Attention Module is Not Only a Weight: Analyzing Transformers with Vector Norms

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Abstract

Because attention modules are core components of Transformer-based models that have recently achieved considerable success in natural language processing, the community has a great deal of interest in why attention modules are successful and what kind of linguistic information they capture. In particular, previous studies have mainly analyzed attention weights to see how much information the attention modules gather from each input to produce an output. In this study, we point out that attention weights alone are only one of the two factors determining the output of self-attention modules, and we propose to incorporate the other factor as well, namely, the transformed input vectors into the analysis. That is, we measure the norm of the weighted vectors as the contribution of each input to an output. Our analysis of self-attention modules in BERT and the Transformer-based neural machine translation system shows that the attention modules behave very intuitively, contrary to previous findings. That is, our analysis reveals that (1) BERT’s attention modules do not pay so much attention to special tokens, and (2) Transformer’s attention modules capture word alignment quite well.

1 Introduction

Transformer-based models have improved the state-of-the-art in a wide range of natural language processing (NLP) tasks (Vaswani et al., 2017; Devlin et al., 2019; Yang et al., 2019; Liu et al., 2019; Lan et al., 2020). As the success of these models has not yet been sufficiently explained, a substantial body of research has focused on their linguistic capabilities (Rogers et al., 2020). Since attention modules (Section 2) are the core components of Transformer-based models, one prominent line of research has been the analysis of correlations of attention weights with various linguistic phenomena (Clark et al., 2019; Kovaleva et al., 2019; Reif et al., 2019; Lin et al., 2019; Mareček and Rosa, 2019; Htut et al., 2019; Raganato and Tiedemann, 2018; Tang et al., 2018). However, the community has not reached a consensus about how and why attention modules work well.

To go a step further in this line of research, in this paper, we propose a novel method of analyzing the behavior of an attention module. The previous approach that tracks attention weights is based on the assumption that if an input vector gains considerable attention weight than the other input vectors, that input vector has a greater contribution to the output. In contrast, we start with the insight that the computation of an output of the attention module can be decomposed into a weighted sum of the transformed input vectors, and point out that analyzing only attention weights is insufficient to investigate the behavior of an entire attention module (Section 2). We then propose an analysis method with the norm (length) of the weighted vectors that considers the previously ignored factor as well, namely, the transformed vectors, to estimate the contribution of each input vector in the computation of the output vector (Section 3).

We first analyze the self-attention modules in BERT (Devlin et al., 2019) in our experiments (Section 4). We empirically show that the figures of the contributions of input tokens to their output hidden vectors are considerably different from what was reported in previous work. In particular, some previous reports showed several non-intuitive observations; for example, specific tokens such as commas, periods, and special tokens (e.g., separator token; [SEP]) tend to gain markedly large attention weights (Clark et al., 2019, etc.). Our experiments demonstrate that, unlike the previous attention weight-tracking approach, our norm-based method produces more intuitive observations.
Finally, we analyze the source-target attention modules in the Transformer-based neural machine translation (NMT) system (Vaswani et al., 2017) (Section 5). The properties of the NMT systems observed by using our norm-based method are markedly different from previous results — their attention modules implicitly learn word alignment in contrast to previous findings from the attention weights analysis.

The contributions of this study are as follows:

- We propose a method of analyzing an attention module based on vector norms, that considers the previously ignored factor as well as attention weights.
- We analyzed the self-attention modules in BERT using our norm-based method and found that (1) the dispersion of norms of the previously ignored vectors is large, (2) the attention module does not pay much attention to special tokens, and (3) the attention module tends to discount frequent words.
- We analyzed the source-target attention modules in a Transformer-based NMT system and found that, contrary to previous findings, the attention module implicitly performs word alignment well.

2 Background

2.1 Attention module

We briefly review the attention module\(^1\) implemented in Transformer (Vaswani et al., 2017). An overview of the attention module is shown in Figure 1. In the attention module, the output vector is calculated using the weighted sum of the input vectors, the weights, and the bias. Intuitively, when the weight assigned to a certain vector (the blue circles in Figure 1) is large, the module pays much attention to the input vector, whereas a vector with a smaller weight is paid less attention.

