Learning Baseline Values for Shapley Values

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Abstract

This paper aims to formulate the problem of estimating optimal baseline values for the Shapley value in game theory. The Shapley value measures the attribution of each input variable of a complex model, which is computed as the marginal benefit from the presence of this variable w.r.t. its absence under different contexts. To this end, people usually set the input variable to its baseline value to represent the absence of this variable (i.e. the no-signal state of this variable). Previous studies usually determine baseline values in an empirical manner, which hurts the trustworthiness of the Shapley value. In this paper, we revisit the feature representation of a deep model from the perspective of game theory, and define the multi-variate interaction patterns of input variables to formulate the no-signal state of an input variable. Based on the multi-variate interaction, we learn the optimal baseline value of each input variable. Experimental results have demonstrated the effectiveness of our method. The code will be released when the paper is accepted.

1 Introduction

Deep neural networks (DNNs) have exhibited significant success in various tasks, but the black-box nature of DNNs makes it difficult for people to understand the internal behavior of the DNN. Many methods have been proposed to explain the DNN, e.g. visualizing appearance patterns encoded by deep models [37, 49, 32], inverting features to the network input [12], extracting receptive fields of neural activations [50], and estimating the attribution/saliency/importance of input variables (e.g. pixels in an image, words in a sentence) w.r.t. the output of the model/network [51, 35, 28].

In terms of estimating the attribution/saliency/importance of input variables, the Shapley value can be considered as an unbiased estimation of an input variable’s attribution [36, 16, 28, 44]. As an attribution metric, the Shapley value satisfies the linearity, nullity, symmetry, and efficiency axioms, which ensure the trustworthiness of the attribution, thereby being widely used.

However, the Shapley value is at present obscured by two clouds. The first comes into existence with out-of-distribution (OOD) samples. The first comes into existence with out-of-distribution (OOD) samples. The Shapley value is measured on different masked samples, which are actually out of the distribution of real samples (as shown in Figure 1). The existence of such OOD samples has been proven to hurt the reliability of the Shapley value [39].

The second cloud is the choice of baseline values (or called reference values). Essentially, the Shapley value of an input variable is computed as the marginal difference of the model output between the case of removing this variable and the case of maintaining this variable (see Figure 1(left)). The removal of an input variable can be implemented as setting this variable to a certain baseline value, which does not provide any meaningful signals for inference (i.e. representing the absence of this variable). In other words, the baseline value is supposed to reflect the no-signal state of this variable. Hence, determining a suitable baseline value for each input variable is an important issue [8].
Therefore, in this paper, we define the no-signal state in game theory, i.e. the same theoretic system of defining the Shapley value. Then, we propose a method to estimate the optimal baseline values for the Shapley value. Given a trained model and input samples, we aim to learn baseline values for different input variables, which satisfy the following two requirements. (1) Our method is supposed to retain all the four axioms of Shapley values, which ensure the solidness of the theoretic system of Shapley values. (2) Our method needs to push the baseline value towards the no-signal state as much as possible.

Before defining the no-signal state of an input variable, let us first revisit the feature representation of a model from the perspective of game theory. Essentially, a model may encode varied interactions between different sets of input variables. Let us consider a toy example with binary input variables \( f(x) = x_1x_2 + x_3x_4, x_i \in \{0, 1\} \). The first term is activated \((x_1x_2 = 1)\) only if \( x_1 = x_2 = 1 \). We consider such input variables collaborate with each other, and the function \( f \) contains two multivariate interaction components \((e.g. x_1x_2\) and \( x_3x_4 \)), namely multi-variate interaction patterns. Each interaction pattern \((x_1x_2)\) represents an AND-relationship between multiple input variables \((x_1, x_2)\).

We further define the numerical utility of the multi-variate interaction patterns in game theory. Given a model and an input variable with \( n \) variables \( N = \{1, 2, \ldots, n\} \), we have proven that the overall utility/influence of an input sample on the model output can be decomposed as the sum of \( 2^n - n - 1 \) multi-variate interaction patterns, \( I(S) \).

In this way, signal states in an input sample can be modeled as salient patterns with significant influences on the model output \((i.e. those with large \( |I(S)| \) values), among all \( 2^n - n - 1 \) interaction patterns. Other patterns with small values of \( |I(S)| \) are considered as noisy patterns with little impact on the model output. Accordingly, for each input variable \( i \), there are \( 2^n - 1 - 1 \) interaction patterns containing the variable \( i \). The number of its signal states is quantified as the number of salient patterns activated by this variable. In order to approximate the no-signal state of an input variable, its baseline value is supposed to activate the least salient patterns. Thus, the objective of learning baseline values of input variables is to reduce the number of salient patterns when we set variables to their baseline values.

However, the cost of enumerating \( 2^n - n - 1 \) interaction patterns is NP-hard. Fortunately, we discover an approximate-yet-efficient method to reduce salient interaction patterns of the model. Experimental results have demonstrated the effectiveness of our method.

Besides the learning of baseline values, let us discuss the problem of OOD samples. This is an inherent problem of the Shapley value because incorrect baseline values usually create OOD interaction patterns. However, our method can be considered to alleviate the OOD problem, because our proposed baseline values are learned to activate as few patterns as possible in the feature space, thereby avoiding generating new OOD interaction patterns.
Contributions of this paper can be summarized as follows. (1) We formulate two requirements for baseline values in game theory. (2) We develop a method to estimate optimal baseline values, which ensures the reliability and trustworthiness of the Shapley value. (3) We define the multi-variate interaction, and prove its theoretical connections to the Shapley value \[36\] and the Shapley interaction index \[16\], which demonstrate the rigorousness of this metric.

2 Related works

Shapley values. The Shapley value \[36\] was first proposed in game theory, which was considered as an unbiased distribution of the overall reward in a game to each player. Lindeman \[27\] and Grömping \[17\] used the Shapley value to attribute the correlation coefficient of a linear regression to input features. Štrumbelj et al. \[42\], Štrumbelj and Kononenko \[41\] used the Shapley value to attribute the prediction of a model to input features. Bork et al. \[6\] used the Shapley value to estimate importances of protein interactions in large, complex biological interaction networks. Keinan et al. \[22\] employed the Shapley value to measure causal effects in neurophysical models. Sundararajan et al. \[42\] proposed Integrated Gradients based on the AumannShapley \[5\] cost-sharing technique. Besides above local explanations, Covert et al. \[9\] focused on the global interpretability.

In order to compute the Shapley value in deep models efficiently, Lundberg and Lee \[28\] proposed various approximations for Shapley values in DNNs. Lundberg et al. \[29\] further computed the Shapley value on tree ensembles. Aas et al. \[1\] generalized the approximation method in \[28\] to the case when features were related to each other. Ancona et al. \[3\] further formulated a polynomial-time approximation of Shapley values for DNNs.

Some previous studies also discussed problems with baseline values in the computation of Shapley values. Most studies \[8, 31, 44, 25\] compared influences of baseline values on explanations, without providing any principle rules for setting baseline values. Besides, Agarwal and Nguyen \[2\] and Frye et al. \[15\] used generative models to alleviate the OOD problem caused by baseline values.

Unlike previous studies, we rethink and formulate baseline values from the perspective of game theory. We define the absence (no-signal states) of input variables based on the multi-variate interaction, and further propose a method to learn optimal baseline values.

Interactions. Interactions between input variables of deep models have been widely investigated in recent years. In game theory, Grabisch and Roubens \[16\], Lundberg et al. \[29\] proposed and used the Shapley interaction index based on Shapley values. Sorokina et al. \[40\] proposed an approach to detect interactions of input variables in an additive model. Tsang et al. \[47\] measured interactions of weights in a DNN. Ren et al. \[34\] defined bivariate interactions of different contextual complexities between input variables. Murdoch et al. \[33\], Singh et al. \[38\], Jin et al. \[21\] used the contextual decomposition (CD) technique to extract variable interactions. Cui et al. \[10\] proposed a non-parametric probabilistic method to measure interactions using a Bayesian neural network. Janizek et al. \[20\] extended the Integrated Gradients method \[45\] to explain pairwise feature interactions in DNNs. Sundararajan et al. \[46\] defined the Shapley-Taylor index to measure interactions over binary features. In this paper, we define the multi-variate interaction of input variables. Our interaction metric has strong connections to \[16\] and \[34\], but represents elementary interaction patterns in a more detailed manner than \[34\], and satisfies the efficiency axiom, unlike \[16\].

