Interpreting Hierarchical Linguistic Interactions in DNNs

Die Zhang Huilin Zhou Xiaoyi Bao Da Huo
Ruizhao Chen Xu Cheng Hao Zhang Mengyue Wu
Quanshi Zhang
Shanghai Jiao Tong University
{zizhan52,zhouhuilin116,zjbaoxiaoyi,sjtuhuoda,
stelledge,xcheng8,1603023-zh,mengyuewu,
zqs1022}@sjtu.edu.cn

Abstract

This paper proposes a method to disentangle and quantify interactions among words that are encoded inside a DNN for natural language processing. We construct a tree to encode salient interactions extracted by the DNN. Six metrics are proposed to analyze properties of interactions between constituents in a sentence. The interaction is defined based on Shapley values of words, which are considered as an unbiased estimation of word contributions to the network prediction. Our method is used to quantify word interactions encoded inside the BERT, ELMo, LSTM, CNN, and Transformer networks. Experimental results have provided a new perspective to understand these DNNs, and have demonstrated the effectiveness of our method.

1 Introduction

Deep neural networks (DNNs) have shown promise in various tasks of natural language processing (NLP), but a DNN is usually considered as a black-box model. In recent years, explaining features encoded inside a DNN has become an emerging direction. Based on the inherent hierarchical structure of natural language, many methods use latent tree structures of language to guide the DNN to learn interpretable feature representations [4, 8, 29, 30, 31, 36, 42, 45]. However, the interpretability usually conflicts with the discrimination power [1]. There is a considerable gap between pursuing the interpretability of features and pursuing superior performance.

Therefore, in this study, we aim to explain a trained black-box DNN in a post-hoc manner, so that the explanation of the DNN does not affect its performance. This is essentially different from previous studies of designing new network architectures or losses to learn interpretable features, e.g. physically embedding tree structures into a DNN.

Given a trained DNN, in this paper, we propose to analyze interactions among input words, which are used by the DNN to make a prediction. Our method generates a tree structure to objectively reflect interactions among words. Mathematically, the interaction of several words is quantified as the difference of the contribution when these words contribute jointly to the prediction w.r.t. when each individual word contributes independently to the prediction. The interaction between words may bring either positive or negative effects on the prediction. For example, the word green and the word hand in the sentence he is a green hand have a strong and positive interaction, because the words green and hand contribute to the person’s identity jointly, rather than independently.

Preprint. Under review.
The core challenge in this study is to guarantee the objectiveness of the explanation. I.e. the tree needs to reflect true interactions among words without significant bias. We notice that the Shapley value is widely considered as a unique unbiased estimation of the word contribution [21], which satisfies four desirable properties (linearity, dummy, symmetry and efficiency) [10]. Thus, we define the interaction benefit among words based on the Shapley value. Let us consider a constituent with \( m \) words. \( \phi_1, \phi_2, \ldots, \phi_m \) denote numerical contributions of each word to the prediction of a DNN, respectively. \( \phi_{all} \) represents the numerical contribution of the entire constituent to the prediction. Hence, \( B = \phi_{all} - \sum_{i=1}^{m} \phi_i \) measures the interaction benefit of this constituent. If \( B > 0 \), interactions among these \( m \) words have positive effects on the prediction; otherwise, negative effects. Here, \( \phi_1, \ldots, \phi_m, \phi_{all} \) can be computed as Shapley values.

Given a trained DNN and an input sentence with \( n \) words, Figure 1 shows the tree structure that reflects word interactions encoded inside the DNN. In the tree, \( \frac{n}{2} \) leaf nodes represent \( n \) input words.

More specifically, there are two types of interactions among words, \textit{i.e.} (1) interactions within a constituent and (2) interactions between constituents.

- **Interactions within a constituent** exist among any two or more words in the constituent. For the sentence \textit{the sun is shining in the sky}, interactions within the constituent \textit{in the sky} consist of interactions among all combinations of words, including interactions (1) between \textit{(in, the)}, (2) between \textit{(the, sky)}, (3) between \textit{(in, sky)} and (4) among \textit{(in, the, sky)}.

- **Interactions between constituents.** In the aforementioned sentence, interactions between the constituent \textit{the sun} and its adjacent constituent \textit{is shining} are composed of all potential interactions among all combinations of words from the two constituents, including interactions (1) between \textit{the} and \textit{is}; (2) between \textit{the} and \textit{shining}; (3) between \textit{sun} and \textit{is}; (4) between \textit{sun} and \textit{shining}; (5) between \textit{the} and \textit{is shining}; (6) between \textit{sun} and \textit{is shining}; (7) between \textit{the sun and is}; (8) between \textit{the sun and shining}; (9) between \textit{the sun and shining}.

We use a tree structure to select and encode the most salient interactions among words, in order to reveal the signal processing in a DNN. We further propose additional metrics to diagnose interactions among words, \textit{e.g.} the quantification of interactions within a constituent, the quantification of interactions between two adjacent constituents, and ratios of interactions that are modeled and unmodeled by the tree.

Theoretically, our method can be used as a generic tool to analyze DNNs with different architectures for various tasks, including the BERT [7], ELMo [25], LSTM [12], CNN [16] and Transformer [39]. Experimental results have demonstrated the effectiveness of our method.

**Contributions** of this paper can be summarized as follows. (1) We propose a method to extract and quantify interactions among words. (2) A tree structure is automatically generated to represent salient interactions encoded in a DNN. (3) We further design six metrics to analyze interactions, which provides new perspectives to understand DNNs.

## 2 Related Work

- **Hierarchical representations of natural language.** Many studies integrated hierarchical structures of natural language into DNNs for better representations [29][40][41]. Other studies learned syntactic parsers [8][13][18][19][20][23], although these methods pursued a high parsing accuracy, instead of explaining the DNN. Essentially, the learning of the syntactic parser aimed to make the parser fit syntactic structures defined by people. Nevertheless, the post-hoc explanation of a DNN was proposed to objectively explain the signal processing in a DNN. In this way, we hope to provide...
a generic tool to analyze DNNs in a post-hoc manner, without being affected by the subjective bias in human annotations.

**Learning interpretable DNNs:** Some studies designed specific network architectures to learn interpretable feature representations, which reflected hierarchical structures of natural language. Chung et al. [3] revised an RNN to generate a hierarchical structure. Shen et al. [30] designed a novel network to automatically capture the latent tree structure of an input sentence.

**Post-hoc explanation of DNNs:** Another important direction was to explain DNNs using hierarchical structures. Yogatama et al. [40] evaluated the ability of various RNNs for natural language to capture syntactic dependencies. Murdoch et al. [24] estimated contributions of input words to the prediction of an LSTM as well as inter-word relationships. Singh et al. [33] generated a tree structure to explain the predictions of a DNN. Reif et al. [22] found that the attention matrices in BERT contained syntactic representations. Raganato and Tiedemann [26] exploited attention weights of the Transformer to analyze what kind of linguistic information was learned by the encoder of the model. Jin et al. [15] provided hierarchical explanations by quantifying the importance of each word or phrase. Voita et al. [40] studied the evolution of token representations across layers in the Transformer under different learning objectives. Lundberg and Lee [21] proposed SHAP value to assign each feature an importance value for a prediction. Simonyan et al. [32] visualized saliency maps for the class prediction to understand deep CNNs.