Here and subsequently, boldface letters such as \(x\) denote row vectors. Formally, the attention module computes each output vector \(y_i \in \mathbb{R}^d\) from the corresponding pre-update vector \(\tilde{y}_i \in \mathbb{R}^d\) and a set of input vectors \(X = \{x_1, \ldots, x_n\} \subseteq \mathbb{R}^d\) to be incorporated:

\[
y_i = \left(\sum_{j=1}^{n} \alpha_{i,j} v(x_j)\right) W^O + b^O \in \mathbb{R}^d \quad (1)
\]

\[
\alpha_{i,j} := \text{softmax} \left(\frac{q(\tilde{y}_i) k(x_j)^\top}{\sqrt{d'}}\right) \in \mathbb{R}, \quad (2)
\]

where \(q(\cdot), k(\cdot), \text{and } v(\cdot)\) are the Query, Key, and Value vectors, respectively.

\[
q(\tilde{y}_i) := \tilde{y}_i W^Q + b^Q \quad \left(W^Q \in \mathbb{R}^{d \times d'}, b^Q \in \mathbb{R}^{d'}\right)
\]

\[
k(x_j) := x_j W^K + b^K \quad \left(W^K \in \mathbb{R}^{d \times d'}, b^K \in \mathbb{R}^{d'}\right)
\]

\[
v(x_j) := x_j W^V + b^V \quad \left(W^V \in \mathbb{R}^{d \times d'}, b^V \in \mathbb{R}^{d'}\right).
\]

That is, the attention weight \(\alpha_{i,j}\) is firstly computed, then the Value vector \(v(x_j)\) is weighted by \(\alpha_{i,j}\), the weighted Value vectors are summed, and finally, the affine transformation by \(W^O \in \mathbb{R}^{d \times d}\) and \(b^O \in \mathbb{R}^d\) is applied (see Figure 1).

In the case of \(\tilde{y}_i \in X\), this module is called the Self-attention module, which is implemented in, e.g., BERT. In the attention module between the encoder and the decoder of the Transformer sequence-to-sequence model, \(X\) corresponds to the representations from the encoder stack, and vectors \(\tilde{y}_i\) and \(y_i\) correspond to the \(i\)-th token in the decoder side.

2.2 Attention module sums weighted vectors

With a simple reformulation, we can see that the attention module computes a weighted sum of input vectors. Using the linearity of the matrix product, we can rewrite Equation 1 as

\[
y_i = \sum_{j=1}^{n} \alpha_{i,j} v(x_j) W^O + b^O \in \mathbb{R}^d \quad (1)
\]
Figure 2: Overview of attention module based on Equation 3. The module computes the output vector by summing weighted vectors, where vectors with larger norms can provide a more dominant contribution. The arrows in the circles represent the corresponding vectors. The sizes of the colored circles illustrate the value of the scalar or the norm of the corresponding vector.

\[ y_i = \sum_{j=1}^{n} \alpha_{i,j} f(x_j) + b^O \]

Equation 3 shows that the attention module firstly transforms each input vector \( x \) to generate \( f(x) \) and computes attention weights \( \alpha \), then sums \( \alpha f(x) \) with a bias \( b^O \) (see Figure 2).

### 2.3 Problems with attention weight analysis

The attention module is designed to update representations by gathering relevant information from the input sequence. Therefore, in prior studies, it has been investigated how much information from each input is used to generate an output by analyzing the magnitude of attention weights (Clark et al., 2019; Kovaleva et al., 2019; Reif et al., 2019; Lin et al., 2019; Mareček and Rosa, 2019; Hüt et al., 2019; Raganato and Tiedemann, 2018; Tang et al., 2018).

Analyses in this line of research are based on the assumption that if an input vector is assigned a larger attention weight than other input vectors, then that input vector contributes more to the output vector than the others. However, this assumption disregards the magnitude of the vectors to be weighted. Intuitively, with attention weights being equal, a larger vector will contribute more to the output vector than a smaller vector.

The problem of neglecting the effect of \( f(x_j) \) is illustrated in Figure 2. Here, the transformed vector \( f(x_1) \) for input \( x_1 \) is assumed to be very small (\( \|f(x_1)\| \approx 0 \)) while it gains considerably greater attention weight \( \alpha_{i,1} \) than other input vectors. In such a case, even if the contribution of input \( x_1 \) to the output vector, say, \( y_i \) is very small, looking at the attention weight alone might lead to a wrong observation that this input vector \( x_1 \) had the greatest contribution to output \( y_i \).

In fact, in previous studies, analysis based on attention weights has produced some non-intuitive observations, probably due to this flaw. For example, Clark et al. (2019) reported that input vectors for specific tokens such as commas, periods, and separator tokens [SEP] tend to gain remarkably large attention weights, whereas intuitively, their contributions to the pre-training tasks (i.e., masked word prediction and next sentence prediction) are expected to be limited compared with more informative content words.

### 3 Proposal: norm as attention degree

As described in Section 2.3, in prior work, only \( \alpha_{i,j} \) has been considered in Equation 3 but the effect of \( f(x_j) \) is neglected. Our main proposal in this paper is to estimate the contribution of the input vector \( x_j \) to the output vector \( y_i \) by \( \alpha_{i,j}f(x_j) \) instead. As we will show, this difference does matter in the exploration of the behavior of attention modules.

