1 Introduction

Deep neural networks (DNNs) have exhibited significant success in various tasks, and the interpretability of DNNs has received increasing attention in recent years. Quantifying the interaction between input variables of the DNN provides a new perspective to explain the signal processing encoded in a DNN [1, 11, 8, 10, 6, 5, 12, 13, 7, 4, 3, 19, 17, 15, 14, 2, 18].

Given a DNN, we quantify interactions of different orders between two input variables of the DNN during the inference process. Previous studies have been proposed to measure the interaction based on game theory [4, 3]. Grabisch and Roubens [4] proposed the interaction index to measure different interaction values for all \(2^n\) combinations of \(n\) variables. Dhamdhere et al. [3] extended the study of [4], and proposed the Shapley-Taylor interaction index. Compared with previous studies, we focus on the interaction between two input variables, and disentangle the interaction into interaction components of different orders, which reflect inter-variable effects w.r.t. contexts of different scales.

In this study, we define interaction components of different orders between two input variables based on game theory. Given a DNN with \(n\) input variables, each input variable can be viewed as a player. In this way, we use \(N = \{1, 2, 3, \cdots, n\}\) to represent the set of all players (indices of all input variables). Let \(v\) denote the output of the DNN, which can be considered as a game function. The function \(v\) maps a set of players to a scalar value, i.e. \(v : 2^N \rightarrow \mathbb{R}\), where \(2^N\) denotes all possible subsets of players in the set \(N\). Let \(\phi(i)\) denote the contribution of the player \(i\) to the game, which can be computed as the Shapley value of the player \(i\). The Shapley value is widely regarded as a unique unbiased estimation of the contribution that satisfies the linearity, dummy, symmetry, and efficiency properties [16].

The overall interaction \(I(i, j)\) between the player \(i\) and the player \(j\) is defined as the change of \(\phi(i)\) when the player \(j\) is absent w.r.t. the case when the player \(j\) is present, i.e. \(I(i, j) = \phi_{w/\, j}(i) - \phi_{w/j}(i)\). If \(I(i, j) > 0\), then we consider players \(i\) and \(j\) have a positive effect. Accordingly, if \(I(i, j) < 0\), then we consider players \(i\) and \(j\) have a negative effect.

More specifically, we explicitly decompose \(I(i, j)\) into 0-order, 1-order, \(\cdots\), \((n-2)\)-order interaction components, i.e. \(I(i, j) = \frac{1}{n-1} \sum_{m=0}^{n-2} I^{(m)}(i, j)\), in order to measure the scale of inference patterns encoded in the DNN. Here, the order \(m\) indicates the scale of the context involved in the computation of interactions between pixels \(i\) and \(j\). For example, given a human face, we consider players \(i\) and \(j\) as two eyes on this face. Besides, we regard other \(m\) players, which are included on the face as the context. The interaction between two eyes depends on such a context of the face, which is measured as \(I^{(m)}(i, j)\). Without the face context, there is supposed not to contain such\footnote{Contribute equally to this paper.}
interaction. Therefore, the order \( n \) reflects the scale of inference patterns that are encoded in the DNN.

Contributions of this study can be summarized as follows. (1) In this study, we define and quantify interaction components of different orders. (2) We further prove that interaction components of different orders satisfy several desirable properties.

2 Algorithm

2.1 Shapley values

Given a game with multiple players, each player is supposed to obtain a high reward. Some players may form a coalition to pursue a high reward. Considering the contribution of each player to the coalition is different, each player should be assigned with different rewards. Let \( N \) denote the set of all players, and \( 2^N \) indicate all potential subsets of \( N \). For each subset of players \( S \), a game \( v : 2^N \to \mathbb{R} \) denotes a scalar reward obtained by \( S \). The Shapley value \( \phi_v(i) \) of the player \( i \) represents the numerical contribution of this player to the game \( v \), which is defined by \( [9] \).

\[
\phi_v(i|N) = \sum_{S \subseteq N \setminus \{i\}} \frac{(n-s-1)!s!}{n!} \Delta_S v(S), \quad \Delta_S v(S) \xrightarrow{\text{def}} v(S \cup \{i\}) - v(S),
\]

where \( |S| = s \) and \( |N| = n \). Weber \( [16] \) have proven that the Shapley value is a unique unbiased method to fairly allocate overall reward to each player with four properties. For simplicity, we use \( \phi(i|N) \) by ignoring the superscript of \( \phi_v(i|N) \) in the following manuscript without causing ambiguity.

