

## TL;DR

We propose the *faithful Shapley interaction index* which is the unique interaction index satisfying the original Shapley axioms while being faithful polynomial approximation to the model.

## Introduction

Quantifying feature interaction is useful in some tasks.

- Question-context interaction in question answering.
- Medicine-medicine interaction in healthcare.

Existing works extend the Shapley values to the interaction context by introducing **less suitable axioms to XAI** to ensure uniqueness.

- The recursive axiom in Shapley interaction indices has almost no physical meaning.
- The interaction distribution axiom in Shapley-Taylor interaction indices causes impoverished lower-order interaction attribution.

We extend the “faithful linear approximation” property of the singleton Shapley value to **“faithful polynomial approximation”** for interaction indices.

- Faithfulness is an important concept in XAI.
- Together with original Shapley axioms, we prove Faith-Shap is the **unique** interaction index satisfying all these axiomatic properties.

Similar theoretical results also apply to the Banzhaf

## Preliminary: Shapley axioms

- Notations: number of input features  $d \in N$ , target set function  $v: 2^d \rightarrow R$ , maximum interaction order:  $\ell \in N$ , number of interactions:  $d_\ell = \sum_{j=0}^{\ell} \binom{\ell}{j}$ , the vector of interaction indices  $\mathcal{E}(v, \ell) \in R^{d_\ell}$ , the set of subsets of size  $\leq \ell: S_\ell$ .

**Axiom 3. (Interaction Linearity):** For any maximum interaction order  $\ell \in [d]$ , and for any two set functions  $v_1$  and  $v_2$ , and any two scalars  $\alpha_1, \alpha_2 \in \mathbb{R}$ , the interaction index satisfies:  $\mathcal{E}(\alpha_1 v_1 + \alpha_2 v_2, \ell) = \alpha_1 \mathcal{E}(v_1, \ell) + \alpha_2 \mathcal{E}(v_2, \ell)$ .

**Axiom 4. (Interaction Symmetry):** For any maximum interaction order  $\ell \in [d]$ , and for any set function  $v: 2^d \mapsto \mathbb{R}$  that is symmetric with respect to elements  $i, j \in [d]$ , so that  $v(S \cup i) = v(S \cup j)$  for any  $S \subseteq [d] \setminus \{i, j\}$ , the interaction index satisfies:  $\mathcal{E}_{T \cup i}(v, \ell) = \mathcal{E}_{T \cup j}(v, \ell)$  for any  $T \subseteq [d] \setminus \{i, j\}$  with  $|T| < \ell$ .

**Axiom 5. (Interaction Dummy):** For any maximum interaction order  $\ell \in [d]$ , and for any set function  $v: 2^d \mapsto \mathbb{R}$  such that  $v(S \cup i) = v(S)$  for some  $i \in [d]$  and for all  $S \subseteq [d] \setminus \{i\}$ , the interaction index satisfies:  $\mathcal{E}_T(v, \ell) = 0$  for all  $T \in S_\ell$  with  $i \in T$ .

**Axiom 6. (Interaction Efficiency):** For any maximum interaction order  $\ell \in [d]$ , and for any set function  $v: 2^d \mapsto \mathbb{R}$ , the interaction index satisfies:  $\sum_{S \in S_\ell \setminus \emptyset} \mathcal{E}_S(v, \ell) = v([d]) - v(\emptyset)$  and  $\mathcal{E}_\emptyset(v, \ell) = v(\emptyset)$ .

(Faithfulness property) The singleton Shapley values are the minimizer of the following weighted linear approximation:

$$\min_{\mathcal{E} \in \mathbb{R}^{d+1}} \sum_{S \subseteq [d]: \mu(S) < \infty} \mu(S) \left( v(S) - \sum_{i \in S} \mathcal{E}_i \right)^2 \text{ s.t. } v(S) = \sum_{i \in S} \mathcal{E}_i, \forall S: \mu(S) = \infty.$$

It has been shown that we can recover the singleton Shapley values as the solution of the weighted regression problem above by setting  $\mu(S) \propto \frac{d-1}{\binom{d}{|S|} |S| (d-|S|)}$  and  $\mu(\emptyset) = \mu([d]) = \infty$  [2].

