantitative comparisons between Anchor and R-LIME in sections 4.1 and 4.3.
- We renamed the section ‘Challenges and Future Work’ to ‘Discussion’.

Please see below for a point-by-point response to each reviewer’s comments.

Responding to Reviewer #1

Suggestions for Rebuttal:

1. Offer guidance on how to select optimal parameters for different datasets and models.

We appreciate your suggestion. We added section 5.3 to provide guidance on how parameters should be selected in practice.

2. Include a discussion of other model-agnostic interpretability methods, such as SHAP, to provide a more comprehensive overview.

Thank you for your valuable suggestion. Although we acknowledge the importance of including an overview of other model-agnostic interpretability methods, due to space constraints, we only mentioned the names of some other methods in section 2.

3. Add experimental comparisons with more other model-agnostic interpretability methods to better evaluate R-LIME’s effectiveness.

We appreciate your sharp observations. We additionally conducted qualitative and quantitative comparisons between Anchor and R-LIME, which demonstrated that R-LIME generates more informative and general explanations than Anchor (see sections 4.1 and 4.3).

Responding to Reviewer #4

The authors should kindly explain why there is not a quantitative comparison between their proposed method R-LIME and Anchor. The lack of the comparison makes it hard to evaluate the impact of the proposed model.

We appreciate your insightful comments. We additionally conducted qualitative and quantitative comparisons between Anchor and R-LIME, which demonstrated that R-LIME generates more informative and general explanations than Anchor (see sections 4.1 and 4.3).

Responding to Reviewer #5

- It would be beneficial to move the comparison of R-LIME with Anchor and LIME to the Related Work section for improved clarity and organization.

We appreciate your insightful suggestion. We interpreted your suggestion to mean that we should move Fig. 1 and its explanation to section 2. After discussing the most understandable structure of our paper, we concluded that we should present effectiveness of R-LIME compared to closely related methods in section 1, before we overview other existing methods in section 2.

- The authors should consider exploring a more compatible method than the KL-LUCB algorithm to achieve higher accuracy. Although the experimental results suggest a minor effect, there may be potential underlying issues that need to be addressed.

Thank you for your valuable feedback. While our results suggest that the practical effect of using the KL-LUCB algorithm is negligible, we acknowledge the need to address its theoretical issues. Our focus is on presenting our novel framework for local interpretability, not the detailed algorithm. Thus, we leave the issues for future work due to space constraints. However, we deeply appreciate your sharp observations.

- The title of the ‘Challenges and Future Work’ section could be more aptly replaced with ‘Discussion’ to better reflect the content.

Thank you for your suggestion. We renamed the section to ‘Discussion’ to clearly reflect the content.

R-LIME: Rectangular Constraints and Optimization for Local Interpretable Model-agnostic Explanation Methods

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Abstract. In recent years, complex machine learning models have been widely introduced in various industrial fields due to their high accuracy. However, their increasing complexity has been a major obstacle to their implementation in sensitive decision-making situations. In order to address this problem, various post-hoc explanation methods have been proposed, but they have not been able to achieve interpretability of both the explanation and its scope. We propose R-LIME, a novel method that interprets complex classifiers within an interpretable scope. R-LIME locally and linearly approximates the complex decision boundary of a black-box classifier within a rectangular region and maximizes the region as long as the approximation accuracy exceeds a given threshold. The resulting rectangular region is interpretable for users because it is expressed as a conjunction of feature predicates. Through qualitative and quantitative comparisons on a real-world dataset, we demonstrate that R-LIME provides more reliable and interpretable explanations than existing methods.

Keywords: Interpretable machine learning · Local surrogate model

1 Introduction

In recent years, complex machine learning models, such as deep neural networks and random forests, have been widely introduced in various industrial fields due to their significant improvements in accuracy. However, their increasing complexity and black-box nature pose challenges, particularly in critical decision-making scenarios such as healthcare and finance, where the lack of transparency becomes a major obstacle to implementation. In order to address this problem, extensive research has focused on post-hoc explanations for complex models [5, 10, 11]. Post-hoc explanation methods are categorized into *model-dependent* and *model-agnostic* methods based on their dependence on the model’s structure, with the latter further classified into *global* and *local* methods based on the locality in the input space [13].

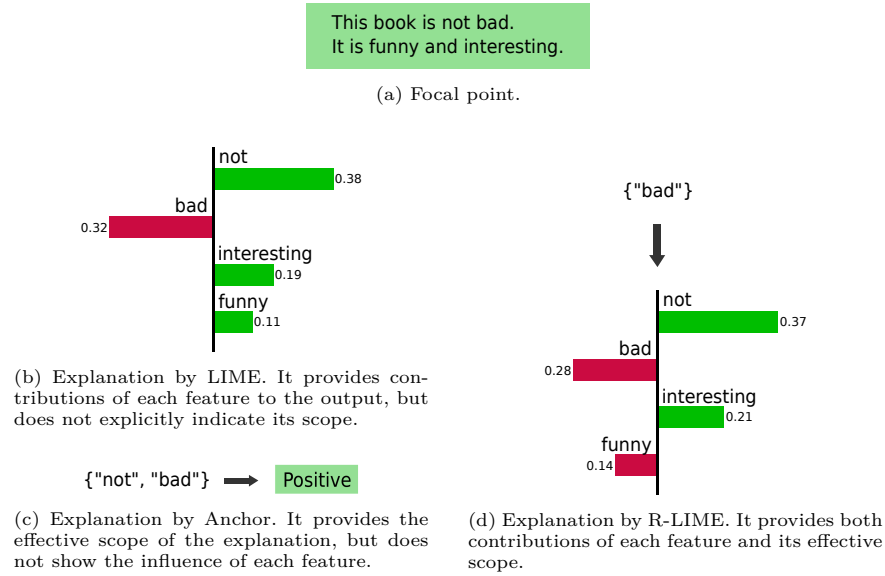


Fig. 1: Example of explanations by LIME [10], Anchor [11] and R-LIME (our proposed method) for a sentiment prediction model.

In this paper, we focus on *local* and *model-agnostic* methods. LIME [10] and Anchor [11] are representative local model-agnostic methods. An example of explanations by LIME and Anchor for a sentiment prediction model is illustrated in Fig. 1. LIME linearly approximates the complex decision boundary around the given focal point (Fig. 1(a)), then provides the weights of the linear model as the contribution of each feature to the output. The explanation by LIME (Fig. 1(b)) suggests that the word “not” mainly contributes to the positive prediction, but does not explicitly indicate its effective scope. Without the scope, users might mistakenly apply the knowledge derived from the explanation to other instances far from the focal point, potentially leading to misunderstanding of the black-box model’s behavior [11]. For this example, users may apply the derived insights to the sentence “This book is not good.” and mistakenly conclude that the word “not” mainly contributes to the positive prediction for this sentence as well, which is obviously incorrect. Anchor maximizes the coverage of a rectangular region containing the focal point as long as the probability of the black-box classifier outputting the same label as the focal point within the region exceeds a given threshold. While Anchor provides an effective scope of the explanation, users can get less insight compared to LIME. The explanation by Anchor (Fig. 1(c)) suggests that replacing words other than “not” and “bad” has little impact on the classifier’s output. While it clearly cannot be applied to the sentence “This book is not good” because of not including the word “bad”, the explanation does not provide details about the influence of each word, resulting in less user insight into the model’s behavior compared to LIME.

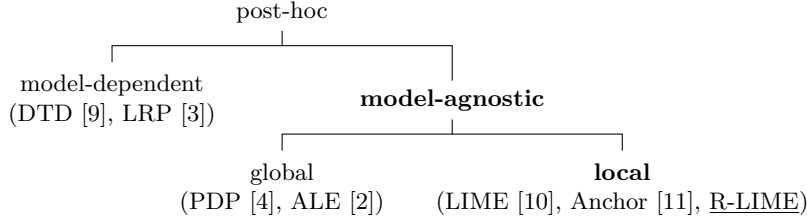


Fig. 2: Categorization of post-hoc explanation methods. We focus on *model-agnostic* and *local* methods, which explain model’s local behavior using only its output.

To address these limitations, we propose R-LIME (Ruled LIME), which provides both the contributions of each feature to the output and the effective scope of the explanation. R-LIME linearly approximates a complex decision boundary in a rectangular region and maximizes the region as long as the accuracy of the linear classifier exceeds a given threshold. The region is interpretable for users because it is expressed as a conjunction of feature predicates. An example of the explanation by R-LIME for a sentiment prediction model is shown in Fig. 1(d). It is clear that users can apply the insights derived from the explanation only to the sentences containing the word “not”.

2 Related Work

In this section, we overview existing research on post-hoc explanation methods, which explain the behavior of black-box models already trained. As shown in Fig. 2, post-hoc methods are classified into several categories.

They are broadly divided into *model-dependent* and *model-agnostic* methods based on their dependence on the model’s structure. Model-dependent methods, such as deep Taylor decomposition (DTD) [9] and layer-wise relevance propagation (LRP) [3], primarily focus on neural networks and explain the model’s behavior using its parameters [13]. While these methods provide detailed explanations (e.g., layer-wise explanations for neural networks), it is often challenging to apply the same method to models with different structures. In contrast, model-agnostic methods use only the model’s output. Although they are applicable to any model, they cannot explain the internal reasoning processes of the model.

Model-agnostic methods are further categorized into *global* and *local* methods based on their locality in the input space. Global methods, such as partial dependence plots (PDP) [4] and accumulated local effects (ALE) [2], aim to explain the model’s behavior across the entire input space. However, providing global explanations becomes challenging as the model’s complexity increases. In contrast, local methods, such as **individual conditional expectation (ICE)** [1], **local interpretable model-agnostic explanations (LIME)** [10], **Anchor** [11] and **shapley additive explanations (SHAP)** [8], explain the model’s behavior in the vicinity of a specific input. While they offer explanations simpler and more accurate than global methods, the scope of the explanation is limited locally.