To address the aforementioned issue, we propose to use \( \|\alpha f(x)\| \), which is the standard Euclidean norm (length) of the weighted, transformed vector in Equation 3, as a novel method for analyzing the behavior of the attention module. Unlike in previous studies in which attention weights alone were observed, we analyze the behavior of \( \|\alpha f(x)\| \) and \( \|f(x)\| \) as well as \( \alpha \) to gain a more in-depth view of how the attention modules work. We call this proposed way of analyzing the attention module the norm-based analysis in contrast to the previous weight-based analysis.

In the experiments section (Section 4 and 5), we empirically show that by using norm-based analysis instead of weight-based analysis, one can gain more intuitive and meaningful observations on the behavior of the attention modules. It is worth noting that our norm-based analysis can be naturally extended to the multi-head attention module implemented in the Transformer, BERT, and others because the multi-head attention module is a natural extension of the attention module and also it
is linearly decomposable; i.e., attention heads (attention modules) are arranged in parallel and the output of the multi-head attention module is the sum of the output vectors of all the heads.

4 Experiments: BERT

Overview: First, we preliminarily show that previously ignored effect, namely, the norm of the transformed vectors, could affect the results in analyzing the attention modules in BERT (Section 4.1). Second, by using our norm-based analysis, we re-examine the reports on BERT in the previous weight-based analysis (Section 4.2). Finally, we introduce the previously overlooked property of BERT (Section 4.3).

General settings: Following previous studies (Clark et al., 2019; Kovaleva et al., 2019; Reif et al., 2019; Lin et al., 2019; Htut et al., 2019), we analyzed the self-attention modules in the pre-trained BERT-base (uncased), which has 12 layers with 12 attention heads. We used the data provided by Clark et al. (2019).

This data consists of 992 input sequences extracted from Wikipedia, each sequence consisting of two continuous paragraphs, in the form of: [CLS] paragraph1 [SEP] paragraph2 [SEP]. Each sequence consists of up to 128 tokens, with an average of 122 tokens.

4.1 Does $f(x)$ have an impact?

As a preliminary demonstration of how much $\|\alpha f(x)\|$ differs from $\alpha$, we analyze the coefficient of variation $\|\alpha f(x)\|$ of $\|f(x)\|$. Based on Equation 3, if $\|f(x)\|$ is almost constant, the attention weights $\alpha$ can be a good approximation of $\|\alpha f(x)\|$. That is, our norm-based analysis is not worth applying if $\|f(x)\|$ is constant.

All the data were first fed into the model; then, we computed the coefficient of variation of $\|f(x)\|$. Table 1 shows that the coefficient of variation is 0.22 on average; the value of $\|f(x)\|$ often varies from 0.78 times to 1.22 times the mean value. Thus, there is a difference between $\alpha$ and $\|\alpha f(x)\|$ owing to this dispersion of $\|f(x)\|$, which motivates to take into account $\|f(x)\|$ in analyzing the attention modules. Appendix A shows the effect of $\|x\|$ and the affine transformation $f$.

4.2 Re-examining previously observed phenomena

In this section, by using our norm-based analysis, we re-investigate the observations of BERT previously reported with the weight-based analysis (Clark et al., 2019).

Settings: All the data were fed into BERT; then, $\alpha$ and $\|\alpha f(x)\|$ were collected from each head. Following Clark et al. (2019), we report the results of the following categories: (i) [CLS], (ii) [SEP], (iii) periods and commas, and (iv) the other tokens.

Results: The values of $\alpha$ and $\|\alpha f(x)\|$ showed completely different trends (Figure 3). Figure 3a

| Head          | $\mu$ | $\sigma$ | CV     | Max  | Min  |
|---------------|-------|----------|--------|------|------|
| Layer 2–Head 4 (max CV) | 4.26  | 1.59     | 0.37   | 12.66| 0.96 |
| Layer 2–Head 7 (min CV)  | 4.00  | 0.50     | 0.12   | 6.15 | 1.35 |
| Average       | 5.15  | 1.17     | 0.22   | -    | -    |

Table 1: Mean ($\mu$), standard deviation ($\sigma$), coefficient of variance (CV), and maximum and minimum values of $\|f(x)\|$; the former three are averaged on all the heads.
shows that the vectors for specific tokens ([CLS], [SEP], and punctuation) gain remarkably large attention weights. However, this observation is not intuitive because those tokens are expected not to have so linguistic information and not to be so useful for pre-training tasks (i.e., masked word prediction and next sentence prediction). However, this trend is indeed consistent with the report by the weight-based analysis (Clark et al., 2019). In contrast, our norm-based method produces an intuitive observation; the contributions of those vectors for specific tokens are generally small (Figure 3b).