3 Learning baseline values for Shapley values

Preliminaries: Shapley values. The Shapley value \[36\] was first introduced in the game theory, which measures the importance/contribution/attribution of each player in a game. Let us consider a game with multiple players. Each player participates in the game and receives a reward individually. Some players may form a coalition and play together to pursue a higher reward. Different players in the game usually contribute differently to the game, and then the question is how to fairly allocate the total reward in the game to each player. To this end, the Shapley value is considered as a unique unbiased approach that fairly allocates the reward to each player \[48, 28, 44\].

Given a game \(v\) with \(n\) players, let \(N = \{1, 2, \cdots, n\}\) denote the set of all players and \(2^N = \{S | S \subseteq N\}\) denote all potential subsets of players. The game \(v : 2^N \rightarrow \mathbb{R}\) is represented as a function that maps a subset of players \(S \subseteq N\) to a real reward \(v(S) \in \mathbb{R}\), i.e. the reward gained by all players in \(S\).
Specifically, \( v(\emptyset) \) represents the baseline score without any players. Considering the player \( i \notin S \), if the player \( i \) joins in \( S \), \( v(S \cup \{i\}) - v(S) \) is considered as the marginal contribution of \( i \). Thus, the Shapley value of the player \( i \) is computed as the weighted marginal contribution of \( i \) w.r.t. all subsets of players \( S \subseteq N \setminus \{i\} \), as follows.

\[
\phi_i = \sum_{S \subseteq N \setminus \{i\}} p(S) [v(S \cup \{i\}) - v(S)], \quad p(S) = \frac{|S|!(n - |S| - 1)!}{n!}
\]  

(1)

The fairness of the Shapley value is ensured by the following four axioms [48].

(a) **Linearity axiom:** If two games can be merged into a new game \( u(S) = v(S) + w(S) \), then the Shapley values of the two old games also can be merged, i.e. \( \forall i \in N, \phi_{i,u} = \phi_{i,v} + \phi_{i,w}; \forall c \in \mathbb{R}, \phi_{i,c \cdot u} = c \cdot \phi_{i,u} \).

(b) **Nullity axiom:** A dummy player \( i \) is defined as a player without any interactions with other players, i.e. satisfying \( \forall S \subseteq N \setminus \{i\}, v(S \cup \{i\}) = v(S) + v(\{i\}) \). Then, the dummy player’s Shapley value is computed as \( \phi_i = v(\{i\}) - v(\emptyset) \).

(c) **Symmetry axiom:** If \( \forall S \subseteq N \setminus \{i,j\}, v(S \cup \{i\}) = v(S \cup \{j\}) \), then \( \phi_i = \phi_j \).

(d) **Efficiency axiom:** The overall reward of the game is equal to the sum of Shapley values of all players, i.e. \( v(N) - v(\emptyset) = \sum_{i \in N} \phi_i \).

**Using Shapley values to explain deep models.** Given a trained model \( f : \mathbb{R}^n \rightarrow \mathbb{R} \) and an input sample \( x \in \mathbb{R}^n \), we can consider each input variable (e.g. a dimension, a pixel, or a word) \( x_i \) as a player \( (i \in N) \), and consider the deep model as a game. The model output \( f(x) \) is regarded as the reward \( v(N) \). Thus, the Shapley value \( \phi_i \) estimates the attribution of the \( i \)-th variable \( x_i \) w.r.t. the model output. In this case, \( v(S) \) represents the model output, when variables in \( S \) are present and variables in \( S = N \setminus S \) are absent. People usually set the input variables in \( S = N \setminus S \) to the variables’ baseline values, in order to represent the states of their absence (i.e. no-signal states of these variables). In this way, \( v(S) \) can be represented as follows.

\[
v(S) = f(\text{mask}(x, S)), \quad \text{mask}(x, S) = x_S \sqcup b_S, \quad (x_S \sqcup b_S)_i = \begin{cases} x_i, & i \in S \\ b_i, & i \in S = N \setminus S \end{cases}
\]  

(2)

where \( \text{mask}(x, S) \) denotes the masked sample, and \( b_i \) denotes the baseline value of the \( i \)-th input variable. \( \sqcup \) indicates the concatenation of \( x \)'s dimensions in \( S \) and \( b \)'s dimensions in \( S = N \setminus S \).

### 3.1 Problems with Shapley values

**Firstly, how to choose baseline values.** According to Equations (1) and (2), the Shapley value computes the marginal contribution of the variable \( i \), \( v(S \cup \{i\}) - v(S) \), under different masked samples (under different contexts \( S \subseteq N \)). All input variables out of \( S \) are set to their baseline values to represent the states of these variables not impacting the inference process, namely no-signal states of these variables. Thus, it is important to set suitable baseline values for these variables to represent their no-signal states in the computation of Shapley values, because we need to avoid bringing in additional noisy signals (i.e. outlier features) to ensure the trustworthiness. To this end, let us discuss existing studies of empirical settings for baseline values (see Table 1).

- **Mean baseline values.** The baseline value of each input variable is set to the mean value of this variable over all samples [11], i.e. \( b_i = \mathbb{E}_x [x_i] \). This method actually introduces additional information to the input. As Figure 7(right) shows, setting pixels to mean baseline values brings in massive additional gray dots to the image, rather than represent no-signal states.

- **Zero baseline values.** Baseline values of all input variables are set to zero [3, 45], i.e. \( \forall i \in N, b_i = 0 \). As Figure 7(right) shows, just like mean baseline values, zero baseline values also introduce additional information to the input. Note that because pixels in the input image are usually normalized to zero mean and a unit variance, the setting of zero baseline values is equivalent to the setting of mean baseline values in this case.

- **Blurring input samples.** Fong and Vedaldi [14] and Fong et al. [13] removed variables in the input image by blurring each input variable \( x_i (i \in S = N \setminus S) \) using a Gaussian kernel. These approaches can only remove high-frequency signals, but fails to remove low-frequency signals.
For each input variable, determining a different baseline value for this variable given each specific context $S$ (neighboring variables). Instead of fixing baseline values as constants, some studies use varying baseline values, which are determined temporarily by the context $S$ in a specific sample $x$, to compute $v(S|x)$ given $x$. Some methods \cite{15,9} define $v(S|x)$ by modeling the conditional distribution of variable values in $S = N \setminus S$ given the context $S$, i.e. $v(S|x) = E_x[p(x'|x_S)]f(x_S \cup x'_S)]$. However, these methods apply varying baseline values, rather than constant baseline values, which may destroy the linearity axiom and the nullity axiom of the Shapley value \cite{9}. Moreover, these methods compute a specific conditional distribution $p(x'|x_S)$ for each of $2^n$ contexts $S$ with a very high computational cost. In contrast, our method learns constant baseline values, which retain the four axioms of Shapley values.

Secondly, discussion on the out-of-distribution (OOD) samples. According to Equations (1) and (2), the Shapley value is computed on the masked samples $mask(x, S)$, which are actually out of the manifold of normal samples, i.e. OOD samples. The OOD problem is inherent in the computation of Shapley values. Previous solutions to the OOD problem are at the cost of violating the linearity axiom and the nullity axiom of Shapley values \cite{9}.

Nevertheless, our method can significantly alleviate the intrinsic OOD problem with the Shapley value, because we aim to learn the baseline values that best represent the no-signal states. To some extent, the main problem with OOD samples is to let the model generate abnormal features out of the manifold of normal features (i.e. generating abnormal interaction patterns, which will be introduced later). To this end, we learn the baseline values that generate the least interaction patterns. Thus, our method is more likely to eliminate existing interaction patterns, instead of triggering new abnormal patterns, to represent the no-signal state. From this perspective, our method generates fewer OOD interaction patterns in intermediate layers, thereby alleviating the OOD problem.

### 3.2 Multi-variate interactions and signal states of input variables

In this study, we propose the multi-variate interaction in game theory as the foundation of representing the full-signal state and the no-signal state of an input variable. In this way, we learn the baseline values that best describe the no-signal states of their corresponding input variables. Meanwhile, the setting of baseline values corresponding to no-signal states also alleviates the OOD problem.

