Evaluating the Correctness of Explainable AI Algorithms for Classification

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Abstract. Explainable AI has attracted much research attention in recent years with feature attribution algorithms, which compute “feature importance” in predictions, becoming increasingly popular. However, there is little analysis of the validity of these algorithms as there is no “ground truth” in the existing datasets to validate their correctness. In this work, we develop a method to quantitatively evaluate the correctness of XAI algorithms by creating datasets with known explanation ground truth. To this end, we focus on the binary classification problems. String datasets are constructed using formal language derived from a grammar. A string is positive if and only if a certain property is fulfilled. Symbols serving as explanation ground truth in a positive string are part of an explanation if and only if they contribute to fulfilling the property. Two popular feature attribution explainers, Local Interpretable Model-agnostic Explanations (LIME) and SHapley Additive exPlanations (SHAP), are used in our experiments. We show that: (1) classification accuracy is positively correlated with explanation accuracy; (2) SHAP provides more accurate explanations than LIME; (3) explanation accuracy is negatively correlated with dataset complexity.

Keywords: Binary classification · Feature importance · Language and grammar.

1 Introduction

Explainable AI (XAI) is a fast growing research area in AI that aims to provide insight into processes that AI uses to conclude [1]. The goal of enabling explainability in AI systems is “to ensure algorithmic predictions and any input data triggering those predictions can be explained to non-experts” [4]. XAI can create practical machine learning methods that produce more human-understandable models while preserving a high accuracy of predictions.

Two main categories of approaches have been proposed in the literature to address the need for explainability in AI systems: (1) intrinsically interpretable methods [23], in which prediction and explanation are both produced by the same underlying mechanism, and (2) model-agnostic methods [17], in which explanations are treated as a post hoc exercise and are separated from the prediction model. In the case for methods (1), while many intrinsically interpretable models, such as short decision trees, linear regression, Naïve Bayes, k-nearest neighbours and decision rules [28] are easy to understand, they can be weak for prediction and suffer from performance loss in complex tasks. On the contrary, model agnostic approaches such as local surrogate [19], global surrogate [2], feature importance [7], and symbolic Bayesian network transformation...
Among the model agnostic methods, giving users explanations in the form of feature importance has been viewed as an effective approach in XAI – as each feature makes some contribution to the prediction, by knowing the “weights” of features, one can better understand how a prediction is made. In addition to the Local Interpretable Model-Agnostic Explanations (LIME) introduced in [20], competing feature importance approaches including the SHapley Additive exPlanations (SHAP) [15] have been developed. Although they have attracted much research attention, there is little work on evaluating the correctness of the explanations produced by the feature importance explainers. After all, what explainers do is to output numbers associated to features. How can we know the feature importance asserted by such explainers is correct explanations? Taking the well known Mushroom dataset [6] as an example, there are 8124 mushroom instances in this dataset where each instance is either edible or poisonous. With a standard random forest classifier, one achieves classification AUC 0.98 on a 80/20 training/testing split. However, upon questioning top features for predicting the 3916 poisonous instances, LIME and SHAP differ on 1527 of them when the highest ranked feature is considered; and 2744 of them when the top two highest ranked features are considered. The question is: Is LIME or SHAP is correct, or are both correct despite they reporting drastically different top features?

With the few exceptions discussed in Section 6, literatures on evaluating correctness are hard to find as only 5% of the researchers that have studied AI interpretability or explainability have focused on assessing them [1]. Existing evaluations, see e.g. [16] for a recent overview, are predominantly based on human inputs. However, as discussed by [5,3,10], any evaluation metric that is completely based on human inputs is fallible due to human bias and subjectivity. Even though some other metrics for XAI methods such as “explanation goodness”, “explanation satisfaction scale”, “explanation usefulness”, and “user trust” are discussed in [8,16], quantitative analysis on explanation correctness without human input is needed.