Unlike above studies of estimating importance/attribution/contribution/saliency of inputs, we focus on interactions among words encoded inside DNNs. Chen and Jordan [3] used a “predefined” syntactic constituency structure to assign an importance score to each word in a sentence, and to quantify interactions between sibling nodes on a parse tree, instead of learning the linguistic structure. Janizek et al. [14] explained pairwise feature interactions by extending the Integrated Gradients explanation method. Lundberg et al. [22] defined the SHAP interaction values to quantify interaction effects between two features. Cui et al. [6] estimated global pairwise interactions from a trained Bayesian neural network. Tsang et al. [37] detected statistical interactions from the weights of feedforward neural networks. An ensemble tree-based method [35] was proposed to detect variable interactions. It compared the predictive performance of two regression trees, one with interactions between two variables of interest, and the other with the absence of the interactions. The neural interaction transparency framework [38] was presented to separate feature interactions by way of regularization, and could only be applied to fully connected vanilla multi-layer perceptrons. Greenside et al. [11] identified interactions between all pairs of discrete features in an input DNA sequence. However, these studies mainly focus on interactions between two variables [6] [11] [14] [22] or are limited to specific network architectures [35] [37] [38]. Instead, we aim to quantify interactions among multiple variables in DNNs with arbitrary architectures without any prior linguistic structure. More specifically, our method uses a tree to organize the extracted interactions hierarchically.

**• Shapley values.** The Shapley value [28] was first introduced in the game theory. Given a game with multiple players, each player is supposed to pursue a high score/award. Sometimes, some players may form a coalition in order to pursue more awards. Since each player contributes differently to the coalition, the final award distributed to each player should be unequal. The Shapley value is widely considered as a unique unbiased approach to fairly allocating the total award to each player, which satisfies four desirable properties, including the linearity, dummy, symmetry and efficiency properties. Please see the supplementary material for details of these properties.

Given a game \( v^N \) with \( n \) players, let \( N = \{1, 2, ..., n\} \) represent the set of \( n \) players. The superscript \( N \) indicates the set of players participating in the game. Let \( 2^N \) denote all the potential subsets of \( N \). For example, there are three players \( a, b \) and \( c \) in a game. Hence, \( N = \{a, b, c\} \) and \( 2^N = \{\emptyset, \{a\}, \{b\}, \{c\}, \{a, b\}, \{a, c\}, \{b, c\}, \{a, b, c\}\} \). \( v^N \) is a set function mapping from each subset to a real number (i.e. \( v^N : 2^N \rightarrow \mathbb{R} \)). For any subset of players \( S \subseteq N \), where \( S \) can be regarded as a coalition, \( v^N(S) \) represents the award of the coalition. Considering that the player \( a \) is not in the coalition \( S \) (i.e. \( a \notin S \)), then if player \( a \) joins the coalition \( S \), the overall award of the coalition would be \( v^N(S \cup \{a\}) \). \( v^N(S \cup \{a\}) - v^N(S) \) is considered as the marginal award of player \( a \). The Shapley value \( \phi^N(a) \) is an unbiased contribution estimation of player \( a \) in the game. \( \phi^N(a) \) is formulated as the weighted sum of marginal awards of player \( a \) brought to all possible

---

1. Although Murdoch et al. [24] called the inter-word relationships interactions, such interactions had essential difference from the interaction defined in this paper.
2. The interaction was defined as deviation of composition from linearity.
coalitions $S \subseteq N \setminus \{a\}$.

$$\phi^v(a) = \sum_{S \subseteq N \setminus \{a\}} \frac{(|N| - |S| - 1)!|S|!}{|N|!} (v^N(S \cup \{a\}) - v^N(S))$$  \hspace{1cm} (1)

Due to the exponential number of coalitions, the computation of Shapley values is NP-hard. A sampling-based method [2] can be used to approximate Shapley values.

3 Algorithm

3.1 Interactions

Interactions between two players. In the game theory, some players may form a coalition to compete with other players and win an award. Considering that the Shapley value is an unbiased estimation of each player’s contribution [21], we quantify interactions based on the Shapley value. Suppose that there are $n$ players $N = \{1, 2, ..., n\}$ in a game $v$. Without loss of generality, we randomly select a pair of players $a, b \in N$. Shapley values of players $a$ and $b$ are denoted by $\phi^v(a)$ and $\phi^v(b)$, respectively. If players $a$ and $b$ cooperate to form a coalition $S_{ab} = \{a, b\}$, we can consider the coalition as a new singleton player, which is represented using brackets, $[S_{ab}]$. In this way, the game can be considered to have $n - 1$ players, and one of them is the singleton $[S_{ab}]$. I.e. $a$ and $b$ always appear together in the game. The interaction benefit between $a$ and $b$ is defined as $B([S_{ab}]) = \phi^v_{N \setminus \{a\}\cup\{S_{ab}\}}([S_{ab}]) - (\phi^v_{N \setminus \{a\}}(a) + \phi^v_{N \setminus \{a\}}(b)), N \setminus \{a, b\} \cup \{[S_{ab}]\}$ represents the set of players in $N$ excluding $a, b$ and being added a new singleton player $[S_{ab}]$. The absolute value of the interaction benefit $|B([S_{ab}])|$ represents the significance of the interaction. $B([S_{ab}]) > 0$ indicates a cooperative relationship between $a$ and $b$. Whereas, $B([S_{ab}]) < 0$ indicates an adversarial relationship between $a$ and $b$.

Extension to interactions among multiple players. We extend the two-player interaction to interactions among multiple players. When the game has $n$ players, let us consider a subset of players $S \subseteq N$ as a coalition, which is regarded as a new singleton player $[S]$. The interaction benefit of the coalition $S$ is defined as follows (please see the supplementary material for more discussions).

$$B([S]) = \phi^v_{N \setminus \{S\}\cup\{[S]\}}([S]) - \sum_{a \in S} \phi^v_{N \setminus \{a\}\cup\{[S]\}}(a)$$  \hspace{1cm} (2)

In this way, the interaction benefit measures the additional award brought by the singleton player $[S]$ w.r.t. the individual contribution of each player computed in Equation (1) without requiring all players in $S$ to appear together. The Shapley value $\phi^v_{N \setminus \{a\}\cup\{[S]\}}([S])$ is computed only considering the set of players when we remove all players in $S$ from $N$ and add a new singleton player $[S]$ in the game. Similarly, $\phi^v_{N \setminus \{a\}\cup\{[S]\}}(a)$ is computed only considering the set of players when we remove all players in $S$ from $N$ and add the player $a$. If $B([S])$ is greater/less than 0, interactions of players in $S$ have positive/negative effects, revealing the cooperative/adversarial relationship among players.

Furthermore, players in $S$ can be divided into two disjoint subsets $S_1, S_2$ (i.e. $S_1 \cap S_2 = \emptyset, S_1 \cup S_2 = S$). Accordingly, the interaction benefit can be decomposed into three terms:

$$B([S]) = B([S_1]) + B([S_2]) + B_{between}(S_1, S_2) \hspace{1cm} (3)$$

The first and second terms $B([S_1])$ and $B([S_2])$ indicate interaction benefits among players within $S_1$ and $S_2$, respectively. The third term $B_{between}(S_1, S_2)$ indicates interaction benefits among players selected from both $S_1$ and $S_2$. $B_{between}(S_1, S_2)$ will be introduced in detail in Section 3.2.