- **Linearity property**: If two independent games can be merged into one game, then the Shapley value of the new game also can be merged, i.e. \( \forall S \subseteq N, \phi_v(i|N) = \phi_v(i|N) + \phi_w(i|N); \forall c \in \mathbb{R}, \phi_{c \cdot v}(i|N) = c \cdot \phi_v(i|N) \).

- **Dummy property**: The dummy player \( i \) is defined as a player satisfying \( \forall S \subseteq N \setminus \{i\}, v(S \cup \{i\}) = v(S) + v(\{i\}) \), which indicates that the player \( i \) has no interactions with other players in \( N \), \( \phi(i|N) = v(\{i\}) - v(\emptyset) \).

- **Symmetry property**: If \( \forall S \subseteq N \setminus \{i\}, v(S \cup \{i\}) = v(S \cup \{j\}) \), then \( \phi(i|N) = \phi(j|N) \).

- **Efficiency property**: Overall reward can be assigned to all players, \( \sum_{i \in N} \phi(i|N) = v(N) - v(\emptyset) \).

2.2 The interaction index \( \mathcal{I}_v(S) \) [4] and its extension [19]

Grabisch and Roubens [4] firstly proposed the interaction index \( \mathcal{I}_v(S) \). Given a game \( v \), and a set of all players \( N \). For a subset of players \( S \subseteq N \), if players in \( S \) cooperate to form a coalition for a high reward, then this coalition can be considered as a new singleton, which is represented using brackets, \( [S] \). In this way, the game \( v \) can be considered to have \((n - s + 1)\) players, and one of them is the singleton \( [S] \). \( \mathcal{I}_v(S) \) quantifies the marginal reward of \( S \), which removes all marginal rewards from all potential subsets of \( S \).

\[
\mathcal{I}_v(S) = \sum_{T \subseteq N \setminus S} \frac{(n - t - s)! t!}{(n - s + 1)!} \Delta_S v(T), \quad \Delta_S v(T) \xrightarrow{\text{def}} \sum_{L \subseteq S} (-1)^{t-s} v(L \cup T).
\]

The physical meaning of the interaction index \( \mathcal{I}_v(S) \) is described by following recursive properties.

- **Recursive property 1**: Let \( \mathcal{I}(S|N) \) denote the interaction index that is computed with the set of players \( N \). Then \( \forall S \subseteq N, s > 1, \mathcal{I}(S|N) = \mathcal{I}([S]|N \setminus S \cup \{[S]\}) - \sum_{K \subseteq S,K \neq \emptyset} \mathcal{I}(K|N \setminus S \cup K) \).

The recursive property 1 indicates that \( \mathcal{I}_v(S) \) contains marginal reward of \( S \), and removes all marginal reward of subsets of \( S \). For example, let \( S = \{a, b, c\} \), then \( \mathcal{I}_v(S) \) contains the marginal reward obtained by \( \{a, b, c\} \), and removes marginal rewards obtained by \( \{a, b\}, \{a, c\}, \{b, c\}, \{a\}, \{b\}, \) and \( \{c\} \).

- **Recursive property 2**: The interaction index in \( S \) is equal to the interaction among players \( S \setminus \{i\} \) with the presence of the player \( i \) minus the interaction among players \( S \setminus \{i\} \) with the absence of the player \( i \), where \( i \) is an arbitrary player inside \( S \). I.e. \( \forall i \in S, \mathcal{I}(S|N) = \mathcal{I}_{v,i}(S \setminus \{i\}|N \setminus \{i\}) \).
The Shapley-Taylor interaction index is computed by averaging all potential orderings. For simplicity, we use $\mathcal{I}(S)$ by ignoring the superscript of $\mathcal{I}_v(S)$ in the following manuscript without causing ambiguity.

- **Linearity property:** If $\forall S \subseteq N$, rewards of games $u$, $v$, and $w$ satisfy $u(S) = v(S) + w(S)$, then $\mathcal{I}_v(S) = \mathcal{I}_v(S) + \mathcal{I}_w(S); \forall c \in \mathbb{R}, \mathcal{I}_v(S) = c \cdot \mathcal{I}_u(S)$.