Various reasons lead to the lack of a quantitative study on correctness of XAI methods. The chief reason is the lack of explanation truth in datasets. For example, in the Mushroom dataset, it is impossible to know what the most important features for a mushroom to be poisonous are from the dataset itself. In other words, there is no ground truth to validate the correctness of XAI methods. Therefore, in this work, we give an approach to generate datasets for binary classification problems with explanation ground truth. In this way, we can compare feature importance XAI methods against the designed explanation ground truth while performing prediction tasks as normal. We do not rely on human inputs in our evaluation as the explanation ground truth are coded into our datasets. Although our dataset generation method may not capture all real world classification tasks, it can be viewed as a systematic and sound benchmark for comparing feature importance XAI methods.

More specifically, we formally define correct explanations for binary classification and introduce an evaluation metric, \( k \)-accuracy, in Section 2. We present an algorithm for generating datasets with correct explanation ground truth using formal grammar in Section 3. We then introduce grammatical complexity (\( G \)-complexity), modelled as
the Kolmogorov Complexity [12], as a controllable complexity measure for dataset generation in Section 4 and show performances of classification and explanation are negatively correlate to it. We experiment with SHAP and LIME throughout in Section 5.

Contributions of this paper are: (1) a method for generating datasets that allow qualitative study of explanation correctness; (2) the discovery of a positive relation between classification accuracy and explanation performance; (3) quantitative evaluation of SHAP and LIME with the proposed method; and (4) the discovery of a negative relation between SHAP performance and dataset complexity.

2 Explanation for Binary Classification

In this work, we focus on the problem of binary classification on categorical data. To construct datasets with explanation ground truth, we need a way to generate data instances that can be labelled in two ways, positive (POS) and negative (npos). For each instance, we need to be able to clearly specify features that are “responsible” for the labelling. Not to trivialise the process, the classification labelling cannot be solely determined by some fixed features in the dataset although such features would explain the classification. For example, “when feature 2 is above 50, then label the instance POS,” would be considered an over simplification for real world classification tasks. We must generate data instances such that the classification labelling is determined by a subset of feature values; yet, the position of explanation subset cannot be fixed throughout the dataset.

To achieve this, we use formal grammars and their corresponding languages. The language and grammar notions we will use are as follows.

2.1 Language and Grammar Notions

– Alphabet $\Sigma$ is a finite set of symbols.
– String is a finite sequence of symbols from $\Sigma$.
– Language $L$ is a subset of $\Sigma^*$.

A Grammar $G$ is a set of production rules and it describes the strings in the language. Formally, given alphabet $\Sigma$, a grammar $G$ is a tuple $\langle N, T, P, S \rangle$, where:

– $N$ is a set of nonterminal symbols, $N \cap \Sigma = \{\}$;
– $T = \Sigma$ is a set of terminal symbols;
– $P$ is a set of production rules from $N$ to $(N \cup T)^*$; and
– $S \in N$ the start symbol.

The parse trees for $G$ are trees with the following conditions:

1. Each interior node is labelled by a symbol in $N$.
2. Each leaf is labelled by either a symbol in $N$, a string of terminal symbols in $T$, or $\epsilon$.
3. If an interior node is labelled as $A$, and its children are labelled as $X_1, X_2, \ldots, X_k$ respectively, from the left, then $A \rightarrow X_1, X_2, \ldots, X_k$ is a production rule in $P$. 


A grammar is ambiguous if there exists a string in the language of the grammar s.t. the string can have more than one parse tree.

2.2 Correct Explanation

We formulate the binary clarification problem on categorical data as the following string classification. Given a set of strings $S$, s.t. each $s \in S$ is of the same length $k > 0$; there exists a labelling function $h$ which maps each string to a class $c \in C$, with $C$ being all possible classes for $S$. The classification task is to identify a classifier $g : S \mapsto C$ s.t. $g(s) = h(s)$. In this process, each symbol in $s$ is a feature of $s$. For instance, the string 0011 has four features, $f_1, f_2, f_3, f_4$, with

$$f_1 = 0, f_2 = 0, f_3 = 1, \text{ and } f_4 = 1;$$

and the string 1100 has four features with

$$f_1 = 1, f_2 = 1, f_3 = 0, \text{ and } f_4 = 0.$$  

Many real binary classification problems are the instances of the string classification. For example, the Mushroom dataset mentioned in Section 1 is a dataset with strings of length 22 on the alphabet \{a, b, c, d, e, f, g, h, k, l, m, n, o, p, r, s, t, u, v, w, x, y, z, ?\}. A instance of the mushroom dampest is shown in Table 1.