Properties of interaction benefits. Theoretically, the overall interaction benefit, $B([S]), S \subseteq N$, can be decomposed into elementary interaction components $I^N(S)$. The elementary interaction component was originally proposed in [10] (please see the supplementary material for details). The elementary interaction component $I^N(S)$ measures the marginal benefit received from the coalition $[S]$, from which benefits of all potential smaller coalitions $S' \subseteq S$ are removed. For example, let $S = \{a, b, c\}$. Then, $I^N(S)$ measures interactions caused by $[S] = \{a, b, c\}$, and ignores all potential interactions caused by coalitions of $(a, b), (a, c), (b, c), (a, b, c)$. Therefore, the elementary interaction component is formulated as follows.

$$I^N(S) = I^{v_{N \setminus \{S\}\cup\{[S]\}}([S])} - \sum_{S' \subset S, S' \neq \emptyset} I^{v_{N \setminus \{S\}\cup\{S'\}}(S')}$$  \hspace{1cm} (4)
In particular, for any singleton player $[S]$, we have $I^{(N \setminus S) \cup \{[S]\}}([[S]]) = \phi^{(N \setminus S) \cup \{[S]\}}([[S]])$. Thus, we can compute $I^{v}(S)$ via dynamic programming. Therefore, $B([S])$ can be decomposed into elementary interaction components as follows (please see the supplementary material for the proof).

$$B([S]) = \sum_{S' \subseteq S, |S'| > 1} I^{(N \setminus S) \cup S'}(S')$$

(5)

3.2 Fine-Grained analysis of interactions between two sets of players

Interactions between two sets of players $B_{between}(S_1, S_2)$ can be further decomposed into three parts $\psi^{inter}_{1}, \psi^{intra}_{1}, \psi^{intra}_{2}$. Please see the supplementary material for the proof.

$$B_{between}(S_1, S_2) = \psi^{inter}_{1} + \psi^{intra}_{1} + \psi^{intra}_{2}$$

(6)

where

$$\psi^{inter}_{1} = \sum_{L \subseteq S_1, L \subseteq S_2, |L| > 1} I^{v(N \setminus S) \cup L} (L)$$

(7)

$$\psi^{intra}_{1} = \sum_{L \subseteq S_1, |L| > 1} I^{v(N \setminus S_1) \cup L} (L) - \sum_{L \subseteq S_1, |L| > 1} I^{v(N \setminus S_1) \cup L} (L) = B([S_1])|N'=(N \setminus S_2) - B([S_1])$$

(8)

$$\psi^{intra}_{2} = \sum_{L \subseteq S_2, |L| > 1} I^{v(N \setminus S_2) \cup L} (L) - \sum_{L \subseteq S_2, |L| > 1} I^{v(N \setminus S_2) \cup L} (L) = B([S_2])|N'=(N \setminus S_1) - B([S_2])$$

(9)

$\psi^{inter}_{1}$ represents all potential interaction benefits caused by coalitions whose elements are selected from both $S_1$ and $S_2$. $B([S_1])|N'=(N \setminus S_2)$ denotes interaction benefits of the singleton $[S_1]$, when the set of players in the game is $N'=(N \setminus S_2)$. $\psi^{intra}_{1}$ indicates the difference of internal interactions among players in the set $S_1$ in the absence and presence of players in the set $S_2$.

3.3 Interactions encoded inside a DNN

We aim to analyze interactions among words, which are encoded inside a trained DNN. Given an input sentence, we construct a tree to disentangle and quantify interactions among input words.

Given an input sentence with $n$ words, we first introduce the Shapley value of input words w.r.t. the prediction of the DNN. Here, we consider each word as a player, and the scalar output of a DNN as the aforementioned reward in the game. If a DNN has a scalar output, we can take the scalar output as the award $v$. If the DNN outputs a vector for multi-category classification, we select the score before the softmax layer corresponding to the true class as the award score. To compute $v(S)$, we mask words in $N \setminus S$ in the input sentence, and feed the modified input into the DNN. The embedding of the masked word is set to a dummy vector, which refers to a padding of the input to the DNN. Then, the Shapley value of each word $a$ is approximated using a sampling-based method [2].

As Figure [1] shows, we construct a binary tree with $n$ leaf nodes. Each leaf node represents a word, while each non-leaf node represents a constituent. Two adjacent nodes with strong interactions will be merged into a node in the next layer. For each sub-structure of a parent node $S$ with two child nodes $S_l$ and $S_r$, we can obtain the following equation according to Equation [4].

$$B([S]) = B([S_l]) + B([S_r]) + B_{between}(S_l, S_r)$$

$$= B([S_l]) + B([S_r]) + B([S_{lr}]) + B_{between}(S_{lr}, S_{rr}) + B_{between}(S_{lr}, S_{rr}) + B_{between}(S_l, S_r)$$

(10)

$B([S])$ can be recursively decomposed into the sum of interaction benefits between two child nodes of all non-leaf nodes. Please see the supplementary material for the proof.

3.4 Metrics for interactions and the construction of a tree

**Metrics for interactions.** Besides $B([S_l])$, $B([S_r])$ and $B_{between}(S_l, S_r)$, we define three additional metrics to provide insightful analysis of interactions among words. Let us consider a sub-structure of
The interaction benefit $B_{ab}$ is more significant than $B_{a'a}$ and $B_{bb'}$, so the tree merges $a$ and $b$ to form a parent node $c$. As Figure 3 shows, $a'$ is the left adjacent node of $a$, and $b'$ is the right adjacent node of $b$. We propose the metric density of modeled interactions for a candidate coalition such as $\{a, b\}$, denoted by $r(a, b)$. This metric measures the ratio of interaction benefits between two adjacent nodes $a$ and $b$ to total interaction benefits related to $a$ and $b$. The density of modeled interactions is approximated as follows.

$$r(a, b) = \frac{\text{interaction benefits between } a \text{ and } b}{\text{total interaction benefits related to } a \text{ and } b} \approx \frac{|B_{ab}|}{|B_{aa'}| + |B_{bb'}| + |\phi_a| + |\phi_b|}$$  \hspace{1cm} (11)

where $B_{ab} = B_{\text{between}}(S_a, S_b)$, $\phi_a$ and $\phi_b$ can be approximated as $\phi^e(S\setminus S_a)\cup(S\setminus S_b)$, respectively. To measure interaction benefits that are not represented by the tree, a metric called density of unmodeled interactions denoted by $s(a, b)$ is given.

$$s(a, b) = \frac{\text{unmodeled interaction benefits}}{\text{total interaction benefits related to } a \text{ and } b} \approx \frac{|B_{a'a}| + |B_{bb'}|}{|B_{aa'}| + |B_{bb'}| + |\phi_a| + |\phi_b|}$$  \hspace{1cm} (12)

Note that neither $r(a, b)$ nor $s(a, b)$ is an accurate estimation of the ratio of interactions. If two constituents are far away (e.g. not adjacent), their interaction benefits are usually small and sometimes can be neglected. Therefore, we only consider interaction benefits between adjacent nodes (i.e. $B_{a'a}$, $B_{ab}$, $B_{bb'}$). We have demonstrated very little effects of such neglection in Table 3. In addition, according to Equation (6), we have $B_{\text{between}}(S_t, S_r) = \psi^{\text{inter}} + \psi^{\text{intra}}_l + \psi^{\text{intra}}_r$. Therefore, we define the following metric to measure the ratio of inter-constituent interactions.

$$t = \frac{\psi^{\text{inter}}}{\psi^{\text{inter}} + \psi^{\text{intra}}_l + \psi^{\text{intra}}_r}$$  \hspace{1cm} (13)

**Construction of a tree.** We introduce a method to construct a tree structure. We use the metric $r(a, b)$ in Equation (11) to quantify the significance of interactions between two adjacent constituents, and to guide the construction of the tree. We are given a trained DNN and an input sentence. The DNN can be trained for various tasks, such as sentiment classification, and estimation of linguistic acceptability. We construct the tree in a bottom-up manner. Let $\Omega$ denote the set of current candidate nodes to merge. In the beginning, each word $a_i$ of the input sentence is initialized as a leaf node, $\Omega = \{a_1, a_2, ..., a_n\}$. In each step, we compute the value of each pair of adjacent nodes $r(a_i, a_{i+1})$. Then, we select and merge two adjacent nodes with the largest value of $r(a_i, a_{i+1})$. In this way, we use a greedy strategy to build up the tree, so that salient interactions among words are represented.