Clark et al. (2019) hypothesized that if there is no necessary information in the input vectors, BERT assigns large weights to [SEP] tokens that guaranteed to appear in any input sequence, not to incorporate any additional information via attention modules. Note that the attention module has the constraint that the sum of the attention weights is no necessary information in the input vectors, not to be so useful for pre-training tasks (i.e., masked word prediction and next sentence prediction). However, this operation “no-op” (no operation). This achieves the “no-op” function of collecting no information from input tokens.

### Analysis — relationship between $\alpha$ and $\| f(x) \|$ in each token category.

Table 2 shows the Spearman rank correlation coefficient between $\alpha$ and $\| f(x) \|$ in each token category.

| Token category | Number of vectors | Spearman’s $\rho$ |
|----------------|------------------|-------------------|
| [CLS]          | 17,443,296       | -0.34             |
| [SEP]          | 34,886,592       | -0.69             |
| comma & period | 182,838,528      | -0.25             |
| Others         | 1,944,928,224    | -0.06             |

Figure 4: The darkness of each cell corresponds to the value of averaged $\alpha$ or $\| f(x) \|$ on a [SEP] category in a given head.

Figure 5: Relationship between $\alpha$ and $\| f(x) \|$ in each token category. Each plot corresponds to a pair of $\alpha_{i,j}$ and $\| f(x_j) \|$ for output vector $y_j$ in either attention head. Each plot is colored by the token category corresponding to $x_j$.

#### 4.3 Relationship between token frequency and $\| f(x) \|$

In the previous section, we demonstrated that $\| f(x) \|$ corresponding to the specific tokens (e.g., [SEP]) is small. Based on the presumption that such special tokens have relatively high frequency, we hypothesize that BERT controls the amount of contribution of highly frequent, less informative tokens by adjusting the norm of $f(x)$.

**Settings:** First, all the data were fed into the model. Then, for each input vector $x^{(r,o)}$ in the data, assigned $\alpha^{(r,o)}$ and $\| f(x^{(r,o)}) \|$ were collected. Here, the vector denoted by $x^{(r,o)}$ is the vectors corresponding to the $o$-th occurrence of
the $r$-th frequent (rank $r$) type (subword)$^5$. Each $\alpha^{(r,o)}$ and $\|f(x^{(r,o)})\|$ denote the averaged score of the values obtained from all the 144 heads.

We analyzed the relationships between the rank of frequency $r$ and $\alpha^{(r,o)}$, and that between $r$ and $\|f(x^{(r,o)})\|$.

**Results:** Figure 6 shows the results of the experiments. Each plot corresponds to $(r, \alpha^{(r,o)})$ or $(r, \|f(x^{(r,o)})\|)$. The Spearman rank correlation coefficient showed no correlation ($\rho = -0.08$) between $r$ and $\alpha^{(r,o)}$ (Figure 6a). On the other hand, the Spearman rank correlation coefficient between $r$ and $\|f(x^{(r,o)})\|$ was 0.75, indicating a strong positive correlation (Figure 6b). These results demonstrate that the self-attention modules in BERT reduce the information from highly frequent tokens by adjusting $\|f(x)\|$ but not $\alpha$. This frequency-based effect is consistent with the intuition that highly frequent tokens such as stop words are unlikely to play an important role in solving the pre-training tasks (masked token prediction and next sentence prediction).

Note that the remarkable behavior in detail might be ignored since $\alpha$ and $\|f(x)\|$ were averaged for all the heads in our experiments. Thus, a more detailed head-level or layer-level analysis is needed in future work.

5 Experiments2: Transformer-based NMT system

We additionally analyze the source-target attention modules in Transformer-based NMT systems. One of the community’s interests in NMT is whether the NMT systems capture word alignment between the source text and the target text, and if so, how to extract it from the black box NMT systems. This is an important issue for interpreting the internal on-line translation process of the systems, conducting detailed error analysis, and showing rich information (which words are translated to which words) for the users of NMT systems (Ding et al., 2017).

Previously, several studies showed that the attention weights in the Transformer’s source-target attention module do not induce word alignment so well (Zenkel et al., 2019; Li et al., 2019; Ding et al., 2019). In this section, we demonstrate that much better word alignments can be extracted from a Transformer-based NMT system simply by applying our norm-based method, i.e., taking into account the norm of the transformed vectors as well.

**Settings:** Following Li et al. (2019), we trained the Transformer-based NMT system with the data used in the WMT2016 news translation task (DE-EN)$^3$. The hyperparameters of the model are shown in Appendix D.

Soft alignments were extracted from the attention module by the following methods:

- **Attention-weights** for each layer were computed by averaging $\alpha$ of all heads following Li et al. (2019).
- For our norm-based method, we merged $\|\alpha f(x)\|$ from all attention heads in each layer by the following strategy: adding all the vec-

$^5$We used the token ids used in BERT’s tokenizer to acquire each token’s frequency rank in the training data of BERT. Special tokens and single characters were excluded from them as we cannot get their exact frequency rank. We considered commas, periods, [SEP], and [CLS] as the top four frequent tokens because they are considered to appear very frequently.