Table 1: Explanation given by SHAP and LIME for a correctly classified data instance from the Mushroom dataset.

| Poisonous mushroom: xwnytffchbtsswpwokpsu |
|-------------------------------------------|
| Cap shape: convex, cap colour: white, gill colour: brown, cap surface: scaly, bruises: t=bruises, odor: foul, gill attachment: free, gill spacing: close, gill size: broad, stalk shape: tapering, stalk root: bulbous, stalk-surface-above-ring: smooth, stalk-surface-below-ring: smooth, stalk-color-above-ring: white, stalk-color-below-ring: white, veil-type: partial, veil-color: white, ring-number: one, ring-type: pendant, spore-print-color: black, population: scattered, habitat: urban. |

Each string in this dataset is labelled in one of the two classes: poisonous or edible. Since each instance can belong to only one of the two classes, classification on this dataset is binary.

Before we define correct explanation, We first give the definition of substring.

**Definition 1.** Given a string $s = a_1 \ldots a_n$ over alphabet $\Sigma$, where $\cdot \notin \Sigma$, $s$ represents a data point $x$ with features $f_1 \ldots f_n$, s.t. $x = \{f_1 = a_1, \ldots, f_n = a_n\}$. A substring $s'$ of $s$ is a string $s' = a'_1 \ldots a'_n$ over alphabet $\Sigma \cup \{\cdot\}$ with $a'_i \in \{a_i, \cdot\}$, $i = 1 \ldots n$. $s'$ represents the set $\{f_i = a_i | a'_i \neq \cdot\}$.

\(^1\) See [6] for the meaning of feature symbols.
For instance, the substring 01· of the string 0011 denotes the set of two feature-values \{f_2 = 0, f_3 = 1\}.

We define our notions of explanation (for a POS classification) and correct explanation as follows.

**Definition 2.** Given a string \( x \in S \) s.t. \( h(x) = \text{POS} \), an explanation \( e_x \) for the label \( h(x) = \text{POS} \) is a substring of \( x \). We also say \( e_x \) is an explanation for \( x \) when there is no ambiguity.

An explanation \( e_x \) is correct (for \( x \) being POS) if and only if for any string \( x' \in S \), if \( e_x \) is a substring of \( x' \), then \( h(x) = h(x') = \text{POS} \). If \( e_x \) is a correct explanation (for some label \( h(x) \)) and the length of \( e_x \) is \( k \), then we say that \( e_x \) is a \( k \)-explanation (for \( h(x) \)).

Definition 2 defines explanations as substrings. Intuitively, a correct explanation for an instance is the “core subset of features” which is “decisive”. In the sense that regardless what other features might be, these “core features” alone determine the outcome of the classification. We focus only on explaining “positive” instances as “core features” can be asymmetrical. An instance is “negative” not because certain features are presented in this instance, but rather the lack of “core features”. In this sense, all features in a negative case “collectively explain” the negative classification.

We illustrate our notion of explanation as follows.

**Example 1.** Let \( S = \{00100, 00001, 10000, 11111, 00111, 10011\} \), the labelling function \( h \) is s.t.

\[
\begin{align*}
h(11111) &= h(00111) = h(10011) = \text{POS}, \\
h(00100) &= h(00001) = h(10000) = \text{NEG}.
\end{align*}
\]

There are \( C(5, 3) = 10 \) 3-explanations for each of the three POS strings. Correct 3-explanations include 111· for \( g(11111) \), ·111 for \( g(00111) \) and 1·11 for \( g(10011) \). The substring 00·1 is not a correct 3-explanation for \( g(00111) \); neither is 100· correct for \( g(10011) \).