### 4 Experiments

- **Instability and accuracy of Shapley values.** According to Equation (1), the accurate computation of Shapley values was NP-hard. Castro et al. [3] proposed a sampling-based method to approximate...
Table 1: The rate of incorrect extractions of word interactions, which verifies the assumption that effects of non-adjacent nodes can be neglected on the SST-2 dataset (see the supplementary material for more results).

| # of merges | BERT  | ELMo  | CNN   | LSTM  |
|-------------|-------|-------|-------|-------|
| 1           | 0.00  | 0.02  | 0.01  | 0.06  |
| 2           | 0.00  | 0.06  | 0.02  | 0.13  |
| 3           | 0.00  | 0.12  | 0.02  | 0.19  |
| 4           | 0.03  | 0.15  | 0.07  | 0.15  |
| 5           | 0.03  | 0.16  | 0.07  | 0.14  |

Table 3: Comparison of the correctness of the extracted interactions on the AND-OR dataset.

| F1       | Recall |
|----------|--------|
| Our method | 45.1%  | 96.8%  |
| SHAP interaction | 38.6%  | 80.9%  |
| Random   | 13.2%  | 27.6%  |
| LB       | 8.4%   | 18.1%  |
| RB       | 4.3%   | 10.0%  |

Figure 5: Examples of the phenomenon that constituents with distinct emotional attitudes have strong interactions and are extracted in the first three steps for BERT learned on the SST-2 dataset.

Table 2: Fitness (the unlabeled F1) between the extracted trees from NLP models and syntactic trees, which demonstrates that interactions encoded in a DNN are not quite related to the syntactic structure.

| Dataset    | BERT  | ELMo  | CNN   | LSTM  |
|------------|-------|-------|-------|-------|
| CoLA       | 39.85%| 17.08%| 16.69%| 14.07%|
| SST-2      | 19.58%| 18.65%| 12.82%| 32.68%|
| Transformer| Random| LB    | RB    |       |
| CoLA       | 3.79% | 15.18%| 2.68% | 60.46%|
| SST-2      | 26.19%| 19.95%| 12.27%| 47.35%|

We aimed to evaluate whether the extracted interaction benefits were accurate enough when the number of sampling times was greater than 1000. We found that when $T \geq 1000$, we obtained stable Shapley values.

In addition, we also evaluated the accuracy of the estimation of interaction benefits $B([S])$. The problem was that the ground truth value of $B([S])$ was computed using the NP-hard brute-force method in Equation (1). Considering the NP-hard computational cost, we only conducted such evaluations on sentences with no more than 10 words. The average absolute difference (i.e. the error) between the estimated $B([S])$ and its ground truth value over all sentences is reported in Figure 2(b).

We found that the estimated interaction benefits were accurate enough when the number of sampling times was greater than 1000.

**Effects of non-adjacent nodes.** To compute $r(a, b)$, we only considered interaction benefits between two adjacent nodes, and assumed that interactions of non-adjacent nodes were much less significant than those of adjacent nodes. To verify this assumption, we defined the following metric to quantify the interaction benefit $r'(a, c)$ between two non-adjacent nodes $a$ and $c$, and evaluated whether the most salient interaction between adjacent nodes $a$, $b$ detected by our method was more significant than interactions between all potential non-adjacent nodes. We use $r'(a, c) = |B_{ac}||B_{ac'}| + |B_{a'c}||B_{ac}| + |B_{a'c'}||B_{ac'}| + |B_{ac'}||B_{c'a}||B_{c'a'}|$ to quantify the interaction density between non-adjacent nodes $a$ and $c$, where $a'$ and $a''$ were the left and right adjacent nodes of $a$, $c'$ and $c''$ were the left and right adjacent nodes of $c$. If the interaction density $r(a, b)$ estimated by our method was higher than that between potential non-adjacent nodes, we considered this as a correct extraction of word interactions. Table 4 reports the rate of incorrect extractions of word interactions over all sentences during the construction of the tree (please see the supplementary material for more results). Based on this assumption, our method performed correctly in most cases.

**Correctness of the extracted interaction.** We aimed to evaluate whether the extracted interaction objectively reflected the true interaction in the model, but the core challenge was that it was impossible...
to annotate ground-truth interactions between words. It was because the human’s understanding of word interactions was not necessarily equivalent to objective interactions encoded in a DNN. In this way, we constructed a dataset with ground-truth interactions between the inputs, as follows.

We constructed a dataset with 2048 models. Each model was implemented as a boolean function, whose input was 11 binary variables \( a_1, a_2, \ldots, a_{11} \in \{0, 1\} \). The output of the model was a binary variable which consisted of AND, OR operations in a tree structure (e.g. the tree in Figure 4). We evaluated whether the extracted interaction could reflect the true AND, OR constituents in the input.

The unlabeled F1 and unlabeled recall were used to evaluate the correctness of the extracted interaction. We compared our method with four baselines. The first baseline was \[22\], which defined a type of two-player interaction (i.e. SHAP interaction), and we extended this technique to construct a tree. I.e. we merged the two adjacent nodes with the largest absolute SHAP interaction value. Since there was no other method to construct a tree for interactions, the other three baselines Random, left-branching (LB) and right-branching (RB) trees (used in \[29\]) were selected to show the performance of trivial solutions. As Table 3 shows, our method outperformed all baselines. Note that theoretically, there did not exist a 100% F1 score, because the extracted binary tree was naturally different from the ground-truth n-ary tree.

### Analysis of DNNs based on interactions

We learned DNNs for binary sentiment classification based on the SST-2 dataset \[34\], and learned DNNs to predict whether a sentence was linguistically acceptable based on the CoLA dataset \[43\]. For each task, we learned five DNNs, including the BERT \[7\], the ELMo \[25\], the CNN proposed in \[16\], the two-layer unidirectional LSTM \[12\], and the Transformer \[39\].

We used our method to extract tree structures that encoded interactions among words inside various trained DNNs. Figure 5 illustrates trees extracted from BERT on different tasks. (1) For the linguistic acceptability task, BERT usually combined noun phrases firstly, while the subject was combined almost at last. ELMo and LSTM were prone to construct a tree with a “subject+verb-phrase+noun/adjective-phrase” structure. CNN usually extracted small constituents including a preposition or an article, e.g. “afraid of,” “fix the.” Transformer tended to encode interactions among adjacent constituents sequentially. (2) For the sentiment analysis task, as Figure 5 shows, most trees of these DNNs usually extracted constituents with distinct positive/negative emotional attitudes in early stages (please see the supplementary material for more results of different models).