**Multi-variate interactions.** Given a trained model and the input sample $x$ with $n$ variables $N = \{1, 2, \ldots, n\}$, we first define the multi-variate interaction of a set of input variables $S \subseteq N$. As aforementioned, let $v(S)$ denote the model output when only variables in $S$ are given, according to Equation (2). Then, $v(N) - v(\emptyset)$ represents the overall inference benefit owing to all input variables in $x$, w.r.t. the model output without given any variables. Thus, our goal is to design a metric for the interaction within each subset of input variables ($S \subseteq N$), $I(S)$, which ensures that the overall benefit $v(N) - v(\emptyset)$ can be decomposed into the sum of $I(S)$ of different subsets $\{S||S| \geq 2\}$.

$$v(N) - v(\emptyset) = \sum_{S \subseteq N, |S| \geq 2} I(S) + \sum_{i \in N} u_i, \quad u_i \overset{\text{def}}{=} v(\{i\}) - v(\emptyset) \quad (3)$$

$u_i$ denotes the marginal benefit from the $i$-th input variable without interactions. Here, $\cdot$ denotes the cardinality of the set.

In order to satisfy Equation (3), the interaction $I(S)$ is defined to measure the additional benefit from the collaboration of input variables in $S$, in comparison with the benefit when they work individually. Specifically, let $v(S) - v(\emptyset)$ denote the overall benefit from all variables in $S$, then we remove benefits of individual variables without collaborations, i.e. $\sum_{i \in S} u_i$, and further remove the marginal benefits owing to collaborations of all smaller subsets $L$ of variables in $S$, i.e. $\{L \subseteq S||L| \geq 2\}$. In this way, we obtain the following definition of the multi-variate interaction, and prove its closed-form

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**Table 1: Analysis about previous choices of baseline values.**

| Setting of baseline values | Baseline values are constant or not | Shortcomings |
|----------------------------|-----------------------------------|--------------|
| Zero \cite{13,15}         | ✓                                 | introduce additional information |
| Mean values \cite{11}     | ✓                                 | introduce additional information |
| Blurring \cite{14,14}     | ✓                                 | cannot remove low-frequency components |
| Marginalize (marginal distribution) \cite{25} | ✓ | assume feature independence and model linearity |
| Marginalize (conditional distribution) \cite{9,15} | ✓ | destroy the linearity and nullity axioms. |

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5
solution (proofs in the supplementary material), as follows.

$$I(S) \overset{\text{def}}{=} \frac{v(S) - v(\emptyset)}{\text{the benefit from all variables in } S} - \sum_{L \subseteq S, |L| \geq 2} I(L) - \sum_{i \in S} u_i \Rightarrow I(S) = \sum_{L \subseteq S} (-1)^{|S| - |L|} v(L)$$ \hspace{1cm} (4)

The above definition of $I(S)$ satisfies the linearity, nullity, symmetry, and efficiency axioms (please see the supplementary material for proofs).

To better understand the meaning of $I(S)$, let us consider the example when a model uses $y_{\text{head}} = \text{sigmoid}(x_{\text{eyes}} + x_{\text{nose}} + x_{\text{mouth}} + x_{\text{ears}} - \text{constant})$ to mimic the detector $y_{\text{head}} = x_{\text{eyes}}x_{\text{nose}}x_{\text{mouth}}x_{\text{ears}}$. In this case, the interaction $I(\{x_{\text{eyes}}, x_{\text{nose}}, x_{\text{mouth}}\})$ measures the marginal benefit when eyes, nose, and mouth collaborate with each other, where the benefits from smaller subsets (e.g., the interaction between eyes and nose) and the individual benefits (e.g., the individual benefit from nose) are removed. According to Equation (4), we have $I(\{x_{\text{eyes}}, x_{\text{nose}}, x_{\text{mouth}}\}) = v(\{x_{\text{eyes}}, x_{\text{nose}}, x_{\text{mouth}}\}) - v(\{x_{\text{eyes}}, x_{\text{nose}}\}) - v(\{x_{\text{eyes}}, x_{\text{mouth}}\}) - v(\{x_{\text{nose}}, x_{\text{mouth}}\}) + v(\{x_{\text{eyes}}\}) + v(\{x_{\text{nose}}\}) + v(\{x_{\text{mouth}}\}) - v(\emptyset)$. Furthermore, Figure 2 visualizes the distribution of contextual pixels $j$ that collaborate with a certain pixel $i$ (the green dot). The pixel value in the heatmap is computed as $p(j|i) = E_{S \ni \Omega}[1(j \in S)], \Omega = \{S||\Delta v_i(S)| \text{ is top-ranked in terms of all } S \subseteq N\}$, where $\Delta v_i(S)$ is defined in Equation (9).

**Number of signal states activated by an input variable.** In fact, we can consider each subset of input variables $S \subseteq N$ as an interaction pattern. If $I(S) > 0$, the collaboration between variables in $S$ has positive effects on model output. If $I(S) < 0$, the collaboration has negative effects. If $I(S) \approx 0$, the collaboration has no effects. According to Equation (3), we can consider the model output as the sum of $2^n - n - 1$ interaction patterns, i.e., $\sum_{S \subseteq N, |S| \geq 2} I(S)$. Some of them are salient patterns with significant influences on the model output (i.e., $|I(S)| \geq \tau$ is large), while others are noisy patterns (i.e., $|I(S)| < \tau$ is small), where $\tau$ is the threshold. In this way, we can consider the number of signal states triggered by an input variable $i$ as the number of salient patterns that contain the variable $i$, i.e., the presence/absence of the variable $i$ will activate/inactivate these salient patterns. The number of signal states provides us a new perspective to guide the learning of baseline values, although we do not need to set the $\tau$ value and count the actual signal states in practice.

**Connection to the Shapley value.** The Shapley value can be represented as the weighted sum of multi-variate interactions of input variables $\phi_i = \sum_{S \subseteq N \setminus \{i\}, S \neq \emptyset} \frac{1}{|S| + 1} I(S \cup \{i\}) + u_i$ (proof in the supplementary material).

**Connection to the Shapley interaction index.** The Shapley interaction index [16], denoted by $I_{\text{shapley}}(S)$, also measures the marginal benefit from variables in $S$, where benefits from all smaller subsets are removed.

$$I_{\text{shapley}}(S) \overset{\text{def}}{=} \sum_{T \subseteq N \setminus S} p(T) \sum_{L \subseteq S} (-1)^{|S| - |L|} v(L \cup T) = \sum_{T \subseteq N \setminus S} p(T) I(S|\text{env}(T))$$ \hspace{1cm} (5)

where $p(T) = \frac{(n-|S|-|T|)!|T|!}{(n-|S|+1)!}$. $I(S|\text{env}(T))$ denotes the specific interaction $I(S)$ when we set the presence of variables in $T$ as a constant environment that are not allowed to be masked. Essentially, $I(S)$ measures the interaction effects exclusively considering variables in $S$, while $I_{\text{shapley}}(S)$ is a weighted average of $I(S)$ when considering the distribution of outside variables $T \subseteq N \setminus S$.

### 3.3 Estimating baseline values to minimize the density of signal states

The computation of the Shapley value is conducted based on the assumption that baseline values represent the absence of input variables. In other words, when we set some variables to their baseline values, the number of salient patterns associated with these variables are supposed to decrease significantly, i.e. the baseline value should not trigger many interaction patterns (nonlinear relationships) between input variables. Otherwise, we may still consider the baseline value is informative enough to trigger massive patterns.

However, learning the optimal baseline values via the enumeration of all potential interaction patterns is NP-hard. Fortunately, the order of interaction patterns provides us a new perspective to solve this
problem. The order of the interaction patterns \( I(S) \) is defined as the cardinality of \( S \), i.e. the order \( m = |S| \). To this end, we obtain the following three propositions.

(1) Each interaction pattern \( I(S) \) represents an AND-relationship between all variables in \( S \). The absence of any variable (i.e. setting this variable to its baseline value) inactivates this pattern. Obviously, high-order interaction patterns depend on massive variables. Thus, high-order interaction patterns are more likely to be inactivated when some variables in the pattern are masked during the computation of Shapley values.

(2) According to Equation (3), the weighted sum of high-order interactions and low-order interactions is relatively stable as \( v(N) - v(\emptyset) \). Therefore, penalizing the influence of low-order interaction patterns will increase the influence of high-order interaction patterns, thereby pushing the model to mainly use high-order interaction patterns to represent the input sample \( x \).