If a dataset is noise free, then every POS sample in the dataset has an explanation, formally:

**Proposition 1.** Given a dataset \( S \), if there is no two strings \( s_1, s_2 \in S \) s.t. \( s_1 = s_2 \) and \( h(s_1) \neq h(s_2) \), then for each \( s \in S \), s.t. \( h(s) = \text{POS} \), \( s \) has a correct non-empty explanation \( e_s \).

**Proof.** (Sketch.) Since each string \( s \) is labelled in only one way, \( e_s = s \) is a correct explanation.

With correct explanation defined, to measure the correctness of an XAI algorithm, we define \( k \)-accuracy as follows.

**Definition 3.** Given a dataset \( S \) over alphabet \( \Sigma \) and a classifier \( g \), for each \( x \in S \) s.t. \( g(x) = h(x) = \text{POS} \), let \( e_x \) be a correct explanation for \( h(x) \). Then, the \( k \)-accuracy of a \( k \)-explanation \( e'_x \) is \(|\{a \in \Sigma | a \text{ is in both } e_x \text{ and } e'_x \}|/k\).
Note that \( k\)-accuracy is defined for correct POS classifications. As we use \( k\)-accuracy to measure explainer performance, we calculate such accuracy only when the prediction matches with the classification ground truth, i.e., when \( g(x) = h(x) \). Intuitively, we ask for explanations only when the prediction is correct. This helps us to separate explainer performance from classifier performance and prevent us from processing meaningless explanations for wrong predictions.

3 Constructing Datasets with Explanation

To construct datasets with explanations, we create a grammar \( G \) with language \( L \). We let \( L' \subseteq L \) be the dataset. A string \( s \in L' \) is labelled as POS if and only if there is some production rule \( r \in G \) used more than \( t > 1 \) times. Terminal symbols associated with the production rule triggering the POS classification form the explanations for \( s \).

We present our dataset and explanation construction with the following example.

**Example 2.** Given a grammar \( G = \langle \{S, B, N, T, Y\}, \{0, 1\}, P, S \rangle \) with \( P \) being the following production rules:

\[
\begin{align*}
S & \rightarrow BB \mid NN \mid \epsilon \\
B & \rightarrow TT \mid YY \mid \epsilon \\
T & \rightarrow 11 \mid 00 \\
N & \rightarrow TY \mid YT \mid \epsilon
\end{align*}
\]

From \( G \), we create a dataset \( L \) containing 8-bit strings such as \( 11000000 \) and \( 00110000 \). We let the threshold \( t = 2 \) and use parse trees to count the times of each production rule is used. For instance, the parse tree for the string \( 11000000 \) is shown in Figure 1 (left). Production rules used to generate the string are follows.

| Production Rule Uses | Production Rule Uses |
|----------------------|----------------------|
| \( S \rightarrow BB \) | \( B \rightarrow TT \) |
| 1                    | 2                    |
| \( T \rightarrow 11 \) | \( T \rightarrow 00 \) |
| 1                    | 3                    |

Since the production rule \( T \rightarrow 00 \) is used 3 times, \( 3 > t = 2 \), \( 11000000 \) is POS. The explanation is \( \cdots 000000 \), which are terminal symbols in the production rule \( T \rightarrow 00 \).

\[
\begin{align*}
S & \rightarrow BB \\
\mid & \\
BB & \\
TT & TT
\end{align*}
\]

\[
\begin{align*}
S & \rightarrow BB \\
\mid & \\
BB & \\
TT & YY
\end{align*}
\]

Fig. 1: Parse trees for \( 11000000 \) (left) and \( 11000110 \) (right).

On the other hand, for the string \( 11000110 \) with its parse tree shown in Figure 1 (right), as shown below, there is no rule triggered more than once. Thus \( 11000110 \) is labelled NEG and there is no explanation for \( 11000110 \).
To formalize our explanation dataset approach, we start by defining *explanation-grammar*, the class of grammar we used to generate datasets, as follows.