**Comparison of the fitness between the extracted trees and syntactic trees:** Furthermore, we compared the fitness between the automatically extracted tree and the syntactic tree of the sentence. To this end, given an input sentence, we used the Berkeley Neural Parser \[17\] to generate the syntactic tree as the ground-truth.\(^\text{3}\) We used the unlabeled F1 to evaluate the fitness. Experimental results are reported in Table 2 which demonstrates the logic of interactions modeled by the DNN was significantly different from human knowledge.

\(^\text{3}\)The parser’s performance was good enough to take its parsing results as ground-truth.
In addition, our method can be also applied to build a tree for interactions w.r.t. the computation of features in an intermediate layer. Please see the supplementary material for details of such experiments.

5 Conclusions

In this paper, we have defined and extracted interaction benefits among words encoded in a DNN, and have used a tree structure to organize word interactions hierarchically. Besides, six metrics are defined to disentangle and quantify interactions among words. Our method can be regarded as a generic tool to objectively diagnose various DNNs for NLP tasks, which provides new insights of these DNNs.

References

[1] David Bau, Bolei Zhou, Aditya Khosla, Aude Oliva, and Antonio Torralba. Network dissection: Quantifying interpretability of deep visual representations. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pages 6541–6549, 2017.

[2] Javier Castro, Daniel Gómez, and Juan Tejada. Polynomial calculation of the shapley value based on sampling. Computers & Operations Research, 36(5):1726–1730, 2009.

[3] Jianbo Chen and Michael I Jordan. Ls-tree: Model interpretation when the data are linguistic. arXiv preprint arXiv:1902.04187, 2019.

[4] Jihun Choi, Kang Min Yoo, and Sang-goo Lee. Learning to compose task-specific tree structures. In Thirty-Second AAAI Conference on Artificial Intelligence, 2018.

[5] Junyoung Chung, Sungjin Ahn, and Yoshua Bengio. Hierarchical multiscale recurrent neural networks. CoRR, abs/1609.01704, 2016. URL http://arxiv.org/abs/1609.01704.

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

[7] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. arXiv preprint arXiv:1810.04805, 2018.

[8] Andrew Drozdov, Patrick Verga, Mohit Yadav, Mohit Iyyer, and Andrew McCallum. Unsupervised latent tree induction with deep inside-outside recursive auto-encoders. In Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long and Short Papers), pages 1129–1141, Minneapolis, Minnesota, June 2019. Association for Computational Linguistics. doi: 10.18653/v1/N19-1116. URL https://www.aclweb.org/anthology/N19-1116.

[9] Chris Dyer, Adhiguna Kuncoro, Miguel Ballesteros, and Noah A. Smith. Recurrent neural network grammars. In Proceedings of the 2016 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, pages 199–209, San Diego, California, June 2016. Association for Computational Linguistics. doi: 10.18653/v1/N16-1024. URL https://www.aclweb.org/anthology/N16-1024.

[10] 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.

[11] Peyton Greenside, Tyler Shimko, Polly Fordyce, and Anshul Kundaje. Discovering epistatic feature interactions from neural network models of regulatory DNA sequences. Bioinformatics, 34(17):i629–i637, 09 2018. ISSN 1367-4803. doi: 10.1093/bioinformatics/bty575. URL https://doi.org/10.1093/bioinformatics/bty575.

[12] Sepp Hochreiter and Jürgen Schmidhuber. Long short-term memory. Neural computation, 9(8):1735–1780, 1997.

[13] Phu Mon Htut, Kyunghyun Cho, and Samuel R Bowman. Inducing constituency trees through neural machine translation. arXiv preprint arXiv:1909.10056, 2019.

[14] Joseph D Janizek, Pascal Sturmels, and Su-In Lee. Explaining explanations: Axiomatic feature interactions for deep networks. arXiv preprint arXiv:2002.04138, 2020.
[15] Xisen Jin, Zhongyu Wei, Junyi Du, Xiangyang Xue, and Xiang Ren. Towards hierarchical importance attribution: Explaining compositional semantics for neural sequence models. In International Conference on Learning Representations, 2020. URL https://openreview.net/forum?id=BkxRRkK5kWz

[16] Yoon Kim. Convolutional neural networks for sentence classification. In Proceedings of the 2014 Conference on Empirical Methods in Natural Language Processing (EMNLP), pages 1746–1751, Doha, Qatar, October 2014. Association for Computational Linguistics. doi: 10.3115/v1/D14-1181. URL https://www.aclweb.org/anthology/D14-1181.

[17] Nikita Kitaev and Dan Klein. Constituency parsing with a self-attentive encoder. In Proceedings of the 56th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers), Melbourne, Australia, July 2018. Association for Computational Linguistics.

[18] Nikita Kitaev, Steven Cao, and Dan Klein. Multilingual constituency parsing with self-attention and pre-training. In Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics, pages 3499–3505, Florence, Italy, July 2019. Association for Computational Linguistics. doi: 10.18653/v1/P19-1340. URL https://www.aclweb.org/anthology/P19-1340.

[19] Bowen Li, Lili Mou, and Frank Keller. An imitation learning approach to unsupervised parsing. In Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics, pages 3485–3492, Florence, Italy, July 2019. Association for Computational Linguistics. doi: 10.18653/v1/P19-1338. URL https://www.aclweb.org/anthology/P19-1338.

[20] Xiang Lisa Li and Jason Eisner. Specializing word embeddings (for parsing) by information bottleneck. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pages 2744–2754, Hong Kong, China, November 2019. Association for Computational Linguistics. doi: 10.18653/v1/D19-1276. URL https://www.aclweb.org/anthology/D19-1276.

[21] Scott M Lundberg and Su-In Lee. A unified approach to interpreting model predictions. In Advances in neural information processing systems, pages 4765–4774, 2017.

[22] Scott M Lundberg, Gabriel G Erion, and Su-In Lee. Consistent individualized feature attribution for tree ensembles. arXiv preprint arXiv:1802.03888, 2018.

[23] Khalil Mrini, Franck Dernoncourt, Trung Bui, Walter Chang, and Ndpaa Nakashole. Rethinking self-attention: An interpretable self-attentive encoder-decoder parser. arXiv preprint arXiv:1911.03875, 2019.

[24] W. James Murdoch, Peter J. Liu, and Bin Yu. Beyond word importance: Contextual decomposition to extract interactions from LSTMs. In International Conference on Learning Representations, 2018. URL https://openreview.net/forum?id=rkRwGg-0Z.

[25] Matthew Peters, Mark Neumann, Mohit Iyyer, Matt Gardner, Christopher Clark, Kenton Lee, and Luke Zettlemoyer. Deep contextualized word representations. In Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 1 (Long Papers), pages 2227–2237, New Orleans, Louisiana, June 2018. Association for Computational Linguistics. doi: 10.18653/v1/N18-1202. URL https://www.aclweb.org/anthology/N18-1202.

[26] Alessandro Raganato and Jörg Tiedemann. An analysis of encoder representations in transformer-based machine translation. In Proceedings of the 2018 EMNLP Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP, pages 287–297, Brussels, Belgium, November 2018. Association for Computational Linguistics. doi: 10.18653/v1/W18-5431. URL https://www.aclweb.org/anthology/W18-5431.

