Abstract

We take a deep look into the behaviour of self-attention heads in the transformer architecture. In light of recent work discouraging the use of attention distributions for explaining a model’s behaviour, we show that attention distributions can nevertheless provide insights into the local behaviour of attention heads. This way, we propose a distinction between local patterns revealed by attention and global patterns that refer back to the input, and analyze BERT from both angles. We use gradient attribution to analyze how the output of an attention attention head depends on the input tokens, effectively extending the local attention-based analysis to account for the mixing of information throughout the transformer layers. We find that there is a significant discrepancy between attention and attribution distributions, caused by the mixing of context inside the model. We quantify this discrepancy and observe that interestingly, there are some patterns that persist across all layers despite the mixing.

1 Introduction

The inception of the transformer architecture, often referred to as NLP’s ImageNet moment, has sparked significant progress across a wide range of language understanding tasks. Variants of transformers currently dominate the popular GLUE (Wang et al., 2019b) and SuperGLUE (Wang et al., 2019a) benchmarks and have even achieved super human performance on multiple tasks. The main innovations behind the transformer architecture are the stacking of self-attention layers into a multi-layer self-attention architecture, as well as an unsupervised pre-training phase that primes the model to be fine-tuned on a wide range of language tasks. Transformers and other self-attention-based models have also been successfully adopted in other areas such as computer vision (Parmar et al., 2018), music processing (Huang et al., 2019) or protein research (Rao et al., 2019). Their extraordinary empirical success has led researchers to investigate transformers more deeply in order to better understand the source of this success, but also in an attempt to explain model decisions.

Much of the research around interpretability and explainability is focused on analyzing the self-attention operation. In multi-layer self-attention, every input computes an attention distribution over itself and all other inputs to produce ever more complex feature representations. In the case of language, a word in a sentence attends to itself and to all other words in order to compute an updated contextual representation of itself. It is tempting to directly rely on attention distributions to explain the model’s predictions. The rationale is that if the attention distribution aligns with human intuition we can conclude that the model learned robust features and obtained a deep understanding of language, in contrast to simply overfitting on spurious patterns. For example, if a transformer classifies an online comment as hate speech, but we find that the model mostly attended to neutral or even positive words, we would conclude that the model did not actually understand the text and that the correct prediction was either due to chance or to the exploitation of an underlying statistical bias in the data (Niven and Kao, 2019).

However, recent studies (Brunner et al., 2020; Pruthi et al., 2019) question the ability of attention maps to provide a faithful explanation of the inner workings of transformer models. In particular, when the explanations refer to the model input attention maps do not account for the mixing of information throughout the model and, since self-attention mixes information among all input tokens, the hidden layers attend over mixtures of tokens.
Therefore, attention maps may be useful to investigate the local behavior of attention heads but not to draw conclusions about how input tokens relate to each other.

In this work we take a detailed look at the inner workings of BERT’s attention heads, both by analyzing the self-attention distributions, as well as by using gradient attribution to account for the mixing of tokens throughout the model. We first show that self-attention distributions correlate strongly with Hidden Token Attribution (Brunner et al., 2020) (HTA) from hidden embedding to head output. We then present novel location based attention patterns, revealing that BERT, despite its bi-directional language modeling objective, attends to the past in earlier layers, and to the future in later layers. Next, we use HTA in order to extend the analysis to take the mixing of information into account, which allows to draw conclusions about the behaviour of an attention head with respect to the original input word. The patterns that emerge are different from the local attention-based patterns, giving us deeper insight into the operation of the model and emphasizing that local attention-based explanations are very different from global attribution-based explanations. Finally, we contrast attention and HTA distributions for individual examples. Our results further highlight the discrepancy between local attention patterns and global attribution patterns.