**Definition 4.** A grammar \( \langle N, T, P, S \rangle \) is an explanation-grammar (e-grammar) if and only if all of the following conditions hold:

1. \( N = N_v \cup N_t, N_v \cap N_t = \{\} \),
2. For each production rule \( r \) in \( P \), \( r \) is of the form:
   - \( A \rightarrow BC | \epsilon \), for \( B, C \in N \), if \( A \in N_v \),
   - \( A \rightarrow abc \ldots \), for \( a, b, c \in T \), if \( A \in N_t \).

*For a production rule \( r = A \rightarrow \ldots \), we say \( r \) is a non-terminal rule if \( A \in N_v \); otherwise, \( r \) is a terminal rule.*

Grammar \( G \) in Example 2 is an e-grammar. Comparing with the standard grammar definition (see Section 2), e-grammar enforces new conditions as follows.

1. Each nonterminal symbol can only be the left-hand side of rules with either terminal or nonterminal symbols on the right-hand side, but not both.
2. Production rules with nonterminal symbols on the right-hand side are called non-terminal rules; otherwise, they are terminal rules.
3. There are either two nonterminal symbols or a single \( \epsilon \) as the right-hand side of a nonterminal rule.
4. There are any positive number of terminal symbols as the right-hand side of a terminal rule.

The following holds trivially from Definition 4.

**Proposition 2.** For any dataset \( D \) consisting strings, there exists an e-grammar \( G \) s.t. the language of \( G \) is \( D \).

**Proof.** Let \( G = \langle N, T, P, S \rangle \) with \( N = \{S\} \), \( T \) be all symbols in \( D \), and \( P = \{S \rightarrow s | s \in D\} \). It is easy to see that the language of \( G \) is \( D \).

Explanation datasets are created from e-grammars using Algorithm 1, as follows.

Algorithm 1 takes an e-grammar \( G \), a string length \( l \), and a threshold \( t \) as its inputs to produce a dataset \( D \) containing strings with classification label and explanation substrings. If a string \( s \) in \( D \) is labelled as POS, then there is a non-empty explanation \( e \) produced for \( s \). The stop condition in Line 2 determines when to exit from the while loop. It is a combination of: (1) whether sufficiently many strings have been added to \( D \); (2) whether \( D \) contains balanced POS and NEG samples; and (3) whether the loop has been running for too long. To generate a random string from a e-grammar \( G \) in

| Production Rule Uses | Production Rule Uses |
|----------------------|----------------------|
| \( S \rightarrow BB \) | \( B \rightarrow TT \) |
| \( B \rightarrow YY \) | \( T \rightarrow 00 \) |
| \( T \rightarrow 11 \) | \( Y \rightarrow 10 \) |
| \( Y \rightarrow 01 \) | \( Y \rightarrow 10 \) |
Input: e-grammar $G$, string length $l$, POS-threshold $t$
Output: strings with classification and explanation labels

1: Let $D$ be empty
2: while stop condition not met do
3: Randomly generate a string $s$ of length $l$ from $G$
4: Let $Rs$ be terminal rules used in generating $s$
   s.t. each $r \in Rs$ is used more than $t$ times
5: if $Rs$ is not empty then
6: Let $e$ be the substring of $s$ formed by terminal symbols in $Rs$
7: add ($\text{POS}$, $s$, $e$) to $D$
8: else
9: add ($\text{NEG}$, $s$, $\emptyset$) to $D$
10: end if
11: end while
12: return $D$

Algorithm 1: Generating explanation datasets containing strings with labels and explanations.

Line 3, we repeatedly perform random derivations until a string with $l$ terminal symbols is produced while prioritising derivations of terminal rules. If there is no more terminal rule can be applied to the string when it reaches $l$ terminal symbols, then this string is returned as all non-terminal symbols can be expanded to $\epsilon$; otherwise, drop this derivation and start again.

Proposition 3 sanctions that Algorithm 1 computes unique explanations from unambiguous grammars.