## Main Theoretical Results

- We say  $\mathcal{E}(v, \ell)$  are Faith-Interaction Indices if there exists a weighting function  $\mu(\cdot)$  such that

$$\mathcal{E}(v, \ell) = \min_{\mathcal{E} \in \mathbb{R}^{d_\ell}} \sum_{S \subseteq [d]} \mu(S) \left( v(S) - \sum_{T \subseteq S, T \leq \ell} \mathcal{E}_T \right)^2.$$

- Our theoretical results:

- (Linearity) Faith-Interaction Indices satisfy the interaction linearity axiom.
- (Symmetry) Faith-Interaction Indices satisfy the interaction symmetry axiom if and only if the weighting function  $\mu(S) = \mu(T)$  for all  $|S| = |T|$ .
- (Linearity, Symmetry, Dummy) Faith-Interaction Indices satisfy the interaction linearity, symmetry, and dummy axiom if and only if the weighting function satisfies:

$$\mu(S) \propto \sum_{i=|S|}^d \binom{d-|S|}{i-|S|} (-1)^{i-|S|} g(a, b, i), \text{ where } g(a, b, i) = \begin{cases} 1 & \text{if } i = 0 \\ \prod_{j=0}^{i-1} \frac{a(a-b)+j(b-a^2)}{a-b+j(b-a^2)} & \text{if } 1 \leq i \leq d, \end{cases}$$

- (Efficiency) Faith-Interaction Indices satisfy the interaction efficiency axiom if and only if  $\mu([d]) = \mu(\emptyset) = \infty$ .
- (Linearity, Symmetry, Dummy, Efficiency) **Faith-Shap is the unique interaction index** that satisfies the interaction linearity, symmetry, dummy, and efficiency axiom. The weighting function is given as

$$\mu(S) \propto \frac{d-1}{\binom{d}{|S|} |S| (d-|S|)} \text{ for all } S \subseteq [d] \text{ with } 1 \leq |S| \leq d-1, \text{ and } \mu(\emptyset) = \mu([d]) = \infty.$$

We term this unique interaction index as the **Faithful Shapley Interaction index (Faith-Shap)**, which has the form:

$$\mathcal{E}_S^{F-Shap}(v, \ell) = a(v, S) + (-1)^{\ell-|S|} \frac{|S|}{\ell+|S|} \binom{\ell}{|S|} \sum_{T \supset S, |T| > \ell} \frac{\binom{|T|-1}{\ell-|S|}}{\binom{|T|+\ell-1}{\ell+|S|}} a(v, T), \forall S \in S_\ell, \quad (16)$$

where  $a(v, \cdot)$  is the Möbius transform of  $v(\cdot)$ . Moreover, its highest-order interaction terms can be expressed as a weighted average of discrete derivatives:

$$\mathcal{E}_S^{F-Shap}(v, \ell) = \frac{(2\ell-1)!}{((\ell-1)!)^2} \sum_{T \subseteq [d] \setminus S} \frac{(\ell+|T|-1)!(d-|T|-1)!}{(d+\ell-1)!} \Delta_S(v(T)) \text{ for all } S \in S_\ell \text{ with } |S| = \ell. \quad (17)$$

- Though the computation of the exact Faith-Shap is exponential, in practice, we use the following procedure to approximate it:

- Sample each coalition  $S_i \subseteq [d]$  with probability  $\mu(S_i) \propto \frac{1}{\binom{d}{|S_i|} |S_i| (d-|S_i|)}$  and compute  $v(S_i)$ .
- Solve the following L1-regularized regression problem:

$$\operatorname{argmin}_{\mathcal{E} \in \mathbb{R}^{d_\ell}} \frac{1}{n} \sum \left( v(S_i) - \sum_{T \subseteq S_i, T \leq \ell} \mathcal{E}_T \right)^2 + \underbrace{\text{INFTY} * \sum_{S \in \{\emptyset, [d]\}} \left( v(S) - \sum_{T \subseteq S, T \leq \ell} \mathcal{E}_T \right)^2}_{\text{Ensure efficiency}} + \underbrace{\lambda |\mathcal{E}|_1}_{\text{Encourage Sparsity}}$$

## Qualitative Examples

- Explain a binary sentiment classification model on the IMDB dataset.
  - A BERT model
  - Faith-Shap with the maximum interaction order  $\ell = 2$ .

Index	Sentences (bold words are the interactions with the highest (absolute) importance values)	Model Prediction	Interaction score
1	I have <b>Never forgot</b> this movie. All these years and it has remained in my life.	Positive	0.818
2	TWINS EFFECT is a poor film in so many respects. The <b>only good</b> element is that it doesn't take itself seriously..	Negative	-0.375
3	I rented this movie to get an easy, entertained view of the history of Texas. I got a <b>headache instead</b> .	Negative	0.396
4	Truly <b>appalling waste</b> of space. Me and my friend tried to watch this film to its conclusion but had to switch it off about 30 minutes from the end.	Negative	0.357
5	I still remember watching Satya for the first time. I was completely <b>blown away</b> .	Positive	0.283

Table 5: Top interactions of different examples on IMDB. See more results in Appendix B.

- (Example 1) While individual words “Never” and “forgot” are negative, their joint effect is positive.
- (Example 2,3,4) non-complementary interaction effect.
- (Example 5) Complementarity effects: words in a phrase are only meaningful when all words are present.