[27] Emily Reif, Ann Yuan, Martin Wattenberg, Fernanda B Viegas, Andy Coenen, Adam Pearce, and Been Kim. Visualizing and measuring the geometry of bert. In H. Wallach, H. Larochelle, A. Beygelzimer, F. d’Alché-Buc, E. Fox, and R. Garnett, editors, Advances in Neural Information Processing Systems 32, pages 8594–8603. Curran Associates, Inc., 2019. URL https://papers.nips.cc/paper/9065-visualizing-and-measuring-the-geometry-of-bert.pdf.

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

[29] Yikang Shen, Zhouhan Lin, Chin wei Huang, and Aaron Courville. Neural language modeling by jointly learning syntax and lexicon. In International Conference on Learning Representations, 2018. URL https://openreview.net/forum?id=rkgULb-0W.
[30] Yikang Shen, Shawn Tan, Alessandro Sordoni, and Aaron Courville. Ordered neurons: Integrating tree structures into recurrent neural networks. In International Conference on Learning Representations, 2019. URL https://openreview.net/forum?id=B1l6qiR5F7

[31] Haoyue Shi, Hao Zhou, Jiaze Chen, and Lei Li. On tree-based neural sentence modeling. In Proceedings of the Conference on Empirical Methods in Natural Language Processing, 2018.

[32] Karen Simonyan, Andrea Vedaldi, and Andrew Zisserman. Deep inside convolutional networks: Visualising image classification models and saliency maps. CoRR, abs/1312.6034, 2014.

[33] Chandan Singh, W. James Murdoch, and Bin Yu. Hierarchical interpretations for neural network predictions. In International Conference on Learning Representations, 2019. URL https://openreview.net/forum?id=SkEzqroOctQ

[34] Richard Socher, Alex Perelygin, Jean Wu, Jason Chuang, Christopher D Manning, Andrew Y Ng, and Christopher Potts. Recursive deep models for semantic compositionality over a sentiment treebank. In Proceedings of the 2013 conference on empirical methods in natural language processing, pages 1631–1642, 2013.

[35] Daria Sorokina, Rich Caruana, Mirek Riedewald, and Daniel Fink. Detecting statistical interactions with additive groves of trees. In Proceedings of the 25th international conference on Machine learning, pages 1000–1007, 2008.

[36] Kai Sheng Tai, Richard Socher, and Christopher D. Manning. Improved semantic representations from tree-structured long short-term memory networks. In Proceedings of the 53rd Annual Meeting of the Association for Computational Linguistics and the 7th International Joint Conference on Natural Language Processing (Volume 1: Long Papers), pages 1556–1566, Beijing, China, July 2015. Association for Computational Linguistics. doi: 10.3115/v1/P15-1150. URL https://www.aclweb.org/anthology/P15-1150

[37] Michael Tsang, Dehua Cheng, and Yan Liu. Detecting statistical interactions from neural network weights. In International Conference on Learning Representations, 2018. URL https://openreview.net/forum?id=ByOzbggRZ

[38] Michael Tsang, Hanpeng Liu, Sanjay Purushotham, Pavankumar Murali, and Yan Liu. Neural interaction transparency (nit): Disentangling learned interactions for improved interpretability. In S. Bengio, H. Wallach, H. Larochelle, K. Grauman, N. Cesa-Bianchi, and R. Garnett, editors, Advances in Neural Information Processing Systems 31, pages 5804–5813. Curran Associates, Inc., 2018.

[39] Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. In Advances in neural information processing systems, pages 5998–6008, 2017.

[40] Elena V oita, Rico Sennrich, and Ivan Titov. The bottom-up evolution of representations in the transformer: A study with machine translation and language modeling objectives. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pages 4396–4406, Hong Kong, China, November 2019. Association for Computational Linguistics. doi: 10.18653/v1/D19-1448. URL https://www.aclweb.org/anthology/D19-1448

[41] Xing Wang, Zhaopeng Tu, Longyue Wang, and Shuming Shi. Self-attention with structural position representations. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pages 1403–1409, Hong Kong, China, November 2019. Association for Computational Linguistics. doi: 10.18653/v1/D19-1145. URL https://www.aclweb.org/anthology/D19-1145

[42] Yaushian Wang, Hung-Yi Lee, and Yun-Nung Chen. Tree transformer: Integrating tree structures into self-attention. In Proceedings of the 2019 Conference on Empirical Methods in Natural Language Processing and the 9th International Joint Conference on Natural Language Processing (EMNLP-IJCNLP), pages 1061–1070, Hong Kong, China, November 2019. Association for Computational Linguistics. doi: 10.18653/v1/D19-1098. URL https://www.aclweb.org/anthology/D19-1098

[43] Alex Warstadt, Amanpreet Singh, and Samuel R Bowman. Neural network acceptability judgments. arXiv preprint arXiv:1805.12471, 2018.

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

[45] Dani Yogatama, Phil Blunsom, Chris Dyer, Edward Grefenstette, and Wang Ling. Learning to compose words into sentences with reinforcement learning. arXiv preprint arXiv:1611.09100, 2016.
[46] Dani Yogatama, Yishu Miao, Gabor Melis, Wang Ling, Adhiguna Kuncoro, Chris Dyer, and Phil Blunsom. Memory architectures in recurrent neural network language models. In *International Conference on Learning Representations*, 2018. URL https://openreview.net/forum?id=SkFqf0lAZ.
A Properties of Shapley values

In this section, we discuss about four desirable properties of Shapley values, which are mentioned in Line 118 of the paper.

In game theory, the Shapley value is a unique value function that satisfies all the following axioms [44]:

• Linearity axiom: When two games \( v \) and \( w \) are combined into a single game \( v + w \), their Shapley values can be added, i.e. \( \phi(v+w)(i) = \phi(v)(i) + \phi(w)(i) \) for each player \( i \) in \( N \). Similarly, for any \( c \in \mathbb{R} \) and \( i \in N \), there will be \( \phi(cv)(i) = c\phi(v)(i) \).

• Dummy axiom: A player \( i \in N \) is referred to as a dummy player if \( v(S \cup \{i\} ) = v(S) + v(i) \) for each subset \( S \subseteq N \setminus \{i\} \). Thus, if \( i \in N \) is a dummy player, \( \phi(v)(i) = v(i) \), which indicates player \( i \) has no interactions to any coalition.

• Symmetry axiom: Given two players \( i, j \in N \), if \( v(S \cup \{i\}) = v(S \cup \{j\}) \) for each subset \( S \subseteq N \setminus \{i, j\} \), \( \phi(v)(i) = \phi(v)(j) \). In other words, if two players have the same interactions with all other players in the game, then they have the same Shapley value.

• Efficiency axiom: The sum of Shapley values of all players in \( N \) is equal to the award of all players in \( N \) (i.e. \( \sum_{i \in N} \phi(i) = v(N) \)). This axiom guarantees the overall award can be distributed to all players in the game.

B Interactions among multiple players

In this section, we mainly discuss about how to extend interactions between two players to interactions among multiple players, which is mentioned in Line 151 of the paper.