Proposition 3. Let $e$ be an explanation for some POS string $s$ in a dataset $D$ generated with Algorithm 1 using grammar $G$ and POS-threshold $t$. If $G$ is unambiguous, then $e$ is an explanation for $s$ in any dataset generated from $G$ with $t$.

Proof. (Sketch.) Since $G$ is unambiguous, $s$ has a unique parse tree. To construct $s$, it always takes more than $t$ invocations of a certain production rule to make $e$ in any dataset.

Theorem 1 below is a key result of this work. It sanctions that Algorithm 1 generates strings with correct explanations.

Theorem 1. Given $D$ generated from Algorithm 1 with some e-grammar $G$ and threshold $t$. If for all terminal rules $r$ in $G$, the right-hand side of $r$ is unique and has the same length, then for each ($\text{POS}$, $s$, $e$) $\in D$, $e$ is a correct explanation for $s$ being $\text{POS}$.

Proof. (Sketch.) To show $e$ is a correct explanation, we need to show for all string $s'$ in $D$, if $e$ is a substring of $s'$, $s'$ is POS. For each string $s$ in $D$, $s$ can be viewed as a sequence of “composition blocks” in which each block is the right-hand side of some terminal rule in $G$. Since $s$ is POS, there must exist a production rule $r^*$ used $t'$ times with $t' > t$. And $e$ contains $t'$ copies of the right-hand side of $r^*$. Since this is the only way of generating $e$ in $D$, for each $s'$ containing $e$, $r^*$ must be used $t'$ time as well, which makes $s'$ POS.
4 Explanation and G-Complexity

Classification and explanation performances are affected by the complexity of the grammar used to construct the dataset. We define grammar complexity (G-complexity) as follows.

**Definition 5.** Given an e-grammar \( G = \langle N, T, P, S \rangle \), \( m = \| \{ r \in P \mid \text{the right-hand side of } r \text{ is not } \epsilon \} \| \) is the G-complexity of \( G \). Let \( D \) be a dataset constructed from \( G \) using Algorithm 1, we say that \( m \) is a G-complexity of \( D \).

Definition 5 uses the number of production rules that are not expanded to \( \epsilon \) to describe complexities of the grammar and any dataset constructed from it. This is in the same spirit as the Kolmogorov Complexity. Kolmogorov Complexity, defined over strings, is the length of the shortest program that generates the string. In our context, as datasets are sets of strings, we draw the analogy between string generating programs and production rules and use the number of rules as a proxy to measure the dataset complexity.

**Example 3.** The G-complexity of grammar \( G \) given in Example 2 is 10. 10 is a G-complexity of any datasets generated from \( G \) using Algorithm 1.

From Definition 5, the following holds.

**Proposition 4.** Every e-grammar has an unique G-complexity. A dataset can have more than one G-complexity.

**Proof.** (Sketch.) As G-complexity is defined on e-grammars, one obtains it by counting production rules in the grammar. As a dataset can be constructed from more than one e-grammar using Algorithm 1, these e-grammars can have different g-complexities, so the dataset can have more than one G-complexity. For instance, let \( \Delta = \{ s_1, \ldots, s_n \} \) be the set of strings in a dataset s.t. the length of strings is 2, and \( s_i \neq s_j \) for \( i \neq j \), then both e-grammars \( G_1 \) and \( G_2 \) construct \( \Delta \) as follows.

\[
G_1 = \langle N, T, P_1, S \rangle, \quad G_2 = \langle N, T, P_2, S \rangle, \quad \text{where}
\]

- \( N = \{ A_1, \ldots, A_n, B_1, \ldots, B_n \} \),
- \( T \) is the set of symbols in \( \Delta \),
- \( P_1 \) is s.t. for each \( s_i = ab \in \Delta \),
  1. \( S \rightarrow A_iB_i \mid \epsilon \in P_1 \),
  2. \( A_i \rightarrow \epsilon \in P_1 \),
  3. \( B_i \rightarrow ab \in P_1 \),
  4. Nothing else is in \( P_1 \).
- \( P_2 \) is s.t. for each \( s_i = ab \in \Delta \),
  1. \( S \rightarrow A_iB_i \mid \epsilon \in P_2 \),
  2. \( A_i \rightarrow a \in P_2 \),
  3. \( B_i \rightarrow b \in P_2 \),
  4. Nothing else is in \( P_2 \).
- \( S \) is the start symbol.