$^6$First, attention weights assigned to $x^{(r,o)}$ for generating each output vector in a sequence are averaged in each head. Then, we calculated the averaged score over the results of 144 heads.

$^7$http://www.statmt.org/wmt16/
tors $\alpha f(x)$ from every head, then calculating the norm of the summed vector (Vector-norms). Adding all $\alpha f(x)$ from every head is the same as the procedure that combines the results from every head into the results of the multi-head attention module.

Next, soft Byte-Pair Encoding (Sennrich et al., 2016) alignments extracted from the methods above converted to hard word alignment following the procedure in Li et al. (2019). Their alignments were evaluated using the alignment error rate (AER) (Och and Ney, 2000) on the gold alignment data provided by Vilar et al. (2006).

We also include the AER results reported by Ding et al. (2019) and Zenkel et al. (2019), obtained using the gradient-based methods and word aligners: fast_align (Dyer et al., 2013) and GIZA++ (Och and Ney, 2003). In the gradient-based methods, SmoothGrad (Smilkov et al., 2017) is applied to the NMT systems (Zenkel et al., 2019; Li et al., 2016).

**Results:** We obtained the following findings: (1) the results obtained using our norm-based method considerably differ from the observation through attention weights (Figure 7 and 8), (2) the norm-based result is much better than existing works — our result is competitive with fast_align, one of the de facto word aligners (Table 3), and (3) These results overturn the previous finding that the attention modules in Transformer do not perform word alignment (Li et al., 2019).

On the difference between norm-based and weight-based results: Figure 7 shows that, especially in the lower layer, the AER scores with our norm-based method significantly improve. The major reason for the difference between the scores obtained using the weight-based and the norm-based methods is probably the same mechanism described in Section 4.2 — while the attention weights assigned to certain tokens (e.g., periods) are large, their vector norms are adjusted to become smaller (Figure 8).

On the comparison of the extracted alignment quality: Our norm-based result is also better than the gradient-based results. While the gradient-based methods introduce some additional hyperparameters, such as the number of augmented samples $n$, our norm-based method does not, which suggests that we succeed in extracting better alignments from the NMT model with more simple way. It is also worth noting that the extracted alignments using our norm-based method, which does not use any external modules, are as clean as those extracted by the existing aligners, fast_align. This result suggests that the Transformer-based NMT system implicitly learned word alignment through the attention modules during training. Therefore, it overturns the previous finding that the attention modules in Transformer fail to capture word alignment (Li et al., 2019).

To sum up, these results suggest that our norm-based method may change the view of our understanding of not only BERT but also other Transformer-based systems.
### 6 Related work

Existing studies investigating Transformer-based models have mainly analyzed the internal representations, outputs (e.g., the scores for predicting masked words in BERT), or attention weights. Studies focusing on internal representations or outputs showed that BERT captures, more or less, syntactic structures and semantic information (Goldberg, 2019; Hewitt and Manning, 2019; Reif et al., 2019; Tenney et al., 2019; Jawahar et al., 2019). The weight-based analyses have shown that BERT or Transformer has attention heads whose attention weight assignments correspond to specific linguistic relations (Clark et al., 2019; Kovaleva et al., 2019; Reif et al., 2019; Lin et al., 2019; Mareček and Rosa, 2019; Htut et al., 2019; Raganato and Tiedemann, 2018; Tang et al., 2018) and that the encoder-decoder attention modules in Transformer do not capture word alignment quite well (Zenkel et al., 2019; Li et al., 2019; Ding et al., 2019). Our study improved the method of analyzing the attention modules considering the effects of conventionally overlooked elements in addition to the attention weights.

Clark et al. (2019) and Brunner et al. (2020) analyzed BERT by observing gradients. To estimate the contribution of each input vector (integral), both the gradient (derivative, sensitivity) and the range of integration are complementary and essential features. While the gradient-based analysis solely focuses on the former factor, our norm-based analysis can consider both of them. Considering both the gradient and the range of integration is similar to multiplying $\alpha$ (coefficient) by $||f(x)||$ to compute the actual summed up vectors in our norm-based analysis.

As a similar study, Brunner et al. (2020) introduced “effective attention”, which ignores certain elements in the attention weights matrix that are canceled out by the transformations in the attention module or the input vectors. While the effective attention approach considers the non-influential elements as zero, our norm-based analysis takes into account the degree of the effects for the output vectors.