Given a game \( v \) with \( n \) players, \( N = \{1, 2, \ldots, n\} \) is the set of \( n \) players. If player \( a \) and player \( b \) form a coalition \( S_{ab} = \{a, b\} \), we regard the coalition as a new singleton player \( [S_{ab}] \). We define the interaction benefit between players \( a \) and \( b \) as \( B([S_{ab}]) \).

\[
B([S_{ab}]) = \phi^{v(N\setminus\{a,b\}) \cup ([S_{ab}])}([S_{ab}]) - (\phi^{v(N\setminus\{a\})}(a) + \phi^{v(N\setminus\{b\})}(b))
\]  

Therefore, we extend the interaction between two players to interactions among multiple players. For example, if a set of players \( S \) form a coalition, which is regarded as a new singleton player \( [S] \), the interaction benefit among players in the coalition is defined as follows (also see Equation (2) of the paper).

\[
B([S]) = \phi^{v(N\setminus\{S\}) \cup ([S])}([S]) - \sum_{a \in S} \phi^{v(N\setminus\{a\}) \cup ([S])}(a)
\]

C Elementary interaction components

In this section, we introduce the elementary interaction component in more detail, which is mentioned in Line 166 of the paper.

In a game \( v \), the elementary interaction component of players among coalition \( S \subseteq N \) is denoted by \( I^v(S) \). The definition of the elementary interaction component [10] is given as follows.

\[
\forall S \subseteq N, \quad I^v(S) = \sum_{T \subseteq N \setminus S} \frac{(n-t-s)!}{(n-s+1)!} \sum_{L \subseteq S} (-1)^{s-l} v(L \cup T)
\]

where \( n, t, s, \) and \( l \) are the size of the corresponding sets \( N, T, S, \) and \( L \), respectively. Note that for a singleton player, the elementary interaction component corresponds to the Shapley value, i.e. \( I^v(a) = \phi^v(a) \) where \( a \) is a singleton player.

If a set of players \( S \) form a coalition, we regard the coalition as a singleton player \( [S] \). Let us take two players \( a \) and \( b \) for example. If players \( a \) and \( b \) form a coalition \( S = \{a, b\} \), which can be considered as a new singleton player \( [S] \). The interaction benefit between players \( a \) and \( b \) is as follows.

\[
I^v(\{a, b\}) = I^v(N\setminus\{a,b\}) \cup ([a,b]) ([a,b]) - I^v(N\setminus\{a\}) (a) - I^v(N\setminus\{b\}) (b)
\]

\[
= \phi^v(N\setminus\{a,b\}) \cup ([a,b]) ([a,b]) - \phi^v(N\setminus\{a\}) (a) - \phi^v(N\setminus\{b\}) (b)
\]
Therefore, if the marginal award of the coalition $\phi^{N\setminus\{a,b\} \cup \{\{a,b\}\}}_S$ is larger than the sum of marginal awards of players $a$ and $b$ (i.e., $\phi^{N\setminus\{a\}}_S(a) + \phi^{N\setminus\{b\}}_S(b)$), players $a$ and $b$ are likely to cooperate in the game $v$. In other words, the positive (or negative) value of $I^v(S)$ indicates a positive (or negative) interaction between players $a$ and $b$.

Besides, $I^v(S)$ satisfies the following recursive axiom for each $S \subseteq N$, $|S| > 1$. $K$ is a non-empty proper subset of $S$.

$$I^v(S) = I^v(N\setminus S \cup \{\{S\}\}) - \sum_{K \subseteq S, K \neq \emptyset} I^v(S \setminus K)$$

$$= I^v(N\setminus S \cup \{\{S\}\}) - \sum_{S' \subseteq S, S' \neq \emptyset} I^v(N\setminus S \cup S')$$

(18)

D Proof of the relationship between interaction benefits and elementary interaction components

In this section, we mainly prove the relationship between interaction benefits and elementary interaction components, which is mentioned in Line 174 of the paper (also see Equation (5) of the paper).

According to Equation (15) and Equation (18), we can establish the relationship between the interaction benefit and the elementary interaction component.

$$B([S]) = \phi^{N\setminus S \cup \{\{S\}\}}_S([S]) - \sum_{a \in S} \phi^{N\setminus S \cup \{\{a\}\}}_S(a)$$

$$= I^v(N\setminus S \cup \{\{S\}\}) - \sum_{a \in S} I^v(N\setminus S \cup \{\{a\}\})$$

$$= \sum_{S' \subseteq S, |S'| > 1} I^v(N\setminus S \cup S')$$

(19)

E Proof of interactions between two sets of players $B_{between}(S_1, S_2)$

In this section, we mainly prove the fine-grained analysis of interactions between two sets of players, which is mentioned in Line 177 of the paper (also see Equation (6) of the paper).

Given a set of players $S$, we can split $S$ into two subsets $S_1$ and $S_2$, $S_1 \cap S_2 = \emptyset$, $S_1 \cup S_2 = S$. According to Equation (19), we have:

$$B([S]) = \sum_{L \subseteq S, |L| > 1} I^v(N\setminus S \cup L)$$

(20)

$$B([S_1]) = \sum_{L \subseteq S_1, |L| > 1} I^v(N\setminus S_1 \cup L)$$

(21)

$$B([S_2]) = \sum_{L \subseteq S_2, |L| > 1} I^v(N\setminus S_2 \cup L)$$

(22)

Therefore, we derive the following equation.

$$B([S]) = B([S_1]) + B([S_2]) + \sum_{L \subseteq S, |L| > 1} I^v(N\setminus S \cup L)$$

$$= \sum_{L \subseteq S_1, |L| > 1} I^v(N\setminus S_1 \cup L) + \sum_{L \subseteq S_2, |L| > 1} I^v(N\setminus S_2 \cup L)$$

$$= B([S_1]) + B([S_2]) + B_{between}(S_1, S_2)$$

(23)
\[ B_{between}(S_1, S_2) = \sum_{L \subseteq S_1 | L > 1} I^{(N \setminus S)_I \cup L}(L) - \sum_{L \subseteq S_2 | L > 1} I^{(N \setminus S_2)_I \cup L}(L) - \sum_{L \subseteq S_1 \cup S_2 | L > 1} I^{(N \setminus S_1 \cup S_2)_I \cup L}(L) \]

\[ = \sum_{L \subseteq S_1, L \subseteq S_2, L \subseteq S_1 \cup S_2 | L > 1} I^{(N \setminus S)_I \cup L}(L) + \sum_{L \subseteq S_1 \setminus | L > 1} I^{(N \setminus S_1)_I \cup L}(L) - \sum_{L \subseteq S_1 \setminus | L > 1} I^{(N \setminus S_2)_I \cup L}(L) + \sum_{L \subseteq S_2 \setminus | L > 1} I^{(N \setminus S_2)_I \cup L}(L) \]

\[ = \psi^{inter} + \psi^{intra} + \psi^{intra} \quad (24) \]

Where

\[ \psi^{inter} = \sum_{L \subseteq S_1, L \subseteq S_2, L \subseteq S_1 \cup S_2 | L > 1} I^{(N \setminus S)_I \cup L}(L) \quad (25) \]

\[ \psi^{intra} = \sum_{L \subseteq S_1 \setminus | L > 1} I^{(N \setminus S_1)_I \cup L}(L) - \sum_{L \subseteq S_2 \setminus | L > 1} I^{(N \setminus S_2)_I \cup L}(L) \]

\[ = B([S_1])_I^{(N \setminus S)_I} - B([S_1]) \quad (26) \]

\[ \psi^{intra} = \sum_{L \subseteq S_2 \setminus | L > 1} I^{(N \setminus S_2)_I \cup L}(L) - \sum_{L \subseteq S_2 \setminus | L > 1} I^{(N \setminus S_2)_I \cup L}(L) \]

\[ = B([S_2])_I^{(N \setminus S)_I} - B([S_2]) \quad (27) \]

\[ B_{between}(S_1, S_2) \] reflects all interactions across players from \( S_1 \) and \( S_2 \).