(3) More crucially, theoretic analysis and preliminary experiments (see the supplementary material) have shown that incorrect baseline values make a model/function consisting of high-order interaction patterns be mistakenly explained as a mixture of low-order and high-order interaction patterns.

Based on the above three propositions, the objective of learning baseline values can be transformed to a loss function that penalizes the influence of low-order interactions. In this way, baseline values are learned to strengthen high-order interaction patterns, which boost the sparsity of salient patterns activated by baseline values. To this end, the influence of low-order interactions can be measured by both the following multi-order Shapley values and the multi-order marginal benefits.

**Multi-order Shapley values and marginal benefits.** We prove that the Shapley value, \( \phi_i \), can be decomposed into the following Shapley values of different orders (\( \phi_i = \frac{1}{n} \sum_{m=0}^{n-1} \phi_i^{(m)} \)), as well as the sum of marginal benefits of different orders (\( \Delta \phi_i = \frac{1}{n} \sum_{m=0}^{n-1} \sum_{|S| = m} \Delta \phi_i(S) \)), in which \( \phi_i^{(m)} \) and \( \Delta \phi_i(S) \) are given as follows (proofs in the supplementary material).

\[
\phi_i^{(m)} \overset{\text{def}}{=} \mathbb{E}_{S \subseteq \mathbb{N} \setminus \{i\}, |S| = m} [v(S \cup \{i\}) - v(S)] \Rightarrow \phi_i^{(m)} = \mathbb{E}_{S \subseteq \mathbb{N} \setminus \{i\}, |S| = m} \left[ \sum_{L \subseteq S, L \neq \emptyset} I(L \cup \{i\}) \right] + u_i
\]

\[
\Delta \phi_i(S) \overset{\text{def}}{=} v(S \cup \{i\}) - v(S) \Rightarrow \Delta \phi_i(S) = \sum_{L \subseteq S, L \neq \emptyset} I(L \cup \{i\}) + u_i
\]

The order of the marginal benefit \( \Delta \phi_i(S) \) is defined as the number of elements in \( S \) (i.e. if \( |S| = m \), the order of \( \Delta \phi_i(S) \) is \( m \)). For a low order \( m \), \( \phi_i^{(m)} \) denotes the attribution of the \( i \)-th input variable, when \( i \) cooperates with a few contextual pixels. For a high order \( m \), \( \phi_i^{(m)} \) corresponds to the impact of \( i \) when it collaborates with massive contextual variables. Similarly, the order of \( \Delta \phi_i(S) \) measures the marginal benefit of the \( i \)-th input variable to the model output with contexts composed of \( m = |S| \) variables.

In Equation (6), we have proven that high-order interaction patterns \( I(S) \) are only contained by high-order Shapley values \( \phi_i^{(m)} \) and high-order marginal benefits \( \Delta \phi_i(S) \). In this way, we propose the following two loss functions to penalize the strength of low-order Shapley values, \( |\phi_i^{(m)}| \), and the strength low-order marginal benefits, \( |\Delta \phi_i(S)| \), respectively, which can boost the influence of high-order interaction patterns according to Equation (3).

\[
L_{\text{Shapley}} = \sum_{m \sim \text{Unif}(0, \lambda)} \sum_{x \in \mathbb{X}} \sum_{i \in \mathbb{N}} |\phi_i^{(m)}|_i \quad L_{\text{marginal}} = \sum_{m \sim \text{Unif}(0, \lambda)} \sum_{x \in \mathbb{X}} \sum_{i \in \mathbb{N}} \mathbb{E}_{S \subseteq \mathbb{N} \setminus \{i\}, |S| = m} |\Delta \phi_i(S)| \quad (7)
\]

where \( \lambda \) denotes the maximum order to penalize. Figure 3 shows the distribution of the ratio of \( \sum_i |\phi_i^{(m)}| \) and the ratio of \( \sum_i \sum_{S \subseteq \mathbb{N} \setminus \{i\}, |S| = m} |\Delta \phi_i(S)| \) of different orders, which demonstrates that our methods effectively boost the influence of high-order interaction patterns.

Figure 3: Our methods successfully boost the influence of high-order Shapley values and high-order marginal benefits, and reduce the influence of low-order Shapley values and low-order marginal benefits, computed on a function in [47].
Figure 4: (Left) The learned baseline values on the MNIST dataset (better viewed in color). (Right) Shapley values produced with different baseline values on the MNIST dataset.

Figure 5: The learned baseline values (left) and Shapley values computed with different baseline values (right) on the UCI Census Income dataset. Results on the UCI South German Credit dataset are shown in the supplementary material.

4 Experiments

Learning baseline values. We used our method to learn baseline values for MLPs and LeNet [26] trained on the UCI South German Credit dataset [4], the UCI Census Income dataset [4], and the MNIST dataset [26], respectively. Based on the UCI datasets, we learned MLPs following settings in [18]. We learned baseline values using either $L_{\text{Shapley}}$ or $L_{\text{marginal}}$ as the loss function. In the computation of $L_{\text{Shapley}}$, we set $v(S) = \log \frac{p(y^{(n)}|\text{mask}(x,S))}{1-p(y^{(n)}|\text{mask}(x,S))}$. In the computation of $L_{\text{marginal}}$, $|\Delta v_i(S)|$ was set to $|\Delta v_i(S)| = \|h(\text{mask}(x,S \cup \{i\}) - h(\text{mask}(x,S))\|_1$, where $h(\text{mask}(x,S))$ denoted the output feature of the second last layer given the masked input $\text{mask}(x,S)$, in order to boost the efficiency of learning. Please see the supplementary material for other potential settings of $v(S)$. We used two ways to initialize baseline values before the learning in experiments, i.e. setting to zero [3,45] or the mean values over different samples [11], namely zero-init and mean-init, respectively. We set $\lambda = 0.2n$ for the MNIST dataset, and $\lambda = 0.5n$ for the simpler data in two UCI datasets. We compared our methods with five previous choices of baseline values introduced in Section 5.4, i.e. zero baseline values [3], mean baseline values [11], blurring images [14,43], and two implementations of varying baseline values (SHAP [28] and SAGE [9]). Zero baseline values, mean baseline values, blurring images, and our learned baseline values allowed us to compute the Shapley value using the sampling-based approximation [7], which ensured the unbiased estimation of Shapley values. For SHAP and SAGE, we used the code released by [28] and [9].

Figure 4(left) shows the learned baseline values on the MNIST dataset. Figure 4(right) compares the computed Shapley values with different choices of baseline values. Compared to zero baseline values, our learned baseline values removed noisy variables on the background, and generated more sparse Shapley values. Compared to mean baseline values and blurring the image, our method yielded more balanced attributions among important variables. Unlike SHAP and SAGE, our settings satisfied the linearity axiom and the nullity axiom. Figure 5 shows the learned baseline values and the computed Shapley values on the UCI Census Income dataset. Unlike our methods, attributions generated by the zero/mean baseline values conflicted with results of all other methods.

Verification on synthetic functions. We usually cannot determine the ground truth of baseline values for real images, such as the MNIST dataset. In order to verify the correctness of the learned baseline values, we conducted experiments on synthetic functions with ground-truth baseline values. We randomly generated 100 functions whose interaction patterns and ground truth of baseline values could be easily determined. This dataset will be released after the paper acceptance. The generated functions

\begin{align*}
\text{Baseline values} = \begin{cases}
\text{Mean} & \text{for MNIST}, \\
\text{Zero} & \text{for UCI},
\end{cases}
\end{align*}

\begin{align*}
\Delta v_i(S) = \|h(\text{mask}(x,S \cup \{i\}) - h(\text{mask}(x,S))\|_1,
\end{align*}
The ground truth of baseline values

Table 2: Examples of generated functions and their ground-truth baseline values.