- **Dummy property:** If the player $i$ is a dummy player, then $\mathcal{I}(S \cup \{i\}) = 0$.

- **Symmetry property:** If $\forall S \subseteq N$ and $i \neq j$, there is $v(S \cup \{i\}) = v(S \cup \{j\})$, then $\mathcal{I}(S \cup \{i\}) = \mathcal{I}(S \cup \{j\})$.

Moreover, Zhang et al. [9] proposed $B([S])$ to measure the overall interaction among players in $S$.

$$B([S]) = \phi([S]\{N \setminus S \cup \{i\}\} - \sum_{i \in S} \phi(i)N \setminus S \cup \{i\} = \sum_{S' \subseteq S, s' > 1} \mathcal{I}(S'). \tag{3}$$

In this way, the interaction $B([S])$ contains $2^s - s - 1$ potential interaction indices inside $S$, where positive and negative interaction indices can counteract each other. Thus, $B'[([S])]$ is used to reflect the significance of interactions among players inside $S$.

$$B'([S]) = \sum_{S' \subseteq S, s' > 1} |\mathcal{I}(S')| = \sum_{S' \subseteq S, s' > 1, \mathcal{I}(S') > 0} \mathcal{I}(S') - \sum_{S' \subseteq S, s' > 1, \mathcal{I}(S') < 0} \mathcal{I}(S'). \tag{4}$$

Zhang et al. [9] proposed an efficient-yet-approximate method to estimate $B'([S])$. Compared with the interaction index, $B'([S])$ provides a more global view to understand the game.

### 2.3 The Shapley-Taylor interaction index $\mathcal{I}_v^{(k)}(S)$ [3]

Dhamdhere et al. [3] proposed the Shapley-Taylor index, which attributed the model’s prediction to interactions among subsets of features up to the size $k$. Specifically, the Shapley-Taylor interaction index is equal to the Taylor Series of the multilinear extension of the set-theoretic behavior of the model. For a fixed ordering $\pi = (i_1, i_2, \ldots, i_n)$ and a set of features $S$, the Shapley-Taylor indices $\mathcal{I}_v^{(k)}(S|\pi)$ is defined as follows.

$$\mathcal{I}_v^{(k)}(S|\pi) = \begin{cases} \Delta_S v(\emptyset), & \text{if } s < k, \\ \Delta_S v(\pi^S), & \text{if } s = k \end{cases} \tag{5}$$

The Shapley-Taylor interaction index is computed by averaging all potential ordering $\pi$, as follows.

$$\mathcal{I}_v^{(k)}(S) = \mathbb{E}_\pi(\mathcal{I}_v^{(k)}(S|\pi)) \tag{6}$$

Dhamdhere et al. [3] have proven that the Shapley-Taylor interaction index satisfies following properties. For simplicity, we use $\mathcal{I}(S)$ by ignoring the superscript of $\mathcal{I}_v^{(k)}(S)$ in the following manuscript without causing ambiguity.

- **Linearity property:** If $\forall S \subseteq N$, three games $u$, $v$, and $w$ satisfy $u(S) = v(S) + w(S)$, then $\mathcal{I}_v^{(k)}(S) = \mathcal{I}_v^{(k)}(S) + \mathcal{I}_w^{(k)}(S)$, and $\mathcal{I}_v^{(k)}(S) = c \cdot \mathcal{I}_w^{(k)}(S)$, where $c$ is a scalar value.

- **Dummy property:** If the player $i$ is a dummy player, then $\mathcal{I}(S \cup \{i\}) = 0$.

- **Symmetry property:** If $\forall S \subseteq N \setminus \{i, j\}$ and $i \neq j$, there is $v(S \cup \{i\}) = v(S \cup \{j\})$, then $\mathcal{I}(i) = \mathcal{I}(j)$.

- **Efficiency property:** The overall reward can be allocated to each potential $S$ with size up to $k$. I.e. $\forall v, \sum_{S \subseteq N, s \leq k} \mathcal{I}(S) = v(N) - v(\emptyset)$.
Interactions between two players:

- Dummy property: A player $i \in N$ is considered as a dummy player if $\forall S \subseteq N \setminus \{i\}, v(S \cup \{i\}) = v(S) + v(\{i\})$. Thus, the player $i$ has no interactions with other players, i.e. $\phi^{(m)}(i|N) = v(\{i\}) - v(\emptyset)$.