### 7 Conclusions and future work

In this paper, we have shown that attention weights alone are only one of two factors determining the output of self-attention modules, and we have proposed to incorporate the other factor as well, namely, the transformed input vectors, into the analysis. Through analysis of self-attention modules in BERT, we have shown that the proposed norm-based method produces insights that better agree with linguistic intuitions than an analysis based on attention weights alone. Our analysis has further revealed that BERT controls the amount of the contribution from highly frequent tokens, not by attention weights but via vector norms. Finally, our norm-based analysis showed that the Transformer-based NMT system implicitly learns word alignment much better than previously estimated by tracking the attention weights.

**Future work:** We believe that our norm-based analysis opens up many new directions for analyzing attention-based models. Our norm-based analysis is directly applicable to analyzing other attention-based models. For future work, we plan to apply it to the attention modules in, such as fine-tuned BERT and RoBERTa. Furthermore, we will extend the scope of analysis from the attention module to an entire architecture to better understand the inner workings and linguistic capabilities of the current powerful black-box NLP systems.

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References

Gino Brunner, Yang Liu, Damián Pascual, Oliver Richter, Massimiliano Ciaramita, and Roger Wattenhofer. 2020. On Identifiability in Transformers. In 8th International Conference on Learning Representations (ICLR).

Kevin Clark, Urvashi Khandelwal, Omer Levy, and Christopher D Manning. 2019. What Does BERT Look At? An Analysis of BERT’s Attention. In Proceedings of the 2019 ACL Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP, pages 276–286.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. 2019. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. 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) (NAACL-HLT), pages 4171–4186.

Shuoyang Ding, Hainan Xu, and Philipp Koehn. 2019. Saliency-driven Word Alignment Interpretation for Neural Machine Translation. In Proceedings of the Fourth Conference on Machine Translation (Volume 1: Research Papers) (WMT), pages 1–12.

Yanzhuo Ding, Yang Liu, Huanbo Luan, and Maosong Sun. 2017. Visualizing and Understanding Neural Machine Translation. In Proceedings of the 55th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers) (ACL), pages 1150–1159.

Chris Dyer, Victor Chahuneau, and Noah A Smith. 2013. A Simple, Fast, and Effective Reparameterization of IBM Model 2. In Proceedings of the 2013 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (NAACL-HLT), pages 644–648.

Yoav Goldberg. 2019. Assessing BERT’s Syntactic Abilities. arXiv preprint arXiv:1901.05287.

John Hewitt and Christopher D Manning. 2019. A Structural Probe for Finding Syntax in Word Representations. 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) (NAACL-HLT), pages 4129–4138.

Phu Mon Htut, Jason Phang, Shikha Bordia, and Samuel R. Bowman. 2019. Do Attention Heads in BERT Track Syntactic Dependencies? arXiv preprint arXiv:1911.12246.

Ganesh Jawahar, Benoît Sagot, and Djâmé Seddah. 2019. What Does BERT Learn about the Structure of Language? In Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics (ACL), pages 3651–3657.

Olga Kovaleva, Alexey Romanov, Anna Rogers, and Anna Rumshisky. 2019. Revealing the Dark Secrets of BERT. 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 4364–4373.

Zhenzhong Lan, Mingda Chen, Sebastian Goodman, Kevin Gimpel, Piyush Sharma, and Radu Soricut. 2020. ALBERT: A Lite BERT for Self-supervised Learning of Language Representations. In 8th International Conference on Learning Representations (ICLR).

Jiwei Li, Xinlei Chen, Eduard Hovy, and Dan Jurafsky. 2016. Visualizing and Understanding Neural Models in NLP. In Proceedings of the 2016 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies (NAACL-HLT), pages 681–691.

Xintong Li, Guanlin Li, Lemao Liu, Max Meng, and Shuming Shi. 2019. On the Word Alignment from Neural Machine Translation. In Proceedings of the 57th Annual Meeting of the Association for Computational Linguistics (ACL), pages 1293–1303.

Yongjie Lin, Yi Chern Tan, and Robert Frank. 2019. Open Sesame: Getting Inside BERT’s Linguistic Knowledge. Proceedings of the 2019 ACL Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP, pages 241–253.

Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. 2019. RoBERTa: A Robustly Optimized BERT Pretraining Approach. arXiv preprint arXiv:1907.11692.

David Mareček and Rudolf Rosa. 2019. From Balustrades to Pierre Vinken: Looking for Syntax in Transformer Self-Attention. In Proceedings of the 2019 ACL Workshop BlackboxNLP: Analyzing and Interpreting Neural Networks for NLP, pages 263–275.

Franz Josef Och and Hermann Ney. 2000. Improved Statistical Alignment Models. In Proceedings of the 38th Annual Meeting of the Association for Computational Linguistics (ACL), pages 440–447.

Franz Josef Och and Hermann Ney. 2003. A Systematic Comparison of Various Statistical Alignment Models. Computational Linguistics, 29(1):19–51.