| Functions ($\forall i \in N, x_i \in [0, 1]$) | The ground truth of baseline values | $b_i^*$  |
|-----------------------------------------------|-------------------------------------|---------|
| $-0.18x_1(x_2 + x_3)^3 + 4x_2x_3x_4$ | $b_i^* = 0$ for $i \in \{1, 2, 3, 4, 6, 7\}$ | $0.43$  |
| $-\text{sigmoid}(4x_1 - 4x_2 - 4x_3 + 2000)$ | $b_i^* = 1$ for $i \in \{1, 2, 3\}$, $b_i^* = 0$ for $i \in \{4, 5, 6, 7, 8, 9\}$ | $0.34$  |
| $-x_1x_2x_3 + \text{sigmoid}(5x_4x_5x_6 + 2.50) - x_2x_3$ | $b_i^* = 1$ for $i \in \{4, 5, 6, 7\}$, $b_i^* = 0$ for $i \in \{1, 2, 3, 8, 9\}$ | $0.11$  |
| $-\text{sigmoid}(-5x_1 + 5x_2x_3 + 2.50) - x_1x_3$ | $b_i^* = 1$ for $i \in \{2, 3\}$, $b_i^* = 0$ for $i \in \{1, 4, 5, 6, 7, 8, 9\}$ | $0.09$  |
| $-\text{sigmoid}(-x_1 + x_2 - x_3 - 0.00) - x_1x_2x_3x_7 - x_1x_4x_5$ | $b_i^* = 1$ for $i = 2, b_i^* = 0$ for $i \in \{1, 3, 4, 5, 6, 7, 8, 9, 10\}$ | $0.10$  |

Table 3: Accuracy of learned baseline values.

| Synthetic functions | Shapley | $\|x^{\text{adv}} - x\|_2$ | $\|b - x\|_2$ | Marginal |
|---------------------|---------|-----------------|---------------|----------|
| Initialize with 0   | 98.06%  | 9.870%          | 9.870%        | 9.870%   |
| Initialize with 0.5 | 88.52%  | 91.80%          | 90.16%        | 9.870%   |
| Initialize with 1   | 98.06%  | 91.80%          | 90.16%        | 9.870%   |

Table 4: The learned baseline values successfully recovered original samples from adversarial samples, demonstrating the effectiveness of our methods.

were composed of addition, subtraction, multiplication, exponentiation, and the sigmoid operations (see Table 2). For example, for the function $y = \text{sigmoid}(3x_1x_2 - 3x_3 - 1.5) - x_1x_3 + 0.25(x_6 + x_7)^2$, $x_i \in (0, 1)$, there were three salient interaction patterns (i.e., $\{x_1, x_2, x_3\}, \{x_4, x_5\}, \{x_6, x_7\}$), which were activated only when $x_i = 1$ for $i \in \{1, 2, 4, 5, 6, 7\}$ and $x_3 = 0$. In this case, the ground truth of baseline values should be $b_i^* = 0$ for $i \in \{1, 2, 4, 5, 6, 7\}$ and $b_3^* = 1$. Please see the supplementary material for more discussions about the setting of ground-truth baseline values. We used our methods to learn baseline values on these functions and tested the accuracy. Note that $|b_i - b_i^*| \leq 0.1$, if $|b_i - b_i^*| < 0.5$, we consider the learned baseline value correct; otherwise incorrect. We set $\lambda = 0.5\delta$ in both Shapley and $L_{\text{marginal}}$. Experimental results are reported in Table 3 and are discussed later.

Verification on functions in [47]. Besides, we also evaluated the correctness of the learned baseline values using functions proposed in [47]. Among all the 92 input variables in these functions, the ground truth of 61 variables could be determined (see the supplementary material). Thus, we used these annotated baseline values to test the accuracy on these functions.

Table 3 reports the accuracy of the learned baseline values on above functions. In most cases, the accuracy was above 90%, showing that our method could effectively learn correct baseline values. A few functions in [47] did not have salient interaction patterns, which caused errors in the estimation of baseline values.

Verification on adversarial examples. We further verified the correctness of the learned baseline values on adversarial examples. Let $x$ denote the normal sample, and let $x^{\text{adv}} = x + \delta$ denote the adversarial example generated by [30]. According to [24], the adversarial example $x^{\text{adv}}$ mainly created out-of-distribution bivariate interactions with high-order contexts, which were actually related to the high-order interactions in this paper.

Thus, in the scenario of this study, the adversarial utility was owing to out-of-distribution high-order interactions. The removal of input variables was supposed to remove most high-order interactions. Therefore, the baseline value can be considered as the recovery of the original sample. In this way, we used the adversarial example $x^{\text{adv}}$ to initialize baseline values before learning, and used $L_{\text{marginal}}$ to learn baseline values. If the learned baseline values $b$ satisfy $\|b - x\|_1 \leq \|x^{\text{adv}} - x\|_1$, we considered that our method successfully recovered the original sample to some extent. We conducted experiments using LeNet [26], AlexNet [24], and ResNet-20 [19] on the MNIST dataset [26] ($\|\delta\|_{\infty} \leq 32/255$) and the CIFAR-10 dataset [23] ($\|\delta\|_{\infty} \leq 8/255$). Table 3 shows that our method recovered adversarial examples to original samples, which demonstrated the effectiveness of our method.

5 Conclusions

In this paper, we have formulated optimal baseline values in game theory. We have innovatively defined the signal state of input variables based on the multi-variate interaction patterns of the model. Then, we have proposed an approximate-yet-efficient method to learn optimal baseline values that represent no-signal states of input variables. Experimental results have demonstrated the effectiveness of our method.
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A Extended discussions about multi-variate interactions

In Section 3.2 of the paper, we define the multi-variate interaction and claim that it satisfies four axioms. In the supplementary material, this section provides extended discussions about the multi-variate interaction, and provides proofs of its axioms.

Given a trained model and the input sample $x$ with $n$ variables $N = \{1, 2, \ldots, n\}$, the multi-variate interaction is defined to measure the benefit from a set of input variables $S \subseteq N$. Let $v(S)$ denote the model output when only variables in $S$ are given. Then, $v(N) - v(\emptyset)$ represents the overall inference benefit owing to all input variables in $x$, w.r.t. the model output without given any variables. The multi-variate interaction $I(S)$ within each subset of input variables ($S \subseteq N$) is supposed to ensure that the overall benefit $v(N) - v(\emptyset)$ can be decomposed into the sum of $I(S)$ of different subsets $\{S| |S| \geq 2\}$.

\[ v(N) - v(\emptyset) = \sum_{S \subseteq N, |S| \geq 2} I(S) + \sum_{i \in N} u_i, \quad u_i \overset{\text{def}}{=} v(\{i\}) - v(\emptyset) \tag{8} \]

$u_i$ denotes the marginal benefit from the $i$-th input variable without interactions. Here, $|\cdot|$ denotes the cardinality of the set.

In order to satisfy Equation (8), the interaction $I(S)$ is defined to measure the additional benefit from the collaboration of input variables in $S$, in comparison with the benefit when they work individually. Specifically, let $v(S) - v(\emptyset)$ denote the overall benefit from all variables in $S$, then we remove benefits of individual variables without collaborations, i.e. $\sum_{i \in S} u_i$, and further remove the marginal benefits owing to collaborations of all smaller subsets $L$ of variables in $S$, i.e. $\{L \subseteq S| |L| \geq 2\}$. In this way, we obtain the following definition of the multi-variate interaction.

\[ I(S) \overset{\text{def}}{=} \frac{v(S) - v(\emptyset)}{\text{the benefit from all variables in } S} - \sum_{L \subseteq S, |L| \geq 2} I(L) - \sum_{i \in S} u_i \tag{9} \]

A.1 Proof of the closed-form solution

We have proven that the closed-form solution to Equation (9) is the following equation.

\[ I(S) = \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L) \]

**Proof:**

Here, let $s = |S|$, $l = |L|$, and $s' = |S'|$ for simplicity. If $s = 2$, then

\[
I(S) = v(S) - v(\emptyset) - \sum_{L \subseteq S, l \geq 2} I(L) - \sum_{i \in S} v(\{i\}) \\
= v(S) - v(\emptyset) - \sum_{i \in S} v(\{i\}) \\
= v(S) - \sum_{i \in S} [v(\{i\}) - v(\emptyset)] \\
= v(S) - \sum_{i \in S} v(\{i\}) + v(\emptyset) \\
= \sum_{L \subseteq S} (-1)^{s-l} v(L)
\]
Let us assume that \( 2 \leq s' < s \), \( I(S') = \sum_{L \subseteq S'} (-1)^{s'-l}v(L) \). Then, we use the mathematical induction to prove \( I(S) = \sum_{L \subseteq S} (-1)^{s'-l}v(L) \), where \( S' \subseteq S \).