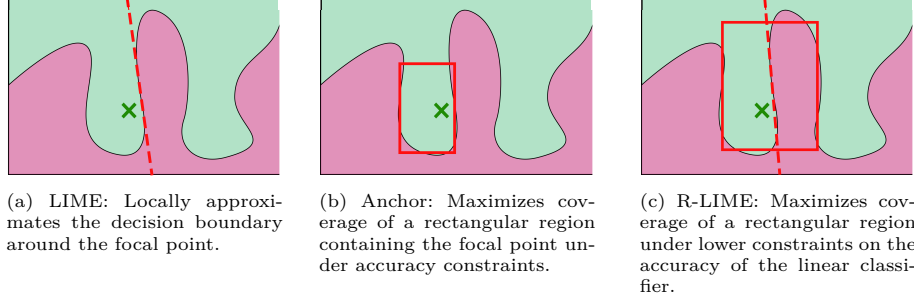


Fig. 3: Visual comparison of LIME, Anchor and R-LIME (our method). The dashed line represents the local linear approximation model, and the solid line represents the rectangular region containing the focal point.

3 Proposed Method

3.1 Previous Work

We specifically focus on *local* and *model-agnostic* methods. This section briefly reviews existing research on local model-agnostic explanations, particularly focusing on studies closely related to our proposed method.

LIME (Local Interpretable Model-agnostic Explanations) [10] LIME locally approximates a black-box classifier $f : \mathbb{R}^m \rightarrow \{0, 1\}$ around a focal point $x \in \mathbb{R}^m$ using a linear classifier $g : \mathbb{R}^m \rightarrow \{0, 1\}$ (Fig. 3(a)). The approximation process involves the following steps:

1. Generate a set of perturbed samples \mathcal{Z}_p around x and their pseudo-labels $f(\mathcal{Z}_p) = \{f(z) \mid z \in \mathcal{Z}_p\}$. (i) Convert x into a binary vector $x' \in \{0, 1\}^{m'}$, (ii) generate perturbed samples by randomly drawing non-zero elements from x' , and (iii) convert the perturbed samples back to the original space.
2. Train a linear classifier g using \mathcal{Z}_p and $f(\mathcal{Z}_p)$ by minimizing the following loss function:

$$\mathcal{L}(f, g, \pi_x) = \sum_{z \in \mathcal{Z}_p} \pi_x(z) (f(z) - g(z))^2, \quad (1)$$

where $\pi_x(z)$ is a weight function that assigns larger weights for samples closer to x , typically defined using an exponential kernel.

LIME provides valuable insights into the local behavior of the model by showing each feature’s contribution to the output $f(x)$. However, it does not explicitly define the region for generating perturbed samples, making it difficult for users to assess the effective scope of the explanation [11].

Anchor [11] Anchor maximizes the coverage of a rectangular region containing the focal point x , expressed as a conjunction of feature predicates (a rule) as long as the probability of the black-box classifier f outputting $f(x)$ within the region exceeds a given threshold τ (Fig. 3(b)). It aims to highlight important features contributing significantly to the output. For a discrete m -dimensional input space \mathbb{D}^m , a trained black-box classifier $f : \mathbb{D}^m \rightarrow \{0, 1\}$, an instance $x \in \mathbb{D}^m$ and a distribution \mathcal{D} over the input space, a rule $A(z) = a_{i_1}(z) \wedge a_{i_2}(z) \wedge \dots \wedge a_{i_t}(z)$ is defined. The predicate $a_i(z)$ evaluates to true ($= 1$) when $z_i = x_i$ and false ($= 0$) otherwise. The reliability of the explanation is defined as the “accuracy” of the rule, and the generality of the explanation is defined as the “coverage” of the rule. The accuracy $\text{acc}(A)$ and coverage $\text{cov}(A)$ of the rule A are defined as follows:

$$\text{acc}(A) = \mathbb{E}_{z \sim \mathcal{D}(z|A)}[\mathbb{1}_{f(z)=f(x)}], \quad (2)$$

$$\text{cov}(A) = \mathbb{E}_{z \sim \mathcal{D}(z)}[A(z)], \quad (3)$$

where $\mathcal{D}(z|A)$ is the conditional distribution in the region where the rule A returns true. $\text{acc}(A)$ represents the probability that the output of f matches between the perturbation $z \sim \mathcal{D}(z|A)$ and the focal point x , and $\text{cov}(A)$ expresses the probability that the perturbation z fits into A . Anchor maximizes coverage as long as the accuracy of the rule A exceeds a given threshold τ . However, eq. (2) is not directly computable. Introducing a confidence level $1 - \delta$ ($0 \leq \delta \leq 1$), the accuracy constraint is relaxed as follows:

$$P(\text{acc}(A) \geq \tau) \geq 1 - \delta. \quad (4)$$

Thus, the following optimization problem is solved:

$$A^* = \arg \max_{A \text{ s.t. } P(\text{acc}(A) \geq \tau) \geq 1 - \delta \wedge A(x)=1} \text{cov}(A). \quad (5)$$

3.2 Overview

We propose R-LIME, a novel method designed to address the limitations of LIME [10] and Anchor [11]. Similar to LIME, it locally approximates the black-box classifier f around the focal point x using a linear classifier g , and similar to Anchor, it generates the perturbed samples for approximation from a rectangular region (Fig. 3(c)).

Anchor maximizes the coverage of region A as long as the probability of the output of the black-box classifier f matching $f(x)$ within A exceeds a given threshold τ . R-LIME, on the other hand, learns a linear classifier g within the rectangular region A and maximizes the coverage of A under lower constraints on the accuracy of g . We modify Anchor’s definition of accuracy in eq. (2) as follows:

$$\text{acc}(A) = \max_{g \in G} \mathbb{E}_{z \sim \mathcal{D}(z|A)}[\mathbb{1}_{f(z)=g(z)}], \quad (6)$$

where G is a hypothesis space of possible linear classifiers. By solving the optimization problem in eq. (5) under the modified definition of accuracy in eq. (6), we can select the rule that enables explanation with high accuracy and generality.

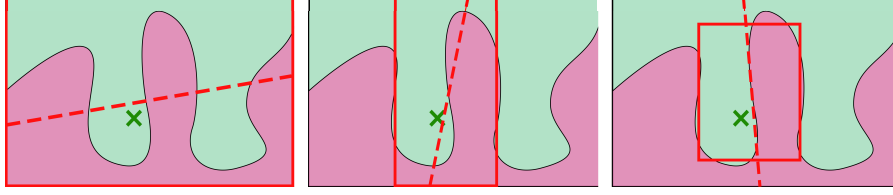


Fig. 4: Overview of the R-LIME algorithm. The progression of the algorithm is illustrated from left to right. The solid line represents the rectangular region A , and the dashed line represents the linear approximation model g learned within A . The initial value of A is an empty rule (entire input space), and predicates are added to A , reducing coverage. The process continues until $\text{acc}(A) \geq \tau$ is satisfied, at which point the rule with the maximum coverage is output.

3.3 Algorithm

The R-LIME algorithm is mainly based on the method used in Anchor[11]. For non-convex optimization problems like eq. (5), greedy search are often used. But greedy methods often converge to local optima, so we use beam search, which selects multiple candidates at each iteration to improve the search robustness. The pseudo-code is shown in Algorithm 5.

Generating New Candidate Rules To generate new candidate rules, one additional predicate is added to each of the B candidate rules selected in the previous iteration. The pseudo-code is shown in Algorithm 6. $T(x)$ is the set of predicates $\{a_1, \dots, a_m\}$, where $a_i(z)$ evaluates to true when $z_i = x_i$ and false otherwise. $T(x) \setminus A$ is the set of predicates in $T(x)$ not included in rule A .

Searching Rules with Highest Accuracy Given the set of candidate rules \bar{A} , the algorithm selects the B candidate rules with the highest accuracy. This problem can be formulated as best arm identification in the multi-armed bandit framework. Each candidate rule $A_i \in \bar{A}$ is considered as an arm, and reward of arm a_i follows a Bernoulli distribution with $P(X = 1) = \text{acc}(A_i)$. By sampling $z \sim \mathcal{D}(\cdot|A_i)$ and obtaining the reward $\mathbb{1}_{f(z)=g_i(z)}$ for each trial, the algorithm updates g_i using z and $f(z)$ after each trial. To efficiently search the rule (arm) with the highest accuracy, we employ the KL-LUCB algorithm [6]. The pseudo-code is shown in Algorithm 7. For tolerance $\epsilon \in [0, 1]$, the KL-LUCB algorithm guarantees below:

$$P(\min_{A \in \bar{A}} \text{acc}(A) \geq \min_{A' \in \bar{A}} \text{acc}(A') - \epsilon) \geq 1 - \delta. \quad (7)$$

However, the KL-LUCB algorithm assumes that the reward distribution for each arm remains unchanged, while our method updates the classifier g_i with each sampling, which may not satisfy the assumption. This issue is discussed further in section 5.2.

Algorithm 1 R-LIME

Input: Black-box model f , Target instance x , Distribution \mathcal{D} , Threshold τ , Beam width B , Tolerance ϵ , Confidence level $1 - \delta$

Output: Rule A^* satisfying Eq. (5)

```

1:  $A^* \leftarrow \text{null}$ ,  $\mathcal{A}_0 \leftarrow \emptyset$ ,  $t \leftarrow 0$   $\triangleright$  Initialize the set of candidate rules  $\mathcal{A}_0$  to  $\emptyset$ 
2: while  $A^* = \text{null}$  do
3:    $t \leftarrow t + 1$ 
4:    $\bar{\mathcal{A}}_t \leftarrow \text{GENERATECANDS}(\mathcal{A}_{t-1})$ 
5:    $\mathcal{A}_t \leftarrow \text{B-BESTCANDS}(\bar{\mathcal{A}}_t, \mathcal{D}, B, \epsilon, \delta)$ 
6:    $A^* \leftarrow \text{LARGESTCAND}(\mathcal{A}_t, \tau, \delta)$ 
7: end while

```

Algorithm 2 Generating new candidate rules

```

1: function GENERATECANDS( $\mathcal{A}, x$ )
2:   if  $\mathcal{A} = \emptyset$  then return  $\{true\}$   $\triangleright$  An initial empty rule always returns true
3:    $\bar{\mathcal{A}} \leftarrow \emptyset$ 
4:   for all  $A \in \mathcal{A}$  do
5:     for all  $a \in (T(x) \setminus A)$  do
6:        $\bar{A} \leftarrow \bar{A} \cup (A \wedge a)$   $\triangleright$  Get a new rule by adding a new predicate  $a$  to  $A$ 
7:     end for
8:   end for
9:   return  $\bar{\mathcal{A}}$ 
10: end function

```

Algorithm 3 Searching rules with highest accuracy (KL-LUCB [6])