Myle Ott, Sergey Edunov, Alexei Baevski, Angela Fan, Sam Gross, Nathan Ng, David Grangier, and Michael Auli. 2019. fairseq: A Fast, Extensible Toolkit for Sequence Modeling. In Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics (Demonstrations), pages 48–53.
Alessandro Raganato and Jörg Tiedemann. 2018. 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.

Emily Reif, Ann Yuan, Martin Wattenberg, Fernanda B Viegas, Andy Coenen, Adam Pearce, and Been Kim. 2019. Visualizing and Measuring the Geometry of BERT. Advances in Neural Information Processing Systems 32 (NIPS), pages 8594–8603.

Anna Rogers, Olga Kovaleva, and Anna Rumshisky. 2020. A Primer in BERTology: What we know about how BERT works. arXiv preprint arXiv:2002.12327.

Rico Sennrich, Barry Haddow, and Alexandra Birch. 2016. Neural Machine Translation of Rare Words with Subword Units. In Proceedings of the 54th Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers) (ACL), pages 1715–1725.

Daniel Smilkov, Nikhil Thorat, Been Kim, Fernanda B Viégas, and Martin Wattenberg. 2017. SmoothGrad: removing noise by adding noise. arXiv preprint arXiv:1706.03825.

Gongbo Tang, Rico Sennrich, and Joakim Nivre. 2018. An Analysis of Attention Mechanisms: The Case of Word Sense Disambiguation in Neural Machine Translation. In Proceedings of the Third Conference on Machine Translation (WMT): Research Papers, pages 26–35.

Ian Tenney, Patrick Xia, Berlin Chen, Alex Wang, Adam Poliak, R Thomas McCoy, Najoong Kim, Benjamin Van Durme, Samuel R Bowman, Dipanjan Das, and Ellie Pavlick. 2019. What do you learn from context? Probing for sentence structure in contextualized word representations. In 7th International Conference on Learning Representations (ICLR).

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Lukasz Kaiser, and Illia Polosukhin. 2017. Attention is All you Need. In Advances in Neural Information Processing Systems 30 (NIPS), pages 5998–6008.

David Vilar, Maja Popović, and Hermann Ney. 2006. AER: Do we need to “improve” our alignments? In International Workshop on Spoken Language Translation (IWSLT) 2006, pages 205–212.

Zhilin Yang, Zihang Dai, Yiming Yang, Jaime Carbonell, Ruslan Salakhutdinov, and Quoc V. Le. 2019. XLNet: Generalized Autoregressive Pretraining for Language Understanding. In Advances in Neural Information Processing Systems 32 (NIPS), pages 1–18.

Thomas Zenkel, Joern Wuebker, and John DeNero. 2019. Adding Interpretable Attention to Neural Translation Models Improves Word Alignment. arXiv preprint arXiv:1901.11359.
A Where the dispersion of $\|f(x)\|$ comes from

As described in Section 4.1, $\|f(x)\|$ has dispersion, but where does it come from? To understand this, we checked the dispersion of $\|x\|$ and scaling effects of transformation $f$.

Dispersion of $\|x\|$ We also checked the coefficient of variation (CV) of $\|x\|$. Table 4 shows that the CV is 0.12 on average; the value of $\|x\|$ often varies from 0.88 times to 1.12 times the mean value. This is less than the dispersion of $\|f(x)\|$.

Scaling effects of $f$ We investigate how much transformation $f$ can change $\|x\|$. Since the affine transformation $f: \mathbb{R}^d \rightarrow \mathbb{R}^d$ can be regarded as a linear transformation $\mathbb{R}^{d+1} \rightarrow \mathbb{R}^{d+1}$ (Appendix B), its scaling effect can be analyzed by checking the singular values of the linear transformation. Figure 9 shows the results of randomly selected heads in BERT. The singular values of the transformation $f$ for each head are in descending order. In each head, there is a difference of at least 1.8 times or more between the maximum and minimum singular values. That is, the value of $\|f(x)\|$ varies greatly due to the transformation $f$.

B Affine transformation as linear transformation

Affine transformation $f: \mathbb{R}^d \rightarrow \mathbb{R}^d$ in Equation 4 can be regarded as a linear transformation $\mathbb{R}^{d+1} \rightarrow \mathbb{R}^{d+1}$. If 1 is added to the end of each input vector $x \in \mathbb{R}^d$ and $\tilde{x} := \begin{bmatrix} x & 1 \end{bmatrix} \in \mathbb{R}^{d+1}$ is given, the affine transformation $f$ can be identified with the linear transformation $\tilde{f}$ as

$$\tilde{f}(\tilde{x}) = \tilde{x} \tilde{W}^V \tilde{W}^O$$

(5)

$$\tilde{W}^V := \begin{bmatrix} W^V & \vdots & 0 \\ 0 & \ddots & 0 \\ b^V & \vdots & 1 \end{bmatrix} \in \mathbb{R}^{(d+1) \times (d'+1)}$$