- Linearity property: If two games $v$ and $w$ can be combined into a single game, their Shapley values can be added, i.e. $\forall i \in N, \phi^{(m)}_v(i|N) = \phi^{(m)}_w(i|N) + \phi^{(m)}_c(i|N)$, and $\phi^{(m)}_c(S) = c \cdot \phi^{(m)}_c(S)$, where $c$ is a scalar value.

- Symmetry property: Given two players $i, j \in N$, if these two players have same interactions with all other players $\forall S \subseteq N \setminus \{i, j\}$, $v(S \cup \{i\}) = v(S \cup \{j\})$, then $\phi^{(m)}(i|N) = \phi^{(m)}(j|N)$.

Interactions between two players: Given two players $i$ and $j$, if these two players always participate in the game together or always do not participate in the game together, we can roughly consider these two players cooperate with each other, and form a singleton player $I_{ij}$, $S_{ij} = \{i, j\}$. Thus, this game can be considered to have $(n - 1)$ players, $N_{ij} = N \setminus \{i, j\} \cup \{S_{ij}\}$. If the player $j$ never participates in the game, then the player $i$ is considered to work individually. Similarly, if the player $i$ is absent in the game, then the player $j$ is also considered to work individually. In this way, the interaction between players $i$ and $j$, $I(i, j)$, is defined as the contribution of $S_{ij}$, when players $i$ and $j$ cooperate with each other w.r.t. the sum of $\phi(i|N \setminus \{j\})$ and $\phi(j|N \setminus \{i\})$, when they work individually [19], as follows.

$$I(i, j) = \phi([S_{ij}]|N_{ij}) - [\phi(i|N \setminus \{j\}) + \phi(j|N \setminus \{i\})] = \sum_{T \subseteq N \setminus \{i, j\}} \frac{(n - t - 2)!t!}{(n - 1)!} \Delta_{ij} v(T),$$

where $\Delta_{ij} v(S) \triangleq v(S \cup \{i, j\}) - v(S \cup \{i\}) - v(S \cup \{j\}) + v(S)$. Eqn. (8) is essentially equivalent to Eqn. (2), when we consider $S$ in Eqn. (2) as $S_{ij}$. If $I(i, j) > 0$, then players $i$ and $j$ cooperate with each other for a higher contribution, i.e. the interaction is positive. If $I(i, j) < 0$, then the interaction between players $i$ and $j$ leads to a lower contribution, i.e. the interaction is negative.

Interaction components of different orders: In this study, we find that the overall interaction $I(i, j)$ can be decomposed into interaction components of different orders $m$, i.e. $I(i, j) = \frac{1}{n-1} \sum^{n-2}_{m=0} I^{(m)}(i, j)$. Here, we use $m$ to measure the scale of contexts. $I^{(m)}(i, j)$ reflects the average interactions between players $i$ and $j$ among all contexts with $m$ players. For example, in the object classification, each pixel of the input image can be considered as a player. The union of $S \subseteq N$ and $\{i, j\}$ can be regarded as an inference pattern. For example, we can consider a human face as an inference pattern. Let players $i$ and $j$ represent two eyes on this face, and other $m$ players on the face represent an inference pattern. In this way, the interaction between two eyes depends on the context of the face, which is measured as $I^{(m)}(i, j)$.

In particular, when $m$ is small, $I^{(m)}(i, j)$ measures the interaction from inference patterns consisting of very few pixels without knowing the global structures of the object. Whereas, when $m$ is large,
Thus, the interaction component $I^{(m)}(i, j)$ corresponds to the interaction from inference patterns computed with relatively rich contextual information, which usually encode global structures of the object. $I^{(m)}(i, j)$ is defined as

\[
I^{(m)}(i, j) = \phi^{(m)}([S_{ij}]|N_{ij}) - \left[ \phi^{(m)}(i|N \setminus \{j\}) + \phi^{(m)}(j|N \setminus \{i\}) \right]
\]

(9)

where $\Delta_{ij}v(S) \overset{\text{def}}{=} v(S \cup \{i, j\}) - v(S \cup \{i\}) - v(S \cup \{j\}) + v(S)$, and Eqn.(9) represents the additional contribution brought by $i$ and $j$ in the context $S$ with $m$ players. In addition, we have proven that for $m \in \{0, \ldots, n - 1\}$, $I^{(m)}(i, j)$ has following properties.