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1: function B-BESTCANDS( $\bar{\mathcal{A}}, \mathcal{D}, B, \epsilon, \delta$ )
2:   initialize  $\text{acc}, \text{acc}_u, \text{acc}_l$  for  $\forall A \in \bar{\mathcal{A}}$ 
3:    $\mathcal{A} \leftarrow \text{B-PROVISIONALLYBESTCANDS}(\bar{\mathcal{A}})$   $\triangleright B$  rules with highest accuracy
4:    $A \leftarrow \arg \min_{A \in \mathcal{A}} \text{acc}_l(A, \delta)$   $\triangleright$  The rule with the smallest lower bound
5:    $A' \leftarrow \arg \max_{A' \notin (\bar{\mathcal{A}} \setminus \mathcal{A})} \text{acc}_u(A', \delta)$   $\triangleright$  The rule with the largest upper bound
6:   while  $\text{acc}_u(A', \delta) - \text{acc}_l(A, \delta) > \epsilon$  do
7:     sample  $z \sim \mathcal{D}(z|A)$ ,  $z' \sim \mathcal{D}(z'|A')$ 
8:     update  $\text{acc}, \text{acc}_u, \text{acc}_l$  for  $A$  and  $A'$ 
9:      $\mathcal{A} \leftarrow \text{B-PROVISIONALLYBESTCANDS}(\bar{\mathcal{A}})$ 
10:     $A \leftarrow \arg \min_{A \in \mathcal{A}} \text{acc}_l(A, \delta)$ 
11:     $A' \leftarrow \arg \max_{A' \notin (\bar{\mathcal{A}} \setminus \mathcal{A})} \text{acc}_u(A', \delta)$ 
12:   end while
13:   return  $\mathcal{A}$ 
14: end function

```

Algorithm 4 Searching a rule with highest coverage under constraint