\[
I(S = S' \cup \{i\}) = v(S' \cup \{i\}) - \sum_{I \subseteq S'} \frac{I(L) - \sum_{j \in S' \cup \{i\}} v(\{j\})}{I(\emptyset) - \sum_{j \in S' \cup \{i\}} v(\{j\})} \quad \% \text{Let } S = S' \cup \{i\}
\]

\[
= v(S' \cup \{i\}) - v(\emptyset) - \sum_{I \subseteq S'} \frac{\sum_{j \in S' \cup \{i\}} (-1)^{t'k}v(K) - \sum_{j \in S' \cup \{i\}} v(\{j\})}{I(\emptyset) - \sum_{j \in S' \cup \{i\}} v(\{j\})} \quad \% \text{Let } T = L \setminus K
\]

\[
= v(S' \cup \{i\}) - v(\emptyset) - \left[ \sum_{t=2}^{s'+1} C_{s' + 1}^t (-1)^t v(\emptyset) + \sum_{t=1}^{s'-1} C_{s'}^t (-1)^t v(\{j\}) \right] + \sum_{K \subseteq S'} \frac{\sum_{t \geq 2} C_{s'+1-k}^t (-1)^t v(K)}{I(\emptyset) - \sum_{j \in S' \cup \{i\}} v(\{j\})} \quad \% \text{Let } T = L \setminus K
\]

\[
= v(S' \cup \{i\}) - v(\emptyset) - (s' - (1 - (-1)^{s'+1})v(\emptyset) + \sum_{j \in S' \cup \{i\}} (1 + (-1)^{s'}) v(\{j\})
\]

\[
+ \sum_{K \subseteq S'} \frac{(-1)^{s'+1-k}v(K)}{I(\emptyset) - \sum_{j \in S' \cup \{i\}} v(\{j\})} - \sum_{j \in S' \cup \{i\}} v(\{j\})
\]

\[
= v(S' \cup \{i\}) + \sum_{j \in S' \cup \{i\}} (-1)^{s'} v(\{j\}) + (-1)^{s'+1}v(\emptyset) + \sum_{K \subseteq S'} (-1)^{s'+1-k}v(K)
\]

\[
= \sum_{K \subseteq S'} (-1)^{s'+1-k}v(K) = \sum_{K \subseteq S} (-1)^{s'-k}v(K)
\]

In this way, Equation [10] is proven as the closed-form solution to the definition of the multi-variate interaction \( I(S) \) in Equation (9).

### A.2 Proof of axioms of the multi-variate interaction

In Line 222, Section 3.2 of the paper, we claim that the proposed multi-variate interaction satisfies the **linearity**, **nullity**, **symmetry**, and **efficiency** properties (axioms). In this section of the supplementary material, we provide proofs for these properties.

1. **Linearity property (axiom):** If we merge outputs of two models, \( u(S) = w(S) + v(S) \), then, \( \forall S \subseteq N \), the interaction \( I_u(S) \) w.r.t. the new output \( u \) can be decomposed into \( I_u(S) = I_w(S) + I_v(S) \).

   \[ I_u(S) = \sum_{L \subseteq S} (-1)^{|S|-|L|}u(L) = \sum_{L \subseteq S} (-1)^{|S|-|L|}[w(S) + v(S)] = \sum_{L \subseteq S} (-1)^{|S|-|L|}w(L) + \sum_{L \subseteq S} (-1)^{|S|-|L|}v(L) = I_w(S) + I_v(S) \]

2. **Nullity property:** The dummy variable \( i \in N \) satisfies \( \forall S \subseteq N \setminus \{i\}, v(S \cup \{i\}) = v(S) + v(\{i\}) \). It means that the variable \( i \) has no interactions with other variables, i.e. \( \forall S \subseteq N \setminus \{i\}, I(S \cup \{i\}) = 0 \).
• **Proof:**

\[
I(S \cup \{i\}) = \sum_{L \subseteq S \cup \{i\}} (-1)^{|S|+1-|L|} v(L)
\]

\[
= \sum_{L \subseteq S} (-1)^{|S|+1-|L|} v(L) + \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L \cup \{i\})
\]

\[
= \sum_{L \subseteq S} (-1)^{|S|+1-|L|} v(L) + \sum_{L \subseteq S} (-1)^{|S|-|L|} [v(L) + v(\{i\})]
\]

\[
= \sum_{L \subseteq S} (-1)^{|S|+1-|L|} [-v(L) + v(L)] + \sum_{L \subseteq S} (-1)^{|S|-|L|} v(\{i\})
\]

\[
= \left(\sum_{L \subseteq S} (-1)^{|S|-|L|}\right) v(\{i\})
\]

\[
= 0
\]

(3) **Symmetry property:** If input variables \(i, j \in N\) have same cooperations with other variables \(\forall S \subseteq N \setminus \{i, j\}, v(S \cup \{i\}) = v(S \cup \{j\})\), then they have same interactions with other variables, \(\forall S \subseteq N \setminus \{i, j\}, I(S \cup \{i\}) = I(S \cup \{j\})\).

• **Proof:**

\[
I(S \cup \{i\}) = \sum_{L \subseteq S \cup \{i\}} (-1)^{|S|-|L|} v(L)
\]

\[
= \sum_{L \subseteq S} (-1)^{|S|+1-|L|} v(L) + \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L \cup \{i\})
\]

\[
= \sum_{L \subseteq S} (-1)^{|S|+1-|L|} v(L) + \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L \cup \{j\})
\]

\[
= \sum_{L \subseteq S \cup \{j\}} (-1)^{|S|-|L|} v(L)
\]

\[
= I(S \cup \{j\})
\]

(4) **Efficiency property:** The output of a model can be decomposed into interactions of different subsets of variables, \(v(N) = v(\emptyset) + \sum_{i \in N} u_i + \sum_{S \subseteq N, |S| \geq 2} I(S)\), where \(u_i \overset{\text{def}}{=} v(\{i\}) - v(\emptyset)\)

• **Proof:**

\[
\text{right} = v(\emptyset) + \sum_{i \in N} u_i + \sum_{S \subseteq N, |S| \geq 2} I(S)
\]

\[
= v(\emptyset) + \sum_{i \in N} [v(\{i\}) - v(\emptyset)] + \sum_{S \subseteq N, |S| \geq 2} \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L)
\]

\[
= \sum_{S \subseteq N} \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L)
\]

\[
= \sum_{L \subseteq N} \sum_{K \subseteq N \setminus L} (-1)^{|K|} v(L) \quad \% \text{Let } K = S \setminus L
\]

\[
= \sum_{L \subseteq N} \left[ \sum_{|K|=0}^{n-|L|} C_{n-|L|}^{|K|} (-1)^{|K|} \right] v(L)
\]

\[
= v(N) = \text{left}
\]

A.3 **Proof of the connection to Shapley values**

In Lines 246-248, Section 3.2 of the paper, we claim that the proposed multi-variate interaction has a close connection with the Shapley value. In this section of the supplementary material, we provide
Proofs for such connection.

\[ \phi_i = \sum_{S \subseteq N \setminus \{i\}, S \neq \emptyset} \frac{1}{|S| + 1} I(S \cup \{i\}) + u_i \]  

*Proof*:

\[
\begin{align*}
\text{right} &= \sum_{S \subseteq N \setminus \{i\}, S \neq \emptyset} \frac{1}{|S| + 1} I(S \cup \{i\}) + u_i \\
&= \sum_{S \subseteq N \setminus \{i\}, S \neq \emptyset} \frac{1}{|S| + 1} \left[ \sum_{L \subseteq S} (-1)^{|S|+1-|L|} v(L) + \sum_{L \subseteq S} (-1)^{|S|-|L|} v(L \cup \{i\}) \right] + u_i \\
&= \sum_{S \subseteq N \setminus \{i\}, S \neq \emptyset} \frac{1}{|S| + 1} \sum_{L \subseteq S} (-1)^{|S|-|L|} [v(L \cup \{i\}) - v(L)] + u_i \\
&= \sum_{L \subseteq N \setminus \{i\}} \sum_{K \subseteq N \setminus L \setminus \{i\}} (-1)^{|K|} \frac{1}{|K| + |L| + 1} [v(L \cup \{i\}) - v(L)] \quad \% \text{Let } K = S \setminus L \\
&= \sum_{L \subseteq N \setminus \{i\}} \left( \sum_{k=0}^{n-1-|L|} (-1)^k \frac{k!}{k+|L|+1} \binom{n-1-|L|}{k} \right) [v(L \cup \{i\}) - v(L)] \quad \% \text{Let } k = |K| \\
&= \sum_{L \subseteq N \setminus \{i\}} \frac{|L|!(n-1-|L|)!}{n!} [v(L \cup \{i\}) - v(L)] \\
&= \phi_i = \text{left}
\end{align*}
\]

**B Multi-order Shapley values and marginal benefits**

In Section 3.3 of the paper, we claim that the Shapley value \( \phi_i \) can be decomposed into the sum of Shapley values of different orders \( \phi^{(m)}_i \), and the sum of marginal benefits of different orders \( \Delta v_i(S) \). Furthermore, the multi-order Shapley values and marginal benefits can be re-written as the sum of multi-variate interactions. In the supplementary material, this section provides proofs for above claims.