- **Linearity property**: If the game $u$ satisfies $u(S) = w(S) + v(S)$, where $v$ and $w$ are another two games. Then, for all $i, j \in N$, $I_{u}^{(m)}(i, j)$ can be decomposed into $I_{w}^{(m)}(i, j) = I_{w}^{(m)}(i, j) + I_{v}^{(m)}(i, j)$, and $I_{w}^{(m)}(i, j) = c \cdot I_{v}^{(m)}(i, j)$, where $c$ is a scalar value.

- **Dummy property**: The dummy player $i \in N$ satisfies $\forall S \subseteq N, v(S \cup \{i\}) = v(S) + v(\{i\})$. It means that the player $i$ has no interactions with other players, i.e. $\forall j \in N, I^{(m)}(i, j) = 0$.

- **Symmetry property**: If players $i, j \in N$ have same interactions with other players $\forall S \subseteq N \setminus \{i, j\}$, then their contributions have same dependence on different contexts, $\forall k \in N \setminus \{i, j\}, I^{(m)}(i, k) = I^{(m)}(j, k)$.

- **Marginal contribution property**: if $\forall i, j \in N, i \neq j, \phi^{(m+1)}(i|N) - \phi^{(m)}(i|N) = \mathbb{E}_{j \in N \setminus \{i\}} I^{(m)}(i, j)$.

- **Accumulation property**: The contribution of $i \in N$ with contexts of $m$ players can be decomposed into interactions dependent on less than $m$ players, $\phi^{(m)}(i|N) = \mathbb{E}_{j \in N \setminus \{i\}} [\sum_{k=0}^{m-1} I^{(k)}(i, j)] + \phi^{(0)}(i|N)$.

- **Recursive property**: $\phi^{(n-1)}(i|N) - \phi^{(0)}(i|N) = \mathbb{E}_{j \in N \setminus \{i\}} [\sum_{m=0}^{n-2} I^{(m)}(i, j)] = I(N \setminus \{i\}, i) = \sum_{j \in N \setminus \{i\}} I(i, j)$.

- **Efficiency property**: The overall reward of the game can be decomposed into interactions of different orders, i.e. $v(N) - v(\emptyset) = \sum_{i \in N} \phi^{(0)}(i|N) + \sum_{i \in N} \sum_{j \in N \setminus \{i\}} \sum_{k=0}^{n-2} \frac{1}{n(n-1)} I^{(k)}(i, j)$.

**Purified interaction components of different orders**: Note that $I^{(m)}(i, j)$ includes the average interaction benefit from 0-order contexts to $(n - 2)$-order contexts. For example, given a specific context $\{a, b\}$, $I^{(2)}(i, j)$ includes marginal interaction benefits from coalitions $\{i, j\}, \{i, j, a\}, \{i, j, b\}$ and $\{i, j, a, b\}$, i.e. $I^{(2)}(i, j)$ reflects a mixture of interactions of different orders. In order to purify the definition of interactions, we propose $J^{(m)}(i, j)$ to exclusively represent the interaction benefit from contexts with exactly $m$ players. Specifically, $R_I(i, j)$ quantifies interaction benefits from the inference pattern of $T \cup \{i, j\}$, which can be computed as follows.

\[
R_I(i, j) = \sum_{T \subseteq T} (-1)^{|T| - 1} \Delta_{ij}v(S)
\]

(10)

Thus, the interaction component $I^{(m)}(i, j)$ can be represented as follows.

\[
I^{(m)}(i, j) = \mathbb{E}_{S \subseteq N \setminus \{i, j\}, s = m} [\sum_{T \subseteq S} R_I(i, j)]
\]

(11)

Similar to Eqn.(11), we define $J^{(m)}(i, j)$ to exclusively measure interactions of the inference pattern with players $i, j$ and other $m$ players as

\[
J^{(m)}(i, j) = \mathbb{E}_{T \subseteq N \setminus \{i, j\}, t = m} [R_T(i, j)]
\]