```

1: function LARGESTCAND( $\mathcal{A}, \tau, \delta$ )
2:    $A^* \leftarrow \text{null}$   $\triangleright$  If no rule satisfies the constraint, return null
3:   for all  $A \in \mathcal{A}$  s.t.  $\text{acc}_l(A, \delta) > \tau$  do
4:     if  $\text{cov}(A) > \text{cov}(A^*)$  then  $A^* \leftarrow A$ 
5:   end for
6:   return  $A^*$ 
7: end function

```

Searching a Rule with Highest Coverage under Constraint To satisfy the constraint imposed by eq. (4), a rule A needs to meet the following condition:

$$\text{acc}_l(A, \delta) > \tau, \quad (8)$$

where $\text{acc}_l(A, \delta)$ is the lower limit of the $100(1 - \delta)\%$ confidence interval for $\text{acc}(A)$. If the set of candidate rules \mathcal{A} includes rules satisfying eq. (8), the one with the maximum coverage among them is selected, then the iteration is terminated. If \mathcal{A} does not contain any rule satisfying eq. (8), it returns **null**, and proceeds to the next iteration. The pseudo-code is presented in Algorithm 8.

3.4 Computational Complexity

Post-hoc explanation methods including LIME, Anchor and R-LIME need to sample a perturbation vector and get the output of the black-box model multiple times, which is computationally expensive. The number of samples required for LIME is $|\mathcal{Z}_p|$, which is the number of samples designated by the user. On the other hand, the expected number of samples required for Anchor and R-LIME is bounded by $\mathcal{O}[m \cdot \mathcal{O}_{\text{MAB}[B \cdot m, B]}]$, where $\mathcal{O}_{\text{MAB}[B \cdot m, B]}$ is the expected number of samples for best arm identification finding the best B arms from $B \cdot m$ arms. For the KL-LUCB algorithm [6],

$$\mathcal{O}_{\text{MAB}[B \cdot m, B]} = \mathcal{O} \left[\frac{Bm}{\epsilon^2} \log \frac{Bm}{\epsilon^2 \delta} \right]. \quad (9)$$

Then the total expected number of samples for Anchor and R-LIME is bounded by

$$\mathcal{O} \left[\frac{Bm^2}{\epsilon^2} \log \frac{Bm}{\epsilon^2 \delta} \right]. \quad (10)$$

For each iteration of the KL-LUCB algorithm, R-LIME needs to update the linear classifier g_i , which is not required in Anchor. If we use logistic regression as the linear classifier and update it by stochastic gradient descent (SGD) [12], the computational complexity of updating g_i is $\mathcal{O}(m)$. It is negligible compared to the complexity of generating a perturbed sample, which is $\mathcal{O}(m^2)$ if we get a sample from a multivariate normal distribution using Cholesky decomposition in advance. Overall, the computational complexity of R-LIME is comparable to that of Anchor.

4 Experiments

To verify the effectiveness of our method, we conducted qualitative and quantitative comparisons of R-LIME with LIME and Anchor, using a real-world dataset. Our code for R-LIME is available on GitHub¹.

¹ <https://github.com/g-ohara/rlime>

Table 1: Attributes of the recidivism dataset used in the experiments. Continuous features are all discretized, and only binary and ordinal features are considered.

Attribute	Overview	# of Possible Values
Race	Race (Black or White)	2
Alcohol	Presence of serious alcohol issues	2
Junky	Drug usage	2
Supervised Release	Supervised release	2
Married	Marital status	2
Felony	Felony or not	2
WorkRelease	Participation in work release program	2
Crime against Property	Crime against property or not	2
Crime against Person	Crime against a person or not	2
Gender	Gender (Female or Male)	2
Priors	Number of prior offenses	4
YearsSchool	Years of formal education completed	4
PrisonViolations	Number of prison rule violations	3
Age	Age	4
MonthsServed	Months served in prison	4
Recidivism	Recidivism or not	2

4.1 Qualitative Evaluation

Experimental Setup We used the recidivism dataset [14] for our experiments. The dataset contains personal information on 9549 prisoners released from North Carolina prisons between July 1, 1979 and June 30, 1980. As shown in Table 1, the dataset includes 19 items such as race (*Race*), gender (*Gender*), presence of alcohol dependence (*Alcohol*), number of prior offenses (*Priors*), and presence of recidivism (*Recidivism*). For this experiment, we treated the binary classification problem of predicting the presence of recidivism (*Recidivism*) as the target label. We discretized continuous features and removed missing values, resulting in 15 features.

We splitted the dataset into training data (7639 instances) and test data (955 instances), and trained a random forest model with 50 trees as the black-box classifier using the training data. Then, we generate LIME, Anchor and R-LIME explanations for two instances extracted from the test data (Fig. 5). For R-LIME, we used logistic regression as the linear approximation model, and a multivariate normal distribution estimated from the training data as the distribution \mathcal{D} . For both Anchor and R-LIME, the beam width was set to $B = 10$, the confidence coefficient to $1 - \delta = 0.95$, and the tolerance of the KL-LUCB algorithm to $\epsilon = 0.05$. The accuracy threshold τ was set to $\tau = 0.70, 0.90$.

This problem setting can be considered as a case where a complex machine learning model is introduced to decide parole for prisoners. Since such decisions can have a significant impact on a person’s life, it is crucial for users to appropriately interpret the outputs of black-box models.

Race	Black (0)
Alcohol	No (0)
Junky	No (0)
Supervised Release	Yes (1)
Married	Yes (1)
Felony	No (0)
WorkRelease	Yes (1)
Crime against Property	No (0)
Crime against Person	No (0)
Gender	Male (1)
Priors	1
YearsSchool	$8.00 < \text{YearsSchool} \leq 10.00$ (1)
PrisonViolations	0
Age	$\text{Age} > 33.00$ (3)
MonthsServed	$4.00 < \text{MonthsServed} \leq 9.00$ (1)
Recidivism	No more crimes (0)

(a) Instance A

Race	Black (0)
Alcohol	Yes (1)
Junky	No (0)
Supervised Release	Yes (1)
Married	No (0)
Felony	No (0)
WorkRelease	Yes (1)
Crime against Property	Yes (1)
Crime against Person	No (0)
Gender	Male (1)
Priors	1
YearsSchool	$\text{YearsSchool} > 11.00$ (3)
PrisonViolations	0
Age	$21.00 < \text{Age} \leq 26.00$ (1)
MonthsServed	$4.00 < \text{MonthsServed} \leq 9.00$ (1)
Recidivism	Re-arrested (1)

(b) Instance B

Fig. 5: Two instances sampled from training data of recidivism dataset. Each number in parentheses represents the integer value assigned to the corresponding categorical value.

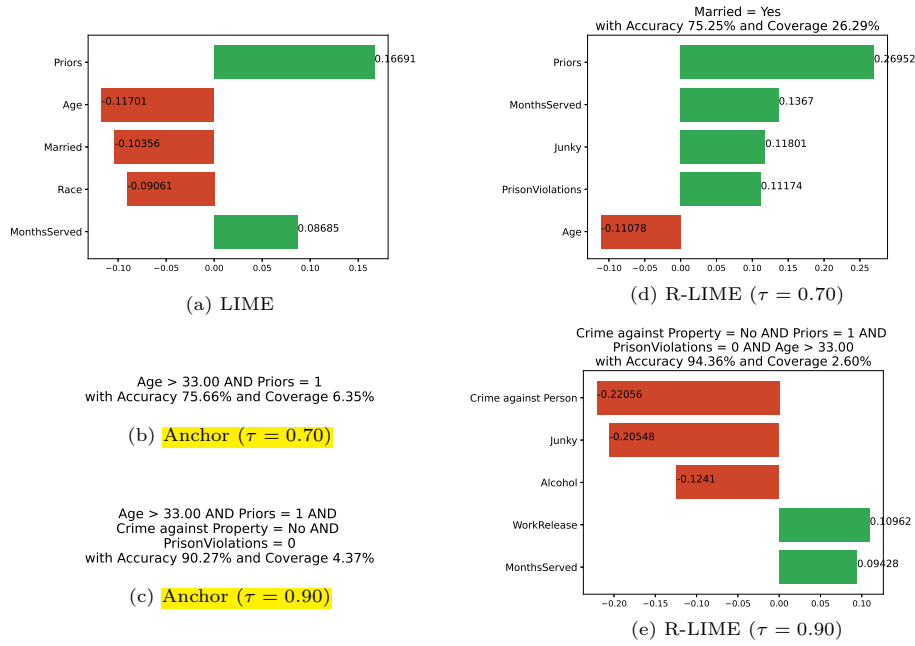


Fig. 6: Explanation for Instance A by LIME and R-LIME.

Experimental Results The results of the experiment are shown in Figs. 6 and 7. The values assigned to each feature name represent the contribution (weight of the linear classifier) to the output of the black-box classifier, normalized such that the absolute sum is 1. The figures display the 5 features with the highest absolute contribution.

Explanations generated by LIME (Figs. 6(a) and 7(a)) provide insights that having a prior offenses (*Priors*), being served for a long time in prison (*MonthsServed*), and committing a crime against property (*Crime against Property*) primarily contribute to the positive prediction (prediction that the prisoner will be re-arrested). On the other hand, being elderly (*Age*), being married (*Married*), and being of white race (*Race*) contribute to the negative prediction (prediction that the prisoner will not be re-arrested). While these LIME explanations provide valuable insights into the behavior of the black-box model, they do not explicitly indicate the application scope of the explanations, leaving users unable to determine to which prisoners the explanations are applicable.

Anchor provides conditions for the model's output to be fixed with high probability. For example, the explanation for instance A under $\tau = 0.70$ (Fig. 6(b)) means that the model will predict with 75.66 % probability that the prisoner will commit no more crimes when a prisoner is older than 33 and has one prior offense. Although it clearly provides the explanation's application scope, it does not provide details about how these conditions affect the model's output.

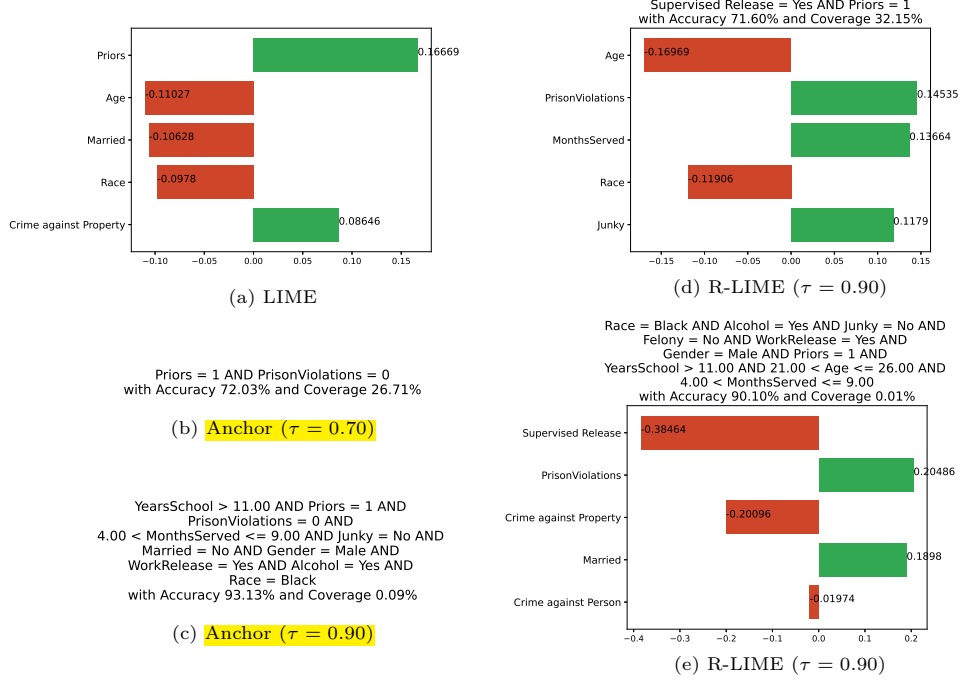


Fig. 7: Explanation for Instance B by LIME and R-LIME.

In contrast to LIME and Anchor, R-LIME provides both contribution of each feature to the output and the application scope of the explanation. For example, the explanation for instance A under $\tau = 0.70$ (Fig. 6(d)) indicates that it is applicable only to married prisoner (*Married* = Yes). R-LIME explanations also provide their accuracy and coverage, allowing users to evaluate reliability and generality of the explanations. For example, the coverage of the explanation for instance B under $\tau = 0.90$ (Fig. 7(e)) is 0.01%, indicating that the decision boundaries around instance B are complex, making it challenging to obtain a high-accuracy linear approximation. This information allows users to discern that the application scope of this explanation is very narrow, limiting its utility.

4.2 Quantitative Evaluation: LIME vs. R-LIME

Experimental Setup To demonstrate that R-LIME learns a highly accurate linear approximation model in the optimized approximation region, we conducted a comparison of the local accuracy of explanations between LIME and R-LIME. Under the same settings as in section 4.1, we randomly sampled 100 instances from the test data of the recidivism dataset and generated explanations using LIME and R-LIME (with $\tau = 0.70, 0.80, 0.90$). We then sampled 10,000 instances within the rectangular region obtained by R-LIME and calculated the local accuracy of both methods.

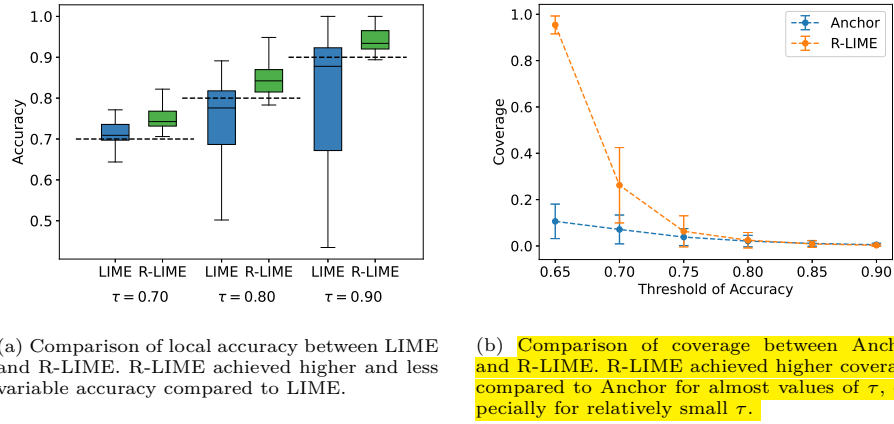


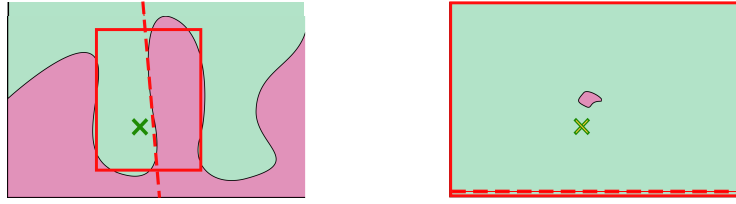
Fig. 8: Comparison of existing methods (LIME, Anchor) and R-LIME.

Experimental Results The results are presented in Fig. 8(a), showing the distribution of the local accuracy of the linear classifiers learned by LIME and R-LIME. R-LIME achieved higher accuracy compared to LIME for all values of τ . This suggests that the linear classifiers learned by LIME and R-LIME differ significantly, and R-LIME learns a high-accuracy linear classifier adapted to the optimized rectangular region. Additionally, as τ increases, the variability in the accuracy of LIME widens. This indicates that the linear classifiers learned by LIME may not function effectively as approximation models depending on how the region is selected.