First, we have proven the following decomposition of the Shapley value.

\[
\phi_i = \frac{1}{n} \sum_{m=0}^{n-1} \phi^{(m)}_i = \frac{1}{n} \sum_{m=0}^{n-1} E_{S \subseteq N \setminus \{i\}, |S| = m} \Delta v_i(S) \tag{11}
\]

where the Shapley value of \( m \)-order \( \phi^{(m)}_i \) def \( E_{S \subseteq N \setminus \{i\}, |S| = m} [v(S \cup \{i\}) - v(S)] \), and the marginal benefit \( \Delta v_i(S) = v(S \cup \{i\}) - v(S) \).
**Proof:**

\[
\phi_i = \sum_{S \subseteq N} \frac{|S|!(n - 1 - |S|!)}{n!} [v(S \cup \{i\}) - v(S)]
\]

\[
= \sum_{m=0}^{n-1} \sum_{S \subseteq N, |S|=m} \frac{|S|!(n - 1 - |S|!)}{n!} [v(S \cup \{i\}) - v(S)]
\]

\[
= \frac{1}{n} \sum_{m=0}^{n-1} \sum_{S \subseteq N, |S|=m} \frac{|S|!(n - 1 - |S|!)}{(n-1)!} [v(S \cup \{i\}) - v(S)]
\]

\[
= \frac{1}{n} \sum_{m=0}^{n-1} \mathbb{E}_{S \subseteq N, |S|=m} [v(S \cup \{i\}) - v(S)]
\]

\[
= \frac{1}{n} \sum_{m=0}^{n-1} \phi_i^{(m)}
\]

\[
= \frac{1}{n} \sum_{m=0}^{n-1} \mathbb{E}_{S \subseteq N \setminus \{i\}, |S|=m} \Delta v_i(S)
\]

**Connection between multi-variate interactions and multi-order marginal benefits.** Equation (6) in the main paper shows that the \(m\)-order marginal benefit can be decomposed as the sum of multi-variate interactions. In the supplementary material, this section provides the proof for such decomposition.

\[
\Delta v_i(S) = \sum_{L \subseteq S, L \neq \emptyset} I(L \cup \{i\}) + u_i
\]  

**Proof:**

\[
\text{right} = \sum_{L \subseteq S, L \neq \emptyset} I(L \cup \{i\}) + u_i
\]

\[
= \sum_{L \subseteq S, L \neq \emptyset} \left[ \sum_{K \subseteq L} (-1)^{|L|-|K|} v(K) + \sum_{K \subseteq L} (-1)^{|L|-|K|} v(K \cup \{i\}) \right] + u_i
\]

\[
= \sum_{L \subseteq S, L \neq \emptyset} \sum_{K \subseteq L} (-1)^{|L|-|K|} [v(K \cup \{i\}) - v(K)] + u_i
\]

\[
= \sum_{L \subseteq S} \sum_{K \subseteq L} (-1)^{|L|-|K|} \Delta v_i(K)
\]

\[
= \sum_{K \subseteq S} \sum_{P \subseteq S \setminus K} (-1)^{|P|} \Delta v_i(K) \quad \% \text{Let } P = L \setminus K
\]

\[
= \sum_{K \subseteq S} \sum_{p=0}^{[S]-|K|} (-1)^p C_{[S]-|K|}^p \Delta v_i(K) \quad \% \text{Let } p = |P|
\]

\[
= \sum_{K \subseteq S} 0 \cdot \Delta v_i(K) + \sum_{K \subseteq S} \sum_{p=0}^{[S]-|K|} (-1)^p C_{[S]-|K|}^p \Delta v_i(K)
\]

\[
= \Delta v_i(S) = \text{left}
\]

**Connection between multi-variate interactions and multi-order Shapley values.** Similarly, Equation (6) in the main paper also shows that the \(m\)-order Shapley value can also be decomposed as the sum of multi-variate interactions. In the supplementary material, this section provides
Using \((zero\text{-init})\)
Using \((mean\text{-init})\)
Using \((zero\text{-init})\)
Using \((mean\text{-init})\)

Baseline values learned by our methods

Figure 6: The learned baseline values on the UCI South German Credit dataset.

the proof for such decomposition.

\[
\phi_i^{(m)} = E_{S \subseteq N \mid |S| = m} \left[ \sum_{L \subseteq S, L \neq \emptyset} I(L \cup \{i\}) \right] + u_i \tag{13}
\]

• Proof:

\[
\phi_i^{(m)} = E_{S \subseteq N, |S| = m} \Delta v_i(S) \\
= E_{S \subseteq N, |S| = m} \left[ \sum_{L \subseteq S, L \neq \emptyset} I(L \cup \{i\}) + u_i \right] \\
= E_{S \subseteq N, |S| = m} \left[ \sum_{L \subseteq S, L \neq \emptyset} I(L \cup \{i\}) \right] + u_i
\]

C  More experimental results

This section provides more experimental results for experiments in Section 4 of the paper.

Other potential settings of \(v(S)\). In the computation of Shapley values, people usually use different settings of \(v(S)\), although the settings of \(v(S)\) do not affect the applicability of our method. Our method of formulating baseline values is applicable to various settings of \(v(S)\). Lundberg and Lee \[28\] directly set \(v(S) = p(y|\text{mask}(x, S))\). Covert et al. \[9\] used the cross-entropy loss as \(v(S)\). In this paper, we use \(v(S) = log \frac{p(y|\text{mask}(x, S))}{1-p(y|\text{mask}(x, S))}\) in \(L_{\text{Shapley}}\). Besides, we use \(|\Delta v_i(S)| = \|h(\text{mask}(x, S \cup \{i\}) - h(\text{mask}(x, S))\|_1\) in \(L_{\text{marginal}}\) on the MNIST dataset to boost the optimization efficiency, where \(h(\text{mask}(x, S))\) denotes the intermediate-layer feature. It is because \(h(\text{mask}(x, S \cup \{i\})\) makes the optimization of \(L_{\text{marginal}}\) receive gradients from all dimensions of the feature.

Experimental results on the UCI South German Credit dataset. This section provides experimental results on the UCI South German Credit dataset \[4\]. Figure 6 shows the learned baseline values by our method, and Figure 7 compares Shapley values computed using different baseline values. Just like results on the UCI Census Income dataset, attributions (Shapley values) generated by our learned baseline values are similar to results of SHAP and SAGE. However, the zero/mean baseline values usually generated conflicting results with all other methods.

Discussion about the setting of ground-truth baseline values. This section discusses the ground truth of baseline values of synthetic functions in Section 4 of the paper. In order to verify the correctness of the learned baseline values, we conducted experiments on synthetic functions with ground-truth baseline values. We randomly generated 100 functions whose interaction patterns and ground truth of baseline values could be easily determined. As Table 5 shows, the generated functions were composed of addition, subtraction, multiplication, exponentiation, and sigmoid operations.
The ground truth of baseline values in these functions was determined based on interaction patterns between input variables. In order to represent no-sign states of variables, baseline values should activate as few interaction patterns as possible, where activation states of interaction patterns were considered as the most infrequent state. Thus, we first identified the activation states of interaction patterns, and the ground-truth of baseline values were set as values that inactivated interaction patterns under different masks. We took the following examples to discuss the setting of ground-truth baseline values (in the following examples, $\forall i \in N, x_i \in \{0, 1\}$ and $b^*_i \in \{0, 1\}$).