G-complexities of \( G_1, G_2 \) are \( 2n \) and \( 3n \), respectively.
5 Evaluation over SHAP and LIME

We evaluate the performance of two popular feature importance XAI methods, SHAP and LIME, over generated benchmark datasets using the proposed approach.

**SHapley Additive exPlanations (SHAP)** is a method that gives individual, thus “local”, explanations to black-box machine learning predictions [15]. It is based on the coalitional game theory concept *Shapley value*. Shapley value is defined to answers the question: “What is the fairest way for a coalition to divide its payout among the players”? It assumes that payouts should be assigned to players in a game depending on their contribution towards total payout. In a machine learning context, feature values are “player”; and the prediction is the “total payout”. The Shapley value of a feature represents its contribution to the prediction and thus explains the prediction. SHAP is “model-agnostic” thus independent of underlying prediction models. For a data point $x$, SHAP computes the marginal contribution of each feature to the prediction of $x$. In this work, we use the tree-based model, TreeSHAP, for estimating Shapley values of features introduced in [14], as which is shown to be a superior method than the Kernel SHAP introduced in [15].

**Local Interpretable Model-Agnostic Explanations (LIME)** is another method to explain individual predictions of machine learning models. LIME also is a model-agnostic approach, so it is applicable to any classifier [20]. LIME tests how predictions change when a user perturbs the input data. Given a black box model $f$ and a data instance $x$, to explain the prediction of $x$ made with $f$, LIME generates a set of perturbed instances around $x$ and compute and their corresponding predictions. It then creates an interpretable model $g$ based on generated data to approximate and explain $f$. LIME provides an explanation as a list of feature contributions to the prediction of the instance $x$. This highlights feature changes that have the most influence to the prediction.

To evaluate the performance of SHAP and LIME, we create 5 datasets containing 1000, …, 5000 strings from each e-grammar (see Definition 4 in Section 3), respectively. Each e-grammar is defined on 8 nonterminal symbols, contains 40 rules and 2 terminal symbols. The maximum length of the right-hand side of terminal rules is 2. The POS-threshold $t$ is 8. We compute $k$-accuracy for $k = 8$. We use a Random Forest classifier with 100 trees, split training and testing with a 80/20 ratio, and returns the average AUC and $k$-accuracy for SHAP and LIME. Results are shown in Figure 2. We see that SHAP performs consistently better than LIME (26% higher on average). Classification and SHAP performances improve as the number of samples increases whereas LIME performance largely remains.

![Fig. 2: Classification AUC and explanation $k$-accuracy under different dataset sizes (Left: mean; Right: standard deviation).](image-url)
To illustrate relations amongst G-complexity, classification and explanation, we create datasets with specified g-complexities by randomly generating e-grammars with the desired number of production rules and evaluate classification and explanation performances. The results are shown in Figure 3. For string lengths 20 to 35 and G-Complexities 20 to 60, we construct 100 e-grammars each generating a dataset containing 10,000 strings with the ratio between POS and NEG samples in the range of [0.4, 0.6]. The POS-threshold $t$ and $k$ in $k$-accuracy are 6 for string length 20, and 8 for the rest.

Fig. 3: Classification AUC and explanation $k$-accuracy for different g-complexities (Top: mean; Bottom: standard deviation).

From Figure 3, we see that for all string lengths, classification accuracy, SHAP and LIME performances all negatively correlate to G-Complexity, as summarised in Table 2, with SHAP performing consistently better than LIME in all cases (37% higher on average). SHAP and LIME accuracies are positively correlated to classification AUC at 0.62 and 0.46, respectively, averaging for all string lengths in Figure 3.