4.3 Quantitative Evaluation: Anchor vs. R-LIME

Experimental Setup To demonstrate that R-LIME explanations are more general than Anchor, we conducted a comparison of the coverage of explanations between Anchor and R-LIME. Under the same settings as in section 4.1, we generated Anchor and R-LIME explanations for 704 instances from the test data of the recidivism dataset, under the values of $\tau = 0.65, 0.70, 0.75, 0.80, 0.85, 0.90$.

Experimental Results The results are presented in Fig. 8(b), showing the coverage of the explanations by Anchor and R-LIME. The coverage of explanations generated by R-LIME is higher compared to Anchor for almost values of τ , especially for relatively small τ . It is because of the flexibility of the linear approximation models learned by R-LIME, which captures the decision boundary more precisely. In contrast, Anchor uses only the intervals of each feature discretized in advance, which cannot capture the decision boundary flexibly and makes its scope narrow.



(a) R-LIME for balanced label distribution. (b) R-LIME for imbalanced label distribution.

Fig. 9: Behavior of R-LIME for balanced and imbalanced label distribution. In case of imbalanced label distribution, the approximation region covers the entire input space and the linear approximation model always outputs the majority label.

Table 2: Deviation between the estimated accuracy and the true accuracy of the linear classifier learned by R-LIME. The deviation 0.012 ± 0.017 was relatively small considering the confidence level $1 - \delta = 0.95$.

	Estimated acc.	True acc.	Deviation
Average	.811	.829	.012
Standard Deviation	.018	.023	.017

5 Discussion

5.1 Behavior for Imbalanced Label Distribution

R-LIME may generate less useful explanations when the distribution of black-box classifier outputs is imbalanced. When the ratio of outputting the minority label is less than $1 - \tau$, where τ is the accuracy threshold, the approximation region generated by R-LIME covers the entire input space, and the learned linear classifier always outputs the majority label (Fig. 9).

A first possible solution to this problem is modifying the loss function. Using weighted logistic loss or Focal Loss [7] as the loss function might lead to the generation of more useful explanations in the case of imbalanced label distribution. Another solution involves adding constraints to limit the label distribution bias within the approximation region. In addition to eq. (4), adding a constraint like

$$\left(\mathbb{E}_{z \sim \mathcal{D}(z|A)} [\mathbb{1}_{f(z)=1}] - \frac{1}{2} \right)^2 < \mu \quad (11)$$

could suppress the excessive expansion of the approximation region.

5.2 Changes in Reward Distribution in Best Arm Identification

For R-LIME, the problem of selecting the rule with the highest accuracy is formulated as the best arm identification problem in multi-armed bandit framework, and solved using the KL-LUCB algorithm [6]. However, this algorithm

assumes that the reward distribution remains constant, while in R-LIME, the reward distribution (accuracy of the linear approximation) changes with every update of the approximation model after sampling. Therefore, rewards obtained at an early stage might influence the estimated value and make it deviate from the true value.

We conducted an experiment to evaluate the deviation between the estimated accuracy and the true accuracy. We generated explanations for 3200 data instances sampled from the dataset, and compared the estimated accuracy with the true accuracy. The true accuracy was calculated based on 1000 instances sampled within the approximation region. The results in Table 2 show a mean deviation of 0.012 with a standard deviation of 0.017. By considering the confidence level $1 - \delta = 0.95$, the deviation was relatively small. While there are concerns about the theoretical validity of using the KL-LUCB algorithm, our results suggest that the deviation is not significant in practice.

5.3 Parameter Selection

In section 3.4, we discussed about the computational complexity of R-LIME, which depends on some hyperparameters. R-LIME requires the hyperparameters to be selected by users, such as the threshold of accuracy τ , beam width B , tolerance ϵ and confidence level δ . B should be large and ϵ and δ should be small for accurate results, as long as the computational cost is acceptable. On the other hand, τ should be carefully selected by users, sometimes interactively, considering the tradeoff between the accuracy and generality of generated explanation.

6 Conclusion

Existing methods for local model-agnostic explanations of black-box classifiers, such as LIME and Anchor, have limitations that they cannot achieve interpretability of both the explanation and its application scope. To address these challenges, we proposed R-LIME, a method that locally and linearly approximates the decision boundary of a black-box classifier and provides a rectangular approximation region, which is interpretable for users due to being expressed as a conjunction of feature predicates. We proposed an algorithm to maximize coverage of the approximation region as long as the accuracy of the linear approximation model exceeds a given threshold. Comparing R-LIME with existing methods on the real-world dataset, we demonstrated that R-LIME achieves interpretability of both the explanation and its application scope, and provides explanations more accurate than LIME and more general than Anchor. Finally, we discussed the instability of behavior with imbalanced label distributions, raised questions about the theoretical validity of using the KL-LUCB algorithm, and hyperparameter tuning in practice.

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R-LIME: Rectangular Constraints and Optimization for Local Interpretable Model-agnostic Explanation Methods

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Abstract. In recent years, complex machine learning models have been widely introduced in various industrial fields due to their high accuracy. However, their increasing complexity has been a major obstacle to their implementation in sensitive decision-making situations. In order to address this problem, various post-hoc explanation methods have been proposed, but they have not been able to achieve interpretability of both the explanation and its scope. We propose R-LIME, a novel method that interprets complex classifiers within an interpretable scope. R-LIME locally and linearly approximates the complex decision boundary of a black-box classifier within a rectangular region and maximizes the region as long as the approximation accuracy exceeds a given threshold. The resulting rectangular region is interpretable for users because it is expressed as a conjunction of feature predicates. Through qualitative and quantitative comparisons on a real-world dataset, we demonstrate that R-LIME provides more reliable and interpretable explanations than existing methods.

Keywords: Interpretable machine learning · Local surrogate model

1 Introduction

In recent years, complex machine learning models, such as deep neural networks and random forests, have been widely introduced in various industrial fields due to their significant improvements in accuracy. However, their increasing complexity and black-box nature pose challenges, particularly in critical decision-making scenarios such as healthcare and finance, where the lack of transparency becomes a major obstacle to implementation. In order to address this problem, extensive research has focused on post-hoc explanations for complex models [5, 10, 11]. Post-hoc explanation methods are categorized into *model-dependent* and *model-agnostic* methods based on their dependence on the model’s structure, with the latter further classified into *global* and *local* methods based on the locality in the input space [13].

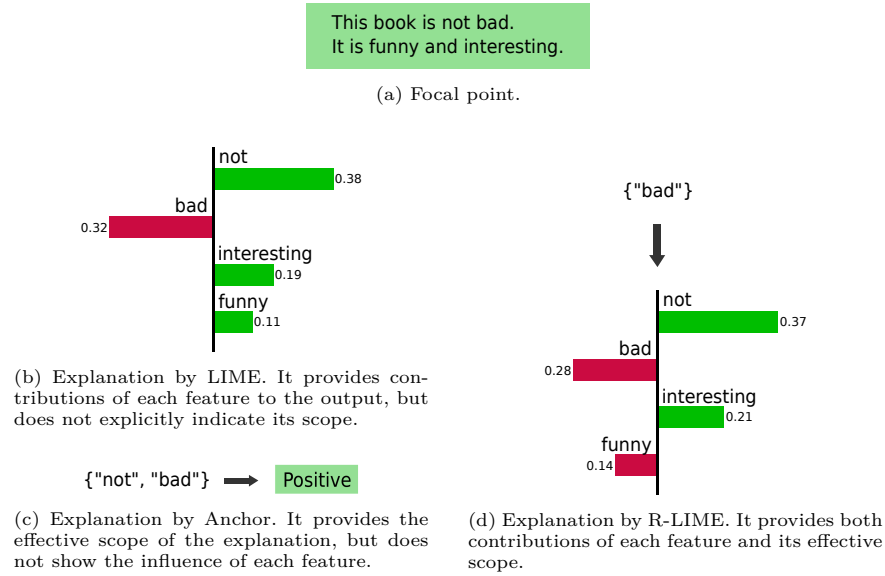


Fig. 1: Example of explanations by LIME [10], Anchor [11] and R-LIME (our proposed method) for a sentiment prediction model.

In this paper, we focus on *local* and *model-agnostic* methods. LIME [10] and Anchor [11] are representative local model-agnostic methods. An example of explanations by LIME and Anchor for a sentiment prediction model is illustrated in Fig. 1. LIME linearly approximates the complex decision boundary around the given focal point (Fig. 1(a)), then provides the weights of the linear model as the contribution of each feature to the output. The explanation by LIME (Fig. 1(b)) suggests that the word “not” mainly contributes to the positive prediction, but does not explicitly indicate its effective scope. Without the scope, users might mistakenly apply the knowledge derived from the explanation to other instances far from the focal point, potentially leading to misunderstanding of the black-box model’s behavior [11]. For this example, users may apply the derived insights to the sentence “This book is not good.” and mistakenly conclude that the word “not” mainly contributes to the positive prediction for this sentence as well, which is obviously incorrect. Anchor maximizes the coverage of a rectangular region containing the focal point as long as the probability of the black-box classifier outputting the same label as the focal point within the region exceeds a given threshold. While Anchor provides an effective scope of the explanation, users can get less insight compared to LIME. The explanation by Anchor (Fig. 1(c)) suggests that replacing words other than “not” and “bad” has little impact on the classifier’s output. While it clearly cannot be applied to the sentence “This book is not good” because of not including the word “bad”, the explanation does not provide details about the influence of each word, resulting in less user insight into the model’s behavior compared to LIME.

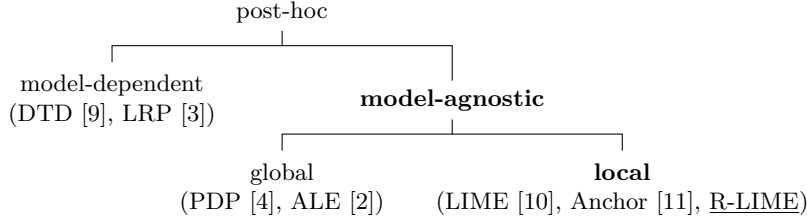