- $f(x) = x_1 x_2 x_3 + \text{sigmoid}(x_4 + x_5 - 0.5) \cdots$. Let us just focus on the term of $x_1 x_2 x_3$ in $f(x)$. The activation state of this interaction pattern is $x_1 x_2 x_3 = 1$ when $\forall i \in \{1, 2, 3\}, x_i = 1$. In order to inactivate the interaction pattern, we set $\forall i \in \{1, 2, 3\}, b^*_i = 0$.
- $f(x) = -x_1 x_2 x_3 + (x_4 + x_5)^3 \cdots$. Let us just focus on the term of $-x_1 x_2 x_3$ in $f(x)$. The activation state of this interaction pattern is $-x_1 x_2 x_3 = -1$ when $\forall i \in \{1, 2, 3\}, x_i = 1$. In order to inactivate the interaction pattern, we set $\forall i \in \{1, 2, 3\}, b^*_i = 0$.
- $f(x) = (x_1 + x_2 - x_3)^3 \cdots$. Let us just focus on the term of $(x_1 + x_2 - x_3)^3$ in $f(x)$. The activation state of this interaction pattern is $(x_1 + x_2 - x_3)^3 = 8$ when $x_1 = x_2 = x_3 = 1$. In order to inactivate the interaction pattern under different masks, we set $b^*_1 = b^*_2 = 0, b^*_3 = 1$.
- $f(x) = \text{sigmoid}(3x_1 x_2 - 3x_3 - 1.5) \cdots$. Let us just focus on the term of $\text{sigmoid}(3x_1 x_2 - 3x_3 - 1.5)$ in $f(x)$. In this case, $x_1, x_2, x_3$ form a salient interaction pattern because $\text{sigmoid}(3x_1 x_2 - 3x_3 - 1.5) > 0.5$ only if $x_1 = x_2 = 1$ and $x_3 = 0$. Thus, in order to inactivate interaction patterns, ground-truth baseline values are set to $b^*_1 = b^*_2 = 0, b^*_3 = 1$.

**Ground-truth baseline values of functions in [47]**. This section provides more details about ground-truth baseline values of functions proposed in [47]. We evaluated the correctness of the learned baseline values using functions proposed in [47]. Among all the 92 input variables in these functions, the ground truth of 61 variables could be determined and are reported in Table 6.
that some variables cannot be 0 or 1 (e.g., $x_8$ cannot be zero in the first function), and we set $\forall i \in N, x_i \notin \{0.001, 0.999\}$ for variables in these functions instead. Similarly, we set the ground truth of baseline values $\forall i \in N, b_i^* \notin \{0.001, 0.999\}$. Some variables did not collaborate/interact with other variables (e.g., $x_4$ in the first function), thereby having no interaction patterns. We did not assign ground-truth baseline values for these individual variables, and these variables are not used for evaluation. Some variables formed more than one interaction pattern with other variables, and had different ground-truth baseline values with different patterns. In this case, the collaboration between input variables was complex and hard to analyze, so we did not consider such input variables with conflicting patterns for evaluation, either.

**Discussion about effects of incorrect baseline values.** This section proves that the setting of incorrect baseline values makes a model/function consisting of high-order interaction patterns be mistakenly explained as a mixture of low-order and high-order interaction patterns. This is mentioned in Section 3.3 of the paper. To show this phenomenon, we compare interaction patterns computed using ground-truth baseline values and incorrect baseline values in Table 7 and the results verify our conclusion. We find that when models/functions contain complex collaborations between multiple variables (i.e., high-order interaction patterns), incorrect baseline values usually generate fewer high-order interaction patterns and more low-order interaction patterns than ground-truth baseline values. In comparison, ground-truth baseline values lead to sparse and high-order salient patterns, which demonstrates that these baseline values represent no-signal states of input variables.

We can understand effects of incorrect baseline values as follows. When we use ground-truth baseline values, the absence of any variable will inactivate the interaction pattern. However, when we use incorrect baseline values, replacing an input variable $i$ with its baseline value cannot completely inactivate the pattern. In other words, the variable $i$ still provides meaningful signals to the output, which damages the trustworthiness of computed interactions and Shapley values.

**Discussion about the verification on adversarial examples.** In Section 4 of the main paper, we discuss the correctness of the learned baseline values on adversarial examples. This section provides more discussions about the verification on adversarial examples.

Let $x$ denote the normal sample, and let $x^{adv} = x + \delta$ denote the adversarial example generated by adversarial attacks [40]. A previous study [34] defined the bivariate interaction with different contextual complexities, and found that adversarial attacks mainly created out-of-distribution bivariate interactions with large contexts. In the scenario of this study, we can consider such sensitive interaction with large contexts related to high-order multi-variate interaction patterns. It is because the bivariate interaction between $(i, j)$ with large contexts (i.e., under many contextual variables $S$) actually considers collaborations between $i, j$ and contextual variables in $S$. Thus, it also partially reflects $I(S \cup \{i, j\})$, which is defined in this paper.

Therefore, from the perspective of multi-variate interaction patterns, the adversarial utility can be considered as introducing out-of-distribution high-order interaction patterns in the model. To this end, setting input variables to baseline values is supposed to remove related interaction patterns to represent no-signal states. Particularly, if we set all input variables to their baseline values, many interaction patterns will be eliminated. Thus, if we initialize baseline values as the adversarial example, and optimize baseline values using our method, the learned baseline values are supposed to remove OOD high-order interaction patterns in the adversarial example, and recover the original sample.
Table 7: Comparison between ground-truth baseline values and incorrect baseline values. The last column shows ratios of individual benefits of input variables $r_1 = \frac{\sum_{i \in N} |u_i|}{\sum_{S \subseteq N, \left| S \right| = 1} |f(S)|}$ and ratios of multi-variate interaction patterns of different orders $r_m = \frac{\sum_{i \in N} |u_i| \sum_{S \subseteq N, \left| S \right| \geq 2} |f(S)|}{\sum_{S \subseteq N, \left| S \right| \geq 2} |f(S)|}$. We consider interactions of input samples that activate interaction patterns. We find that when models/functions contain complex collaborations between multiple variables (i.e. high-order interaction patterns), incorrect baseline values usually generate fewer high-order interaction patterns and more low-order interaction patterns than ground-truth baseline values. In comparison, ground-truth baseline values lead to sparse and high-order salient patterns, which demonstrates that these baseline values represent no-signal states of input variables.

| Functions ($y_t \in N, i \in \{0, 1\}$) | Baseline values $b$ | Ratios $r$ |
|----------------------------------------|----------------------|------------|
| $f(x) = x_1x_2x_3x_4x_5$ $x = [1, 1, 1, 1, 1]$ | ground truth: $b^* = [0, 0, 0, 0, 0]$ | $r_1$ $r_m$ |
|                                                                  | incorrect: $b^{(1)} = [0.5, 0.5, 0.5, 0.5, 0.5]$ |            |
|                                                                  | incorrect: $b^{(2)} = [0.1, 0.2, 0.6, 0.0, 0.1]$ |            |
|                                                                  | incorrect: $b^{(3)} = [0.7, 0.1, 0.3, 0.5, 0.1]$ |            |
| $f(x) = \text{sigmoid}(5x_1x_2x_3 + 5x_4 - 7.5)$ $x = [1, 1, 1, 1]$ | ground truth: $b^* = [0, 0, 0, 0]$ | $r_1$ $r_m$ |
|                                                                  | incorrect: $b^{(1)} = [0.5, 0.5, 0.5, 0.5]$ |            |
|                                                                  | incorrect: $b^{(2)} = [0.6, 0.4, 0.7, 0.3]$ |            |
|                                                                  | incorrect: $b^{(3)} = [0.3, 0.6, 0.5, 0.8]$ |            |
| $f(x) = x_1(x_2 + x_3 - x_4)^3$ $x = [1, 1, 1, 0]$ | ground truth: $b^* = [0, 0, 0, 1]$ | $r_1$ $r_m$ |
|                                                                  | incorrect: $b^{(1)} = [0.5, 0.5, 0.5, 0.5]$ |            |
|                                                                  | incorrect: $b^{(2)} = [0.2, 0.3, 0.6, 0.1]$ |            |
|                                                                  | incorrect: $b^{(3)} = [1.0, 0.3, 1.0, 0.1]$ |            |