(12)

Hence, $J^{(m)}(i, j)$ can be computed recursively as follows.

\[
I^{(m)}(i, j) = \sum_{0 \leq p \leq m} \binom{p}{m} \cdot J^{(p)}(i, j) \Rightarrow J^{(m)}(i, j) = I^{(m)}(i, j) - \sum_{p=0}^{m-1} \binom{p}{m} \cdot J^{(p)}(i, j)
\]

(13)
References

[1] Jacob Bien, Jonathan Taylor, and Robert Tibshirani. A lasso for hierarchical interactions. *Annals of Statistics*, 41(3):1111–1141, 2013.

[2] Tianyu Cui, Pekka Marttinen, and Samuel Kaski. Learning global pairwise interactions with bayesian neural networks. *arXiv: Learning*, 2019.

[3] Kedar Dhamdhere, Ashish Agarwal, and Mukund Sundararajan. The shapley taylor interaction index. *arXiv preprint arXiv:1902.05622*, 2019.

[4] Michel Grabisch and Marc Roubens. An axiomatic approach to the concept of interaction among players in cooperative games. *International Journal of Game Theory*, 28:547–565, 1999.

[5] Joseph D Janizek, Pascal Sturmefels, and Suin Lee. Explaining explanations: Axiomatic feature interactions for deep networks. *arXiv:2002.04138*, 2020.

[6] Xisen Jin, Junyi Du, Zhongyu Wei, Xiangyang Xue, and Xiang Ren. Towards hierarchical importance attribution: Explaining compositional semantics for neural sequence models. *arXiv:1911.06194*, 2019.

[7] Scott Lundberg, Gabriel G Erion, and Suin Lee. Consistent individualized feature attribution for tree ensembles. *arXiv: Learning*, 2018.

[8] W James Murdoch, Peter J Liu, and Bin Yu. Beyond word importance: Contextual decomposition to extract interactions from lstms. *arXiv:1801.05453*, 2018.

[9] Lloyd S Shapley. A value for n-person games. *Contributions to the Theory of Games*, 2(28):307–317, 1953.

[10] Chandan Singh, W James Murdoch, and Bin Yu. Hierarchical interpretations for neural network predictions. *arXiv:1806.05337*, 2018.

[11] Daria Sorokina, Rich Caruana, Mirek Riedewald, and Daniel Fink. Detecting statistical interactions with additive groves of trees. In *ICML*, pages 1000–1007, 2008.

[12] Mukund Sundararajan, Ankur Taly, and Qiqi Yan. Axiomatic attribution for deep networks. In *ICML*, pages 3319–3328, 2017.

[13] Michael Tsang, Dehua Cheng, and Yan Liu. Detecting statistical interactions from neural network weights. In *ICLR*, 2018.

[14] Michael Tsang, Dehua Cheng, Hanpeng Liu, Xue Feng, Eric Zhou, and Yan Liu. Feature interaction interpretability: A case for explaining ad-recommendation systems via neural interaction detection. In *International Conference on Learning Representations*, 2020. URL https://openreview.net/forum?id=BkgnhTETdS

[15] Xin Wang, Jie Ren, Shuyun Lin, Xiangming Zhu, Yisen Wang, and Quanshi Zhang. A unified approach to interpreting and boosting adversarial transferability. *arXiv: 2010.04055*, 2020.

[16] Robert J Weber. Probabilistic values for games. *The Shapley Value. Essays in Honor of Lloyd S. Shapley*, pages 101–119, 1988.

[17] Die Zhang, Huilin Zhou, Xiaoyi Bao, Da Huo, Ruizhao Chen, Xu Cheng, Hao Zhang, Mengyue Wu, and Quanshi Zhang. Interpreting hierarchical linguistic interactions in dnns. *arXiv*: 2007.04298, 2020.

[18] Hao Zhang, Sen Li, Yinchao Ma, Mingjie Li, Yichen Xie, and Quanshi Zhang. Interpreting and boosting dropout from a game-theoretic view. *arXiv: 2009.11729*, 2020.

[19] Hao Zhang, Yichen Xie, Longjie Zheng, Die Zhang, and Quanshi Zhang. Interpreting multivariate interactions in dnns. *arXiv: 2010.05045*, 2020.