Fig. 2: Categorization of post-hoc explanation methods. We focus on *model-agnostic* and *local* methods, which explain model’s local behavior using only its output.

To address these limitations, we propose R-LIME (Ruled LIME), which provides both the contributions of each feature to the output and the effective scope of the explanation. R-LIME linearly approximates a complex decision boundary in a rectangular region and maximizes the region as long as the accuracy of the linear classifier exceeds a given threshold. The region is interpretable for users because it is expressed as a conjunction of feature predicates. An example of the explanation by R-LIME for a sentiment prediction model is shown in Fig. 1(d). It is clear that users can apply the insights derived from the explanation only to the sentences containing the word “not”.

2 Related Work

In this section, we overview existing research on post-hoc explanation methods, which explain the behavior of black-box models already trained. As shown in Fig. 2, post-hoc methods are classified into several categories.

They are broadly divided into *model-dependent* and *model-agnostic* methods based on their dependence on the model’s structure. Model-dependent methods, such as deep Taylor decomposition (DTD) [9] and layer-wise relevance propagation (LRP) [3], primarily focus on neural networks and explain the model’s behavior using its parameters [13]. While these methods provide detailed explanations (e.g., layer-wise explanations for neural networks), it is often challenging to apply the same method to models with different structures. In contrast, model-agnostic methods use only the model’s output. Although they are applicable to any model, they cannot explain the internal reasoning processes of the model.

Model-agnostic methods are further categorized into *global* and *local* methods based on their locality in the input space. Global methods, such as partial dependence plots (PDP) [4] and accumulated local effects (ALE) [2], aim to explain the model’s behavior across the entire input space. However, providing global explanations becomes challenging as the model’s complexity increases. In contrast, local methods, such as individual conditional expectation (ICE) [1], local interpretable model-agnostic explanations (LIME) [10], Anchor [11] and shapley additive explanations (SHAP) [8], explain the model’s behavior in the vicinity of a specific input. While they offer explanations simpler and more accurate than global methods, the scope of the explanation is limited locally.

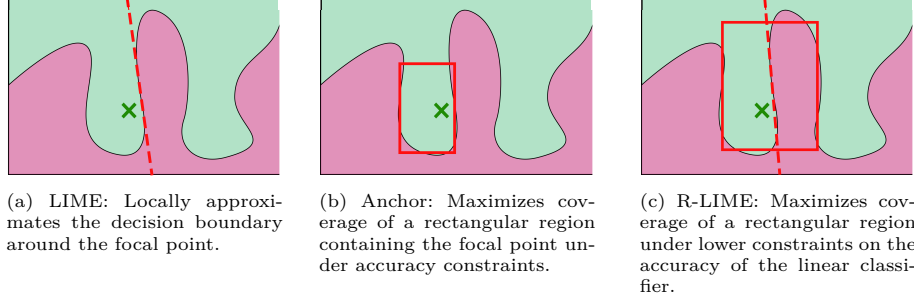


Fig. 3: Visual comparison of LIME, Anchor and R-LIME (our method). The dashed line represents the local linear approximation model, and the solid line represents the rectangular region containing the focal point.

3 Proposed Method

3.1 Previous Work

We specifically focus on *local* and *model-agnostic* methods. This section briefly reviews existing research on local model-agnostic explanations, particularly focusing on studies closely related to our proposed method.

LIME (Local Interpretable Model-agnostic Explanations) [10] LIME locally approximates a black-box classifier $f : \mathbb{R}^m \rightarrow \{0, 1\}$ around a focal point $x \in \mathbb{R}^m$ using a linear classifier $g : \mathbb{R}^m \rightarrow \{0, 1\}$ (Fig. 3(a)). The approximation process involves the following steps:

1. Generate a set of perturbed samples \mathcal{Z}_p around x and their pseudo-labels $f(\mathcal{Z}_p) = \{f(z) \mid z \in \mathcal{Z}_p\}$. (i) Convert x into a binary vector $x' \in \{0, 1\}^{m'}$, (ii) generate perturbed samples by randomly drawing non-zero elements from x' , and (iii) convert the perturbed samples back to the original space.
2. Train a linear classifier g using \mathcal{Z}_p and $f(\mathcal{Z}_p)$ by minimizing the following loss function:

$$\mathcal{L}(f, g, \pi_x) = \sum_{z \in \mathcal{Z}_p} \pi_x(z) (f(z) - g(z))^2, \quad (1)$$

where $\pi_x(z)$ is a weight function that assigns larger weights for samples closer to x , typically defined using an exponential kernel.

LIME provides valuable insights into the local behavior of the model by showing each feature’s contribution to the output $f(x)$. However, it does not explicitly define the region for generating perturbed samples, making it difficult for users to assess the effective scope of the explanation [11].

Anchor [11] Anchor maximizes the coverage of a rectangular region containing the focal point x , expressed as a conjunction of feature predicates (a rule) as long as the probability of the black-box classifier f outputting $f(x)$ within the region exceeds a given threshold τ (Fig. 3(b)). It aims to highlight important features contributing significantly to the output. For a discrete m -dimensional input space \mathbb{D}^m , a trained black-box classifier $f : \mathbb{D}^m \rightarrow \{0, 1\}$, an instance $x \in \mathbb{D}^m$ and a distribution \mathcal{D} over the input space, a rule $A(z) = a_{i_1}(z) \wedge a_{i_2}(z) \wedge \dots \wedge a_{i_t}(z)$ is defined. The predicate $a_i(z)$ evaluates to true ($= 1$) when $z_i = x_i$ and false ($= 0$) otherwise. The reliability of the explanation is defined as the “accuracy” of the rule, and the generality of the explanation is defined as the “coverage” of the rule. The accuracy $\text{acc}(A)$ and coverage $\text{cov}(A)$ of the rule A are defined as follows:

$$\text{acc}(A) = \mathbb{E}_{z \sim \mathcal{D}(z|A)}[\mathbb{1}_{f(z)=f(x)}], \quad (2)$$

$$\text{cov}(A) = \mathbb{E}_{z \sim \mathcal{D}(z)}[A(z)], \quad (3)$$

where $\mathcal{D}(z|A)$ is the conditional distribution in the region where the rule A returns true. $\text{acc}(A)$ represents the probability that the output of f matches between the perturbation $z \sim \mathcal{D}(z|A)$ and the focal point x , and $\text{cov}(A)$ expresses the probability that the perturbation z fits into A . Anchor maximizes coverage as long as the accuracy of the rule A exceeds a given threshold τ . However, eq. (2) is not directly computable. Introducing a confidence level $1 - \delta$ ($0 \leq \delta \leq 1$), the accuracy constraint is relaxed as follows:

$$P(\text{acc}(A) \geq \tau) \geq 1 - \delta. \quad (4)$$

Thus, the following optimization problem is solved:

$$A^* = \underset{A \text{ s.t. } P(\text{acc}(A) \geq \tau) \geq 1 - \delta \wedge A(x)=1}{\arg \max} \text{cov}(A). \quad (5)$$

3.2 Overview

We propose R-LIME, a novel method designed to address the limitations of LIME [10] and Anchor [11]. Similar to LIME, it locally approximates the black-box classifier f around the focal point x using a linear classifier g , and similar to Anchor, it generates the perturbed samples for approximation from a rectangular region (Fig. 3(c)).

Anchor maximizes the coverage of region A as long as the probability of the output of the black-box classifier f matching $f(x)$ within A exceeds a given threshold τ . R-LIME, on the other hand, learns a linear classifier g within the rectangular region A and maximizes the coverage of A under lower constraints on the accuracy of g . We modify Anchor’s definition of accuracy in eq. (2) as follows:

$$\text{acc}(A) = \max_{g \in G} \mathbb{E}_{z \sim \mathcal{D}(z|A)}[\mathbb{1}_{f(z)=g(z)}], \quad (6)$$

where G is a hypothesis space of possible linear classifiers. By solving the optimization problem in eq. (5) under the modified definition of accuracy in eq. (6), we can select the rule that enables explanation with high accuracy and generality.

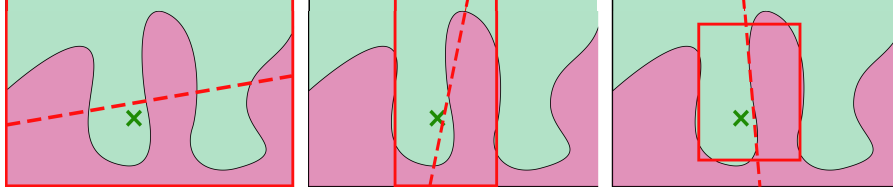


Fig. 4: Overview of the R-LIME algorithm. The progression of the algorithm is illustrated from left to right. The solid line represents the rectangular region A , and the dashed line represents the linear approximation model g learned within A . The initial value of A is an empty rule (entire input space), and predicates are added to A , reducing coverage. The process continues until $\text{acc}(A) \geq \tau$ is satisfied, at which point the rule with the maximum coverage is output.

3.3 Algorithm

The R-LIME algorithm is mainly based on the method used in Anchor[11]. For non-convex optimization problems like eq. (5), greedy search are often used. But greedy methods often converge to local optima, so we use beam search, which selects multiple candidates at each iteration to improve the search robustness. The pseudo-code is shown in Algorithm 5.

Generating New Candidate Rules To generate new candidate rules, one additional predicate is added to each of the B candidate rules selected in the previous iteration. The pseudo-code is shown in Algorithm 6. $T(x)$ is the set of predicates $\{a_1, \dots, a_m\}$, where $a_i(z)$ evaluates to true when $z_i = x_i$ and false otherwise. $T(x) \setminus A$ is the set of predicates in $T(x)$ not included in rule A .

Searching Rules with Highest Accuracy Given the set of candidate rules $\bar{\mathcal{A}}$, the algorithm selects the B candidate rules with the highest accuracy. This problem can be formulated as best arm identification in the multi-armed bandit framework. Each candidate rule $A_i \in \bar{\mathcal{A}}$ is considered as an arm, and reward of arm a_i follows a Bernoulli distribution with $P(X = 1) = \text{acc}(A_i)$. By sampling $z \sim \mathcal{D}(\cdot | A_i)$ and obtaining the reward $\mathbb{1}_{f(z)=g_i(z)}$ for each trial, the algorithm updates g_i using z and $f(z)$ after each trial. To efficiently search the rule (arm) with the highest accuracy, we employ the KL-LUCB algorithm [6]. The pseudo-code is shown in Algorithm 7. For tolerance $\epsilon \in [0, 1]$, the KL-LUCB algorithm guarantees below:

$$P(\min_{A \in \bar{\mathcal{A}}} \text{acc}(A) \geq \min_{A' \in \bar{\mathcal{A}}} \text{acc}(A') - \epsilon) \geq 1 - \delta. \quad (7)$$

However, the KL-LUCB algorithm assumes that the reward distribution for each arm remains unchanged, while our method updates the classifier g_i with each sampling, which may not satisfy the assumption. This issue is discussed further in section 5.2.

Algorithm 5 R-LIME

Input: Black-box model f , Target instance x , Distribution \mathcal{D} , Threshold τ , Beam width B , Tolerance ϵ , Confidence level $1 - \delta$

Output: Rule A^* satisfying Eq. (5)