2 Related Work

The success of attention (Graves, 2013; Bahdanau et al., 2015) models in Natural Language Processing (NLP) arises from their ability to learn alignments between words. The transformer architecture (Vaswani et al., 2017) is a multi-layer multi-head self-attention architecture that is unsupervisedly pre-trained. The extraordinary performance of transformer models has produced an accelerated progress in the field of NLP. Currently, there is a growing number of different transformer models that vary in size, pre-training objective and/or in other architectural elements (Radford et al., 2018, 2019; Liu et al., 2019; Lan et al., 2020; Yang et al., 2019; Sanh et al., 2019; Kitaev et al., 2020; Raffel et al., 2019).

The success of transformers and the possibility of visualizing attention distributions (Vaswani et al., 2017), has motivated a line of research aiming to understand the inner workings of transformers and explain their decisions. Many of these studies have focused on BERT (Devlin et al., 2019a), a well-known transformer model, leading to a body of research grouped under the term BERTology (Rogers et al., 2020).

Aforementioned research builds on previous work on the interpretability of attention distributions in other models other than transformers. In particular, (Jain and Wallace, 2019) examine the attention distributions of LSTM based encoder-decoder models and show a weak to moderate correlation between attention and dot-product gradient attribution. Furthermore, they show that adversarial attention distributions that do not change the model’s decision can be constructed. In the same line, (Serrano and Smith, 2019) find, through zeroing out attention weights, that gradient attribution is a better predictor of feature importance with respect to the model’s output than attention weights. (Wiegrefe and Pinter, 2019) find that although adversarial attention distributions can be easily obtained, they perform worse on a simple diagnostic task. All of these works raise concerns about the ability of attention distributions to explain the decisions of a model.

Nevertheless, attention distributions have been extensively used to study BERT. (Clark et al., 2019) and (Htut et al., 2019) study the attention distributions of BERT’s heads to draw conclusions about the syntactic knowledge of the heads. (Kovaleva et al., 2019) analyse the impact of individual heads on model performance and classify the attention heads into five classes according to their attention patterns. (Voita et al., 2019) also study the syntactic abilities of BERT’s heads in the context of machine translation, devise a different head classification and show that pruning heads results in surprisingly little degradation in performance.

Despite being commonly acknowledged that interpreting attention distributions is problematic, very few works have studied how this problem affects transformers. (Pruthi et al., 2019) shows that, just as in other attention models, it is possible to manipulate self-attention in transformers in order to generate different attention masks that produce only a small drop in performance. (Brunner et al., 2020) find that attention distributions are not unique when the sequence length is larger than the head dimension and show that this can lead to the discovery of spurious patterns. Furthermore, they show that although it is possible to identify input tokens from hidden tokens, there is a very large de-
gree of information mixing inside the model, which questions a straightforward interpretation of attention maps.

Our work addresses this important issue by distinguishing between local and global aggregation patterns, where the former can be explained by attention distributions and the latter by attribution. We analyze BERT from both angles and quantify the mismatch between these interpretations. We show that attention correlates well with attribution locally but not globally and therefore attention maps are inadequate to draw conclusions that refer to the input of the model.

3 Background on Transformers

The original transformer architecture (Vaswani et al., 2017) is a sequence-to-sequence model consisting of an encoder and a decoder, both of which follow a multi-layer multi-head self-attention structure. Conversely, most of the pre-trained transformer models that can be fine-tuned on supervised language tasks only consist of a decoder. Each transformer layer consists of a self-attention block and a non-linear feed forward block (MLP).

The input to a transformer layer is a sequence of embeddings $E^l = [e^l_0, ..., e^l_{d_s}] \in \mathbb{R}^{d_s \times d_e}$, where $l$ denotes the layer number, $d_s$ is the embedding dimension, and $d_e$ is the sequence length. We refer to the sequence of non-contextual input word embeddings as $E^0$, and to the hidden contextual embeddings as $E^l$, where $l > 0$. Note that $E^0$ denotes the sum of the raw word embeddings with any additional embeddings, such as position and sequence embeddings. A self-attention block consists of $d_h$ separate attention heads. The attention heads independently perform the self-attention operation, and the results are then concatenated and projected back into the embedding space by a linear layer. The output of the attention block is then fed into the MLP.