(6)

$$\tilde{W}^O := \begin{bmatrix} W^O & \vdots & 0 \\ 0 & \ddots & 0 \\ 0 & \ldots & 0 & 1 \end{bmatrix} \in \mathbb{R}^{(d+1) \times (d+1)}.$$  

(7)

| Layer | $\mu$ | $\sigma$ | CV  | Max  | Min  |
|-------|-------|---------|-----|------|------|
| 12 (max CV) | 20.49 | 4.62 | 0.23 | 32.84 | 4.13 |
| 7 (min CV)  | 21.64 | 1.40 | 0.06 | 23.03 | 11.87 |
| Average     | 19.93 | 2.39 | 0.12 | -    | -    |

Table 4: Mean ($\mu$), standard deviation ($\sigma$), coefficient of variance (CV), and maximum and minimum values of $\|f(x)\|$; the former three are averaged on all the layers.

Figure 9: Singular values of $f$ at randomly selected heads in each layer. We use $\langle$layer$\rangle$-$\langle$head number$\rangle$ to denote a particular attention head.

C Relationship between $\alpha$ and $\|f(x)\|$ corresponding to the other token categories

As described in Section 4.2, for vectors corresponding to [SEP], $\alpha$ and $\|f(x)\|$ were canceled out in almost all heads. In this section, we show the trends of other vectors. Figures 10 and 11 show that the vectors corresponding to [CLS], periods and commas have the same tendency as the vectors corresponding to [SEP]. On the other hand, Figure 12 shows that the vectors corresponding to the other tokens do not strongly have the same tendency. Note that in the heatmaps of $\|f(x)\|$, the color scale is determined by the maximum value for all heads.

D Hyperparameters of NMT system

We used Transformer (Vaswani et al., 2017) NMT model implemented in fairseq (Ott et al., 2019) for the experiments in Section 5. Table 5 shows the hyperparameters of the model. We used the same data and word segmentation method as Li et al. (2019).

E Alignment examples extracted from other layers

In Section 5, alignment examples extracted from the attention modules in layer 2 were shown. Here, examples from the other layers are shown in Figure 13 to Figure 17).
| Fairseq model architecture | transformer_lm |
|---------------------------|---------------|
| **Loss**                  | label smoothed cross entropy |
| type                      | 0.1           |
| label smoothing            |               |
| **Optimizer**             |               |
| algorithm                 | Adam          |
| learning rates             | 5e-4          |
| $\beta_1$                 | 0.9           |
| $\beta_2$                 | 0.98          |
| weight decay               | 0.0001        |
| clip norm                  | 0.0           |
| **Learning rate scheduler**|               |
| type                      | inverse_sqrt  |
| warmup updates             | 4000          |
| warmup init learning rate  | 5e-4          |
| **Training**              |               |
| batch size                | $2^{15}$ tokens |
| epochs                    | 40            |
| encoder embed dim.        | 512           |
| decoder embed dim.        | 512           |
| encoder layers            | 6             |
| decoder layers            | 6             |
| encoder attention heads   | 8             |
| decoder attention heads   | 8             |

Table 5: Hyperparameters of the NMT model.

(a) Averaged $\alpha$ assigned to vectors corresponding to $[CLS]$.  
(b) Averaged $\|f(x)\|$ of vectors corresponding to $[CLS]$.  

Figure 10: $\alpha$ and $\|f(x)\|$ corresponding to $[CLS]$ token, averaged on all the input text.

(a) Averaged $\alpha$ assigned to vectors corresponding to periods and commas.  
(b) Averaged $\|f(x)\|$ of vectors corresponding to periods and commas.  

Figure 11: $\alpha$ and $\|f(x)\|$ corresponding to periods and commas, averaged on all the input text.

(a) Averaged $\alpha$ assigned to vectors corresponding to the other tokens.  
(b) Averaged $\|f(x)\|$ of vectors corresponding to the other tokens.  

Figure 12: Comparison between assigned $\alpha$ and $\|f(x)\|$ for vectors corresponding to the other tokens.
Figure 13: Examples of soft alignment extracted from the attention modules in layer 1 of the model and reference of word alignment. Word pairs with a green frame are extracted as the alignments.

Figure 14: Examples of soft alignments extracted from layer 3. Word pairs with a green frame are extracted as the alignments.

Figure 15: Examples of soft alignments extracted from layer 4. Word pairs with a green frame are extracted as the alignments.

Figure 16: Examples of soft alignments extracted from layer 5. Word pairs with a green frame are extracted as the alignments.

Figure 17: Examples of soft alignments extracted from layer 6. Word pairs with a green frame are extracted as the alignments.