```

1:  $A^* \leftarrow \text{null}$ ,  $\mathcal{A}_0 \leftarrow \emptyset$ ,  $t \leftarrow 0$   $\triangleright$  Initialize the set of candidate rules  $\mathcal{A}_0$  to  $\emptyset$ 
2: while  $A^* = \text{null}$  do
3:    $t \leftarrow t + 1$ 
4:    $\bar{\mathcal{A}}_t \leftarrow \text{GENERATECANDS}(\mathcal{A}_{t-1})$ 
5:    $\mathcal{A}_t \leftarrow \text{B-BESTCANDS}(\bar{\mathcal{A}}_t, \mathcal{D}, B, \epsilon, \delta)$ 
6:    $A^* \leftarrow \text{LARGESTCAND}(\mathcal{A}_t, \tau, \delta)$ 
7: end while

```

Algorithm 6 Generating new candidate rules

```

1: function GENERATECANDS( $\mathcal{A}, x$ )
2:   if  $\mathcal{A} = \emptyset$  then return  $\{true\}$   $\triangleright$  An initial empty rule always returns true
3:    $\bar{\mathcal{A}} \leftarrow \emptyset$ 
4:   for all  $A \in \mathcal{A}$  do
5:     for all  $a \in (T(x) \setminus A)$  do
6:        $\bar{A} \leftarrow \bar{A} \cup (A \wedge a)$   $\triangleright$  Get a new rule by adding a new predicate  $a$  to  $A$ 
7:     end for
8:   end for
9:   return  $\bar{\mathcal{A}}$ 
10: end function

```

Algorithm 7 Searching rules with highest accuracy (KL-LUCB [6])

```

1: function B-BESTCANDS( $\bar{\mathcal{A}}, \mathcal{D}, B, \epsilon, \delta$ )
2:   initialize  $\text{acc}, \text{acc}_u, \text{acc}_l$  for  $\forall A \in \bar{\mathcal{A}}$ 
3:    $\mathcal{A} \leftarrow \text{B-PROVISIONALLYBESTCANDS}(\bar{\mathcal{A}})$   $\triangleright B$  rules with highest accuracy
4:    $A \leftarrow \arg \min_{A \in \mathcal{A}} \text{acc}_l(A, \delta)$   $\triangleright$  The rule with the smallest lower bound
5:    $A' \leftarrow \arg \max_{A' \notin (\bar{\mathcal{A}} \setminus \mathcal{A})} \text{acc}_u(A', \delta)$   $\triangleright$  The rule with the largest upper bound
6:   while  $\text{acc}_u(A', \delta) - \text{acc}_l(A, \delta) > \epsilon$  do
7:     sample  $z \sim \mathcal{D}(z|A)$ ,  $z' \sim \mathcal{D}(z'|A')$ 
8:     update  $\text{acc}, \text{acc}_u, \text{acc}_l$  for  $A$  and  $A'$ 
9:      $\mathcal{A} \leftarrow \text{B-PROVISIONALLYBESTCANDS}(\bar{\mathcal{A}})$ 
10:     $A \leftarrow \arg \min_{A \in \mathcal{A}} \text{acc}_l(A, \delta)$ 
11:     $A' \leftarrow \arg \max_{A' \notin (\bar{\mathcal{A}} \setminus \mathcal{A})} \text{acc}_u(A', \delta)$ 
12:   end while
13:   return  $\mathcal{A}$ 
14: end function

```

Algorithm 8 Searching a rule with highest coverage under constraint