### F Proof of the decomposition of \( B([S]) \)

In this section, we mainly prove the decomposition of the interaction benefit \( B([S]) \), which is mentioned in Line 199 of the paper (also see Equation (10) of the paper).

\[ B([S]) = B([S_1]) + B([S_2]) + B_{between}(S_1, S_2) \]

\[ = B([S_1]) + B([S_2]) + B_{between}(S_1, S_2) + B_{between}(S_1, S_{1r}) + B_{between}(S_2, S_{2r}) \]

\[ = \sum_{H \in \text{non-leaf nodes}} B_{between}(H_l, H_r) \quad (28) \]

Note that the interaction benefit of a leaf node is zero, so only interaction benefits between two child nodes of non-leaf nodes will be left at the end of the recursion in Equation (28).

### G Experimental Results

We provided more results of “Effects of non-adjacent nodes” (Line 246) and “Analysis of DNNs based on interactions” (Line 277) experiments in Section 4 (Line 227) of the paper, as well as further experiments to analyze interactions encoded in intermediate layers, which were mentioned in Line 297 of the paper.

- **Effects of non-adjacent nodes.** Here, we provided more results of this experiment. Specifically, as Table 4 shows, we reported the rate of incorrect extractions of word interactions over all sentences during the construction of the tree on the SST-2 dataset, and the CoLA dataset, respectively. Note that Table 4 was a complement to Table 1 of the paper.

- **Analysis of DNNs based on interactions.** (1) For the linguistic acceptability task, we provided more results of trees extracted from different NLP models on the SST-2 dataset and the CoLA dataset, respectively (see Figures 9 – 13, which were complements to Figure 6 of the paper). We found that BERT usually combined noun phrases firstly, while the subject was combined almost at last. ELMo and LSTM were prone to construct a tree with a “subject+verb-phrase+noun/adjective-phrase” structure. CNN usually extracted small constituents including a preposition or an article. Transformer tended to encode interactions among adjacent constituents sequentially. (2) For the sentiment analysis task, we found that most trees of these DNNs usually extracted constituents with distinct positive/negative emotional attitudes in early stages of the construction of the tree. More examples of this phenomenon were given in Tables 5 – 8, which were complements to Figure 5 of the paper.
Table 4: The rate of incorrect extractions of word interactions, which verifies the assumption that effects of non-adjacent nodes can be neglected on the SST-2 dataset (left) and the CoLA dataset (right).

| # of merges | BERT | ELMo | CNN | LSTM |
|-------------|------|------|-----|------|
| 1           | 0.00 | 0.02 | 0.01| 0.06 |
| 2           | 0.00 | 0.06 | 0.02| 0.13 |
| 3           | 0.00 | 0.12 | 0.02| 0.19 |
| 4           | 0.03 | 0.15 | 0.07| 0.15 |
| 5           | 0.03 | 0.16 | 0.07| 0.14 |

Table 5: Constituents extracted from ELMo in the first three steps during the construction of the tree.

| sentence                                      | 1st merge | 2nd merge | 3rd merge |
|-----------------------------------------------|-----------|-----------|-----------|
| I just loved every minute of this film .      | just      | loved     | this film |
| But it could have been worse .                | it        | could     | But       |
| Too much of humor falls flat .                | falls     | flat      | falls flat |
| There is no pleasure in watching a child suffer . | no pleasure | no pleasure | in no pleasure in watching |
| It all adds up to good fun .                  | good      | fun       | good      |

Table 6: Constituents extracted from CNN in the first three steps during the construction the tree.

| sentence                                      | 1st merge | 2nd merge | 3rd merge |
|-----------------------------------------------|-----------|-----------|-----------|
| A deep and meaningful film .                  | A deep    | meaningful film | meaningful film |
| Dense with characters and contains some thrilling moments . | thrilling moments | Dense with | and contains |
| It treats women like idiots .                  | like      | idiots    | treats     |
| Just embarrassment and a vague sense of shame . | sense     | of        | shame      |
| Just one bad idea after another .             | one       | bad       | idea after |

Table 7: Constituents extracted from LSTM in the first three steps during the construction of the tree.

| sentence                                      | 1st merge | 2nd merge | 3rd merge |
|-----------------------------------------------|-----------|-----------|-----------|
| No way i can believe this load of junk .      | this      | load      | i can     |
| Just one bad idea after another .             | bad       | idea      | one bad idea after another |
| But it could have been worse .                | been      | worse     | But       |
| There is no pleasure in watching a child suffer . | no pleasure | is no pleasure | child suffer |
| Too slow , too long and too little happens .   | too slow  | too long  | too slow  |
| It treats women like idiots .                  | like      | idiots    | It treats |

Table 8: Constituents extracted from Transformer in the first three steps during the construction of the tree.

| sentence                                      | 1st merge | 2nd merge | 3rd merge |
|-----------------------------------------------|-----------|-----------|-----------|
| No way i can believe this load of junk .      | this      | load      | i can     |
| Just one bad idea after another .             | bad       | idea      | one bad idea |
| There is no pleasure in watching a child suffer . | no pleasure | is no pleasure | child suffer |
| I just loved every minute of this film .      | loved     | every     | just loved every |
| But it could have been worse .                | been      | worse     | it could   |

16
G.1 Interactions encoded in intermediate layers.

Besides interactions w.r.t. the network output, we used our method to analyze interactions w.r.t. the computation of an intermediate-layer feature \( f \). More specifically, we used \( f_N \) and \( f_S \) to represent the intermediate-layer features when the input of the network was a set of words \( N \) and \( S \) in the sentence, respectively. Since the intermediate-layer features \( f_N \) and \( f_S \) were high dimensional vectors, we used the scalar \( \langle f_N, f_S \rangle / \|f_N\| \) to represent the award \( v(S) \), where \( \|f_N\| \) was used for normalization. In this way, we evaluated interactions encoded in different layers of BERT. The extracted trees from different intermediate layers of BERT are shown in Figure 7 (for the BERT learned on the SST-2 dataset) and Figure 8 (for the BERT learned on the CoLA dataset).

![Figure 7: The extracted trees of interactions encoded in different intermediate layers of BERT learned on the SST-2 dataset.](image-url)
Figure 8: The extracted trees of interactions encoded in different intermediate layers of BERT learned on the CoLA dataset.
Figure 9: Extracted trees of different NLP models trained on the SST-2 dataset.
Figure 10: Extracted trees of different NLP models trained on the SST-2 dataset.
Figure 11: Extracted trees of different NLP models trained on the SST-2 dataset.
Figure 12: Extracted trees of different NLP models trained on the SST-2 dataset.
Figure 13: Extracted trees of different NLP models trained on the SST-2 dataset.
Figure 14: Extracted trees of different NLP models trained on the CoLA dataset.
Figure 15: Extracted trees of different NLP models trained on the CoLA dataset.
Figure 16: Extracted trees of different NLP models trained on the CoLA dataset.
Figure 17: Extracted trees of different NLP models trained on the CoLA dataset.
Figure 18: Extracted trees of different NLP models trained on the CoLA dataset.