Table 2: Correlations between G-Complexity and mean performances of classification AUC, SHAP and LIME $k$-accuracies.

| String Length | Classification | SHAP $k$-acc. | LIME $k$-acc. |
|---------------|----------------|----------------|---------------|
| 20            | -0.88          | -0.97          | -0.92         |
| 25            | -0.76          | -0.95          | -0.91         |
| 30            | -0.95          | -0.93          | -0.53         |
| 35            | -0.94          | -0.88          | -0.45         |

To further validate these results, we expand the size of alphabet to 4, set string length to 25 and repeat the experiment. Results are in Figure 4. Classification and explanation performances are negatively correlate to G-Complexity with SHAP performing better than LIME (49% higher on average).

Fig. 4: Classification AUC and explanation $k$-accuracy for alphabet size 4 (Left: mean; Right: standard deviation).
6 Related Work

A survey on machine learning interpretability is presented in [4]. It provides an overview on interpretability while focusing on the societal impact and interpretability metrics. It presents 12 model-agnostic explanation methods including SHAP and LIME as well as Anchors [21] and Influence Functions [11]. There is no quantitative comparison of these methods in the study.

A comparison of LIME, DeepLIFT [25] and SHAP with human explanations is conducted in [15]. They report a stronger agreement between human explanations and SHAP than with LIME. [13] show that SHAP is more consistent with human intuition in their experiments than other approaches. [9] present a comparison of SHAP and LIME using their Explanation Consistency Framework. Three requirements are proposed: Identity - identical objects must have identical explanations; Separability - nonidentical objects cannot have identical explanations; and Stability - similar objects must have similar explanations. They show that SHAP meets all requirements LIME fails at identity. However, they do not measure explanation accuracy. [22] define properties for outputs generated by explanation methods including accuracy, fidelity, consistency, stability, comprehensibility, importance, novelty, and others. However, they do not provide any concrete approach for measuring these properties. While presenting an algorithm for generating counterfactual explanation, [18] show that LIME does not guarantee to perfectly distribute prediction amongst feature values whereas SHAP does. Thus LIME does not offer a globally consistent explanation as SHAP. While pointing out this theoretical difference, no quantitative evaluation is performed. [26] present the concept of “Three Cs of Interpretability”, completeness, correctness and compactness. Completeness refers to the coverage of the explanation in terms of the number of instances comprised by the explanation. Correctness means the explanation must be true. Compactness means the explanation should be succinct. They present their study in a healthcare setting with similar examples to the query instance considered as explanations. They do not study explanations in terms of features.

A framework to hide the biases of black-box classifier is proposed in [27]. Specifically, they use biases to make black-box classifier discriminatory to effectively fool explanation techniques such as SHAP and LIME into generating incorrect explanations which do not reflect the discriminatory biases in the data. They find that LIME is more vulnerable than SHAP to their attacks.

7 Conclusion

A key challenge in current XAI research is to develop robust ways to evaluate explanation methods. The lack of qualitative evaluation is largely due to the missing of explanation ground truth in the existing literature. In this work, while focusing on binary classification, we present a definition for correct explanation, a metric for explanation evaluation and provide an algorithm for constructing datasets with correct explanation ground truth for quantitatively evaluating model agnostic explanation algorithms. We create datasets as languages of grammars and set explanations as substrings created from repeated application of production rules. We introduce G-complexity, modelled after the
Kolmogorov Complexity of strings, to describe dataset complexity and show that both
classification and explanation become harder as datasets become more complex. We
evaluate SHAP and LIME with our approach and show that SHAP perform better than
LIME throughout and SHAP has a stronger correlation to classification performance
than LIME. For future work, we will perform human user studies to see whether our
notion of correct explanation corresponds to human explanations. We will experiment
with other model-agnostic explainer such as Anchors [21]. As our notion of correct ex-
planation is similar to theirs in spirit, it will be interesting to see how Anchors performs
against SHAP. Lastly, we will also extend our approach to multi-class classification and
regression.

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