```

1: function LARGESTCAND( $\mathcal{A}, \tau, \delta$ )
2:    $A^* \leftarrow \text{null}$   $\triangleright$  If no rule satisfies the constraint, return null
3:   for all  $A \in \mathcal{A}$  s.t.  $\text{acc}_l(A, \delta) > \tau$  do
4:     if  $\text{cov}(A) > \text{cov}(A^*)$  then  $A^* \leftarrow A$ 
5:   end for
6:   return  $A^*$ 
7: end function

```

Searching a Rule with Highest Coverage under Constraint To satisfy the constraint imposed by eq. (4), a rule A needs to meet the following condition:

$$\text{acc}_l(A, \delta) > \tau, \quad (8)$$

where $\text{acc}_l(A, \delta)$ is the lower limit of the $100(1 - \delta)\%$ confidence interval for $\text{acc}(A)$. If the set of candidate rules \mathcal{A} includes rules satisfying eq. (8), the one with the maximum coverage among them is selected, then the iteration is terminated. If \mathcal{A} does not contain any rule satisfying eq. (8), it returns **null**, and proceeds to the next iteration. The pseudo-code is presented in Algorithm 8.

3.4 Computational Complexity

Post-hoc explanation methods including LIME, Anchor and R-LIME need to sample a perturbation vector and get the output of the black-box model multiple times, which is computationally expensive. The number of samples required for LIME is $|\mathcal{Z}_p|$, which is the number of samples designated by the user. On the other hand, the expected number of samples required for Anchor and R-LIME is bounded by $\mathcal{O}[m \cdot \mathcal{O}_{\text{MAB}[B \cdot m, B]}]$, where $\mathcal{O}_{\text{MAB}[B \cdot m, B]}$ is the expected number of samples for best arm identification finding the best B arms from $B \cdot m$ arms. For the KL-LUCB algorithm [6],

$$\mathcal{O}_{\text{MAB}[B \cdot m, B]} = \mathcal{O} \left[\frac{Bm}{\epsilon^2} \log \frac{Bm}{\epsilon^2 \delta} \right]. \quad (9)$$

Then the total expected number of samples for Anchor and R-LIME is bounded by

$$\mathcal{O} \left[\frac{Bm^2}{\epsilon^2} \log \frac{Bm}{\epsilon^2 \delta} \right]. \quad (10)$$

For each iteration of the KL-LUCB algorithm, R-LIME needs to update the linear classifier g_i , which is not required in Anchor. If we use logistic regression as the linear classifier and update it by stochastic gradient descent (SGD) [12], the computational complexity of updating g_i is $\mathcal{O}(m)$. It is negligible compared to the complexity of generating a perturbed sample, which is $\mathcal{O}(m^2)$ if we get a sample from a multivariate normal distribution using Cholesky decomposition in advance. Overall, the computational complexity of R-LIME is comparable to that of Anchor.

4 Experiments

To verify the effectiveness of our method, we conducted qualitative and quantitative comparisons of R-LIME with LIME and Anchor, using a real-world dataset. Our code for R-LIME is available on GitHub¹.

¹ <https://github.com/g-ohara/rlime>

Table 1: Attributes of the recidivism dataset used in the experiments. Continuous features are all discretized, and only binary and ordinal features are considered.

Attribute	Overview	# of Possible Values
Race	Race (Black or White)	2
Alcohol	Presence of serious alcohol issues	2
Junky	Drug usage	2
Supervised Release	Supervised release	2
Married	Marital status	2
Felony	Felony or not	2
WorkRelease	Participation in work release program	2
Crime against Property	Crime against property or not	2
Crime against Person	Crime against a person or not	2
Gender	Gender (Female or Male)	2
Priors	Number of prior offenses	4
YearsSchool	Years of formal education completed	4
PrisonViolations	Number of prison rule violations	3
Age	Age	4
MonthsServed	Months served in prison	4
Recidivism	Recidivism or not	2

4.1 Qualitative Evaluation

Experimental Setup We used the recidivism dataset [14] for our experiments. The dataset contains personal information on 9549 prisoners released from North Carolina prisons between July 1, 1979 and June 30, 1980. As shown in Table 1, the dataset includes 19 items such as race (*Race*), gender (*Gender*), presence of alcohol dependence (*Alcohol*), number of prior offenses (*Priors*), and presence of recidivism (*Recidivism*). For this experiment, we treated the binary classification problem of predicting the presence of recidivism (*Recidivism*) as the target label. We discretized continuous features and removed missing values, resulting in 15 features.

We splitted the dataset into training data (7639 instances) and test data (955 instances), and trained a random forest model with 50 trees as the black-box classifier using the training data. Then, we generate LIME, Anchor and R-LIME explanations for two instances extracted from the test data (Fig. 5). For R-LIME, we used logistic regression as the linear approximation model, and a multivariate normal distribution estimated from the training data as the distribution \mathcal{D} . For both Anchor and R-LIME, the beam width was set to $B = 10$, the confidence coefficient to $1 - \delta = 0.95$, and the tolerance of the KL-LUCB algorithm to $\epsilon = 0.05$. The accuracy threshold τ was set to $\tau = 0.70, 0.90$.

This problem setting can be considered as a case where a complex machine learning model is introduced to decide parole for prisoners. Since such decisions can have a significant impact on a person’s life, it is crucial for users to appropriately interpret the outputs of black-box models.

Race	Black (0)
Alcohol	No (0)
Junky	No (0)
Supervised Release	Yes (1)
Married	Yes (1)
Felony	No (0)
WorkRelease	Yes (1)
Crime against Property	No (0)
Crime against Person	No (0)
Gender	Male (1)
Priors	1
YearsSchool	$8.00 < \text{YearsSchool} \leq 10.00$ (1)
PrisonViolations	0
Age	$\text{Age} > 33.00$ (3)
MonthsServed	$4.00 < \text{MonthsServed} \leq 9.00$ (1)
Recidivism	No more crimes (0)

(a) Instance A

Race	Black (0)
Alcohol	Yes (1)
Junky	No (0)
Supervised Release	Yes (1)
Married	No (0)
Felony	No (0)
WorkRelease	Yes (1)
Crime against Property	Yes (1)
Crime against Person	No (0)
Gender	Male (1)
Priors	1
YearsSchool	$\text{YearsSchool} > 11.00$ (3)
PrisonViolations	0
Age	$21.00 < \text{Age} \leq 26.00$ (1)
MonthsServed	$4.00 < \text{MonthsServed} \leq 9.00$ (1)
Recidivism	Re-arrested (1)

(b) Instance B

Fig. 5: Two instances sampled from training data of recidivism dataset. Each number in parentheses represents the integer value assigned to the corresponding categorical value.

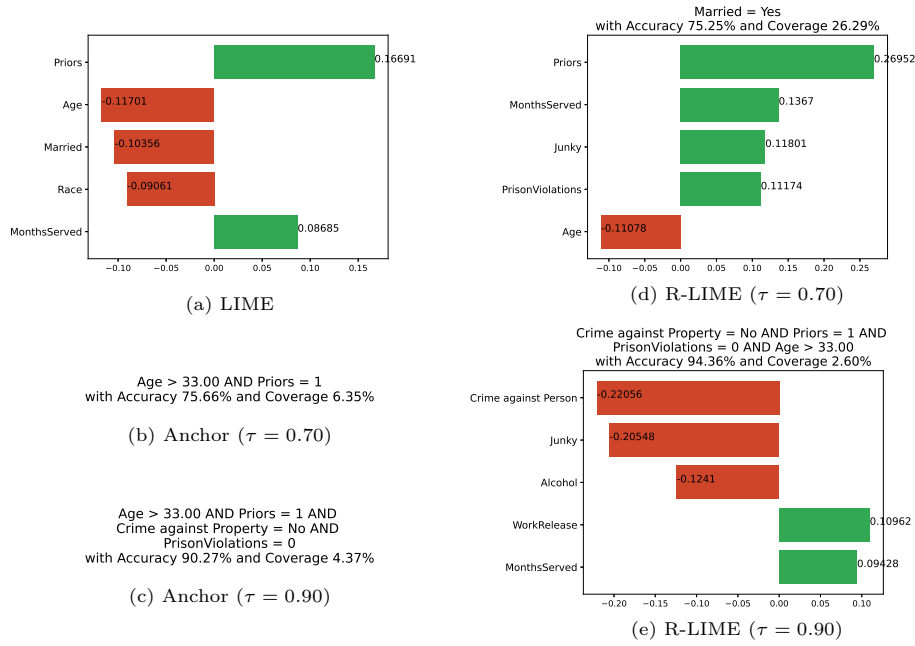


Fig. 6: Explanation for Instance A by LIME and R-LIME.

Experimental Results The results of the experiment are shown in Figs. 6 and 7. The values assigned to each feature name represent the contribution (weight of the linear classifier) to the output of the black-box classifier, normalized such that the absolute sum is 1. The figures display the 5 features with the highest absolute contribution.

Explanations generated by LIME (Figs. 6(a) and 7(a)) provide insights that having a prior offenses (*Priors*), being served for a long time in prison (*MonthsServed*), and committing a crime against property (*Crime against Property*) primarily contribute to the positive prediction (prediction that the prisoner will be re-arrested). On the other hand, being elderly (*Age*), being married (*Married*), and being of white race (*Race*) contribute to the negative prediction (prediction that the prisoner will not be re-arrested). While these LIME explanations provide valuable insights into the behavior of the black-box model, they do not explicitly indicate the application scope of the explanations, leaving users unable to determine to which prisoners the explanations are applicable.

Anchor provides conditions for the model's output to be fixed with high probability. For example, the explanation for instance A under $\tau = 0.70$ (Fig. 6(b)) means that the model will predict with 75.66 % probability that the prisoner will commit no more crimes when a prisoner is older than 33 and has one prior offense. Although it clearly provides the explanation's application scope, it does not provide details about how these conditions affect the model's output.

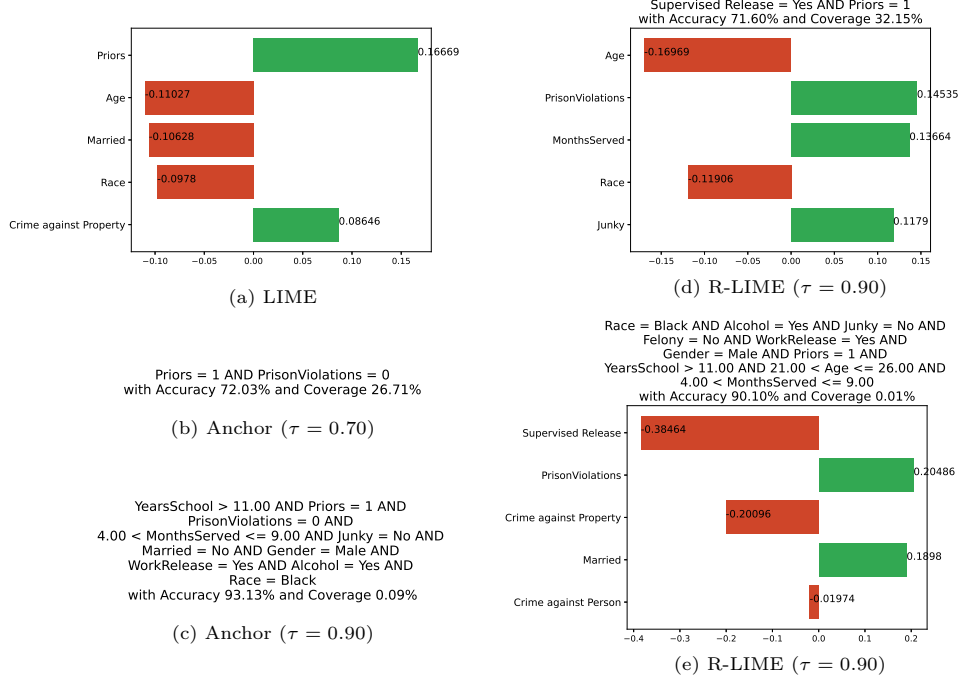


Fig. 7: Explanation for Instance B by LIME and R-LIME.

In contrast to LIME and Anchor, R-LIME provides both contribution of each feature to the output and the application scope of the explanation. For example, the explanation for instance A under $\tau = 0.70$ (Fig. 6(d)) indicates that it is applicable only to married prisoner (*Married* = Yes). R-LIME explanations also provide their accuracy and coverage, allowing users to evaluate reliability and generality of the explanations. For example, the coverage of the explanation for instance B under $\tau = 0.90$ (Fig. 7(e)) is 0.01%, indicating that the decision boundaries around instance B are complex, making it challenging to obtain a high-accuracy linear approximation. This information allows users to discern that the application scope of this explanation is very narrow, limiting its utility.

4.2 Quantitative Evaluation: LIME vs. R-LIME

Experimental Setup To demonstrate that R-LIME learns a highly accurate linear approximation model in the optimized approximation region, we conducted a comparison of the local accuracy of explanations between LIME and R-LIME. Under the same settings as in section 4.1, we randomly sampled 100 instances from the test data of the recidivism dataset and generated explanations using LIME and R-LIME (with $\tau = 0.70, 0.80, 0.90$). We then sampled 10,000 instances within the rectangular region obtained by R-LIME and calculated the local accuracy of both methods.

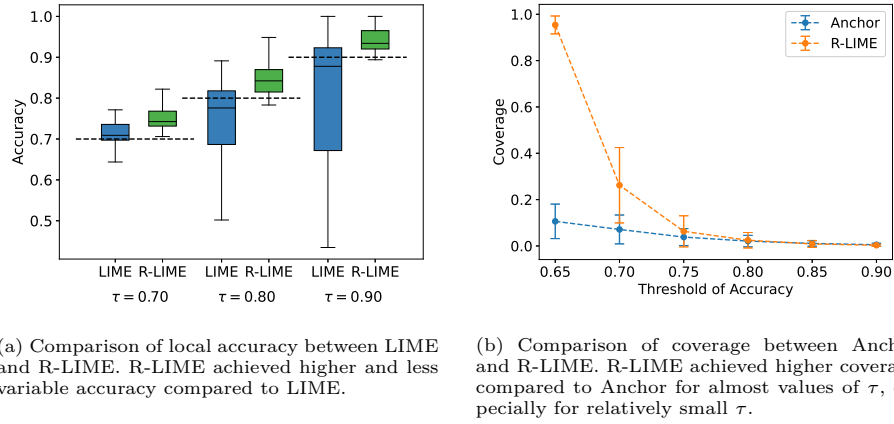


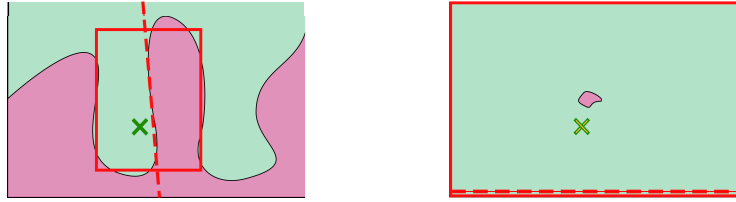
Fig. 8: Comparison of existing methods (LIME, Anchor) and R-LIME.

Experimental Results The results are presented in Fig. 8(a), showing the distribution of the local accuracy of the linear classifiers learned by LIME and R-LIME. R-LIME achieved higher accuracy compared to LIME for all values of τ . This suggests that the linear classifiers learned by LIME and R-LIME differ significantly, and R-LIME learns a high-accuracy linear classifier adapted to the optimized rectangular region. Additionally, as τ increases, the variability in the accuracy of LIME widens. This indicates that the linear classifiers learned by LIME may not function effectively as approximation models depending on how the region is selected.

4.3 Quantitative Evaluation: Anchor vs. R-LIME

Experimental Setup To demonstrate that R-LIME explanations are more general than Anchor, we conducted a comparison of the coverage of explanations between Anchor and R-LIME. Under the same settings as in section 4.1, we generated Anchor and R-LIME explanations for 704 instances from the test data of the recidivism dataset, under the values of $\tau = 0.65, 0.70, 0.75, 0.80, 0.85, 0.90$.

Experimental Results The results are presented in Fig. 8(b), showing the coverage of the explanations by Anchor and R-LIME. The coverage of explanations generated by R-LIME is higher compared to Anchor for almost values of τ , especially for relatively small τ . It is because of the flexibility of the linear approximation models learned by R-LIME, which captures the decision boundary more precisely. In contrast, Anchor uses only the intervals of each feature discretized in advance, which cannot capture the decision boundary flexibly and makes its scope narrow.



(a) R-LIME for balanced label distribution. (b) R-LIME for imbalanced label distribution.

Fig. 9: Behavior of R-LIME for balanced and imbalanced label distribution. In case of imbalanced label distribution, the approximation region covers the entire input space and the linear approximation model always outputs the majority label.

Table 2: Deviation between the estimated accuracy and the true accuracy of the linear classifier learned by R-LIME. The deviation 0.012 ± 0.017 was relatively small considering the confidence level $1 - \delta = 0.95$.

	Estimated acc.	True acc.	Deviation
Average	.811	.829	.012
Standard Deviation	.018	.023	.017

5 Discussion

5.1 Behavior for Imbalanced Label Distribution

R-LIME may generate less useful explanations when the distribution of black-box classifier outputs is imbalanced. When the ratio of outputting the minority label is less than $1 - \tau$, where τ is the accuracy threshold, the approximation region generated by R-LIME covers the entire input space, and the learned linear classifier always outputs the majority label (Fig. 9).

A first possible solution to this problem is modifying the loss function. Using weighted logistic loss or Focal Loss [7] as the loss function might lead to the generation of more useful explanations in the case of imbalanced label distribution. Another solution involves adding constraints to limit the label distribution bias within the approximation region. In addition to eq. (4), adding a constraint like

$$\left(\mathbb{E}_{z \sim \mathcal{D}(z|A)} [\mathbb{1}_{f(z)=1}] - \frac{1}{2} \right)^2 < \mu \quad (11)$$

could suppress the excessive expansion of the approximation region.

5.2 Changes in Reward Distribution in Best Arm Identification

For R-LIME, the problem of selecting the rule with the highest accuracy is formulated as the best arm identification problem in multi-armed bandit framework, and solved using the KL-LUCB algorithm [6]. However, this algorithm

assumes that the reward distribution remains constant, while in R-LIME, the reward distribution (accuracy of the linear approximation) changes with every update of the approximation model after sampling. Therefore, rewards obtained at an early stage might influence the estimated value and make it deviate from the true value.

We conducted an experiment to evaluate the deviation between the estimated accuracy and the true accuracy. We generated explanations for 3200 data instances sampled from the dataset, and compared the estimated accuracy with the true accuracy. The true accuracy was calculated based on 1000 instances sampled within the approximation region. The results in Table 2 show a mean deviation of 0.012 with a standard deviation of 0.017. By considering the confidence level $1 - \delta = 0.95$, the deviation was relatively small. While there are concerns about the theoretical validity of using the KL-LUCB algorithm, our results suggest that the deviation is not significant in practice.

5.3 Parameter Selection

In section 3.4, we discussed about the computational complexity of R-LIME, which depends on some hyperparameters. R-LIME requires the hyperparameters to be selected by users, such as the threshold of accuracy τ , beam width B , tolerance ϵ and confidence level δ . B should be large and ϵ and δ should be small for accurate results, as long as the computational cost is acceptable. On the other hand, τ should be carefully selected by users, sometimes interactively, considering the tradeoff between the accuracy and generality of generated explanation.

6 Conclusion

Existing methods for local model-agnostic explanations of black-box classifiers, such as LIME and Anchor, have limitations that they cannot achieve interpretability of both the explanation and its application scope. To address these challenges, we proposed R-LIME, a method that locally and linearly approximates the decision boundary of a black-box classifier and provides a rectangular approximation region, which is interpretable for users due to being expressed as a conjunction of feature predicates. We proposed an algorithm to maximize coverage of the approximation region as long as the accuracy of the linear approximation model exceeds a given threshold. Comparing R-LIME with existing methods on the real-world dataset, we demonstrated that R-LIME achieves interpretability of both the explanation and its application scope, and provides explanations more accurate than LIME and more general than Anchor. Finally, we discussed the instability of behavior with imbalanced label distributions, raised questions about the theoretical validity of using the KL-LUCB algorithm, and hyperparameter tuning in practice.

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