The self-attention operation itself is implemented by projecting each input token $e_i \in \mathbb{R}^{d_e}$ into a query vector $q_i \in \mathbb{R}^{d_h}$, key vector $k_i \in \mathbb{R}^{d_h}$ and value vector $v_i \in \mathbb{R}^{d_e}$. We present the self-attention operation from the perspective of a single token $e_i$ attending to all input tokens. For that, the key vectors $k_i$ are aggregated into the key matrix $K = [k_0, ..., k_{d_s}] \in \mathbb{R}^{d_h \times d_s}$ and the value vectors $v_i$ are aggregated into the value matrix $V = [v_0, ..., v_{d_s}] \in \mathbb{R}^{d_e \times d_s}$. The attention distribution $a_i$ of token $e_i$ over all input tokens is then computed as

$$a_i = \text{softmax} \left( \frac{q_i \cdot K}{\sqrt{d_q}} \right) \quad (1)$$

The attention vector $a_i \in \mathbb{R}^{d_h}$ now contains an attention weight for each input token. $a_i$ is then multiplied with the value matrix $V$ to compute the output of the self-attention operation for a token $i$ and a head $h$ as

$$o_{h,i} = a_i \cdot V \quad (2)$$

The outputs of all heads $[o_{0,i}, ..., o_{d_h,i}] \in \mathbb{R}^{d_e}$ are then concatenated and fed through a linear layer to compute the output of the self-attention block for a single token. This linear layer can be thought of as an aggregation operation that projects the output of the independent heads back into embedding space. In practice, the attention distributions for all tokens are computed in parallel.

4 Extending Hidden Token Attribution

Hidden Token Attribution (Brunner et al., 2020) is a gradient-based attribution method that quantifies how much information from each input token is contained in a given hidden embedding. For each layer $l$, this method defines the relative contribution $c^l_{i,j}$ of an input token $x_i$ to a hidden embedding $e^l_j$ as:

$$c^l_{i,j} = \frac{\|\nabla^l_{i,j}\|_2^2}{\sum_{k=0}^{d_s} \|\nabla^l_{k,j}\|_2^2} \quad \text{with} \quad \nabla^l_{i,j} = \frac{\delta e^l_j}{\delta x_i} \quad (3)$$

The contribution $c^l_{i,j}$ is normalized by the sum of the attribution values to all input tokens and hence, ranges between 0 and 1.

In this work, we apply Hidden Token Attribution to the individual attention heads of BERT. For a token $e^l_j$ at layer $l$ we back-propagate the gradients from the output $o^l_{h,j}$ of each attention head $h$ independently. This differs from the original method in that Hidden Token Attribution propagates the gradients from the layer output. In general, using Equation 3, we can compute the contribution between any two vectors in the model, as long as they are connected in the computation graph. We hence denote the contribution of any vector $x$ to another vector $y$ as $C(x, y)$.

In particular, we calculate two different contributions to the head output:
Previous layer contribution: Contribution from the hidden embeddings at the input of the attention head to the output of the attention head:
\[ C(e^{l-1}_i, o^l_{h,j}) \]

Input contribution: Contribution from tokens at the input of the transformer model to the output of an attention head \( h \) at layer \( l \):
\[ C(e^0_i, o^l_{h,j}) \]

Previous layer contribution allows us to study how attention heads operate locally and how HTA distributions compare to attention distributions. Input contribution enables us to extend the head attention patterns all the way back to the input, thereby controlling for the effect of information mixing.

5 Setup

For our experiments we use the non-finetuned, uncased BERT base model (Devlin et al., 2019b) as provided in the original repository.\(^1\) Despite the recent explosion of new transformer variants, BERT remains the most popular model for research into the interpretability of transformer models. The reason for this is that most of the newer models are architecturally similar to BERT, and therefore, studies performed on BERT either directly generalize to these models or can be repeated with relatively little effort.

We perform our experiments on 1800 examples from the development set of the MNLI matched (MNLI\textsubscript{m}) dataset. (Brunner et al., 2020) show that when the sequence length is larger than the head output dimension, there exists a non-trivial null space that may lead to significant parts of the attention distributions to be mapped to zero. Therefore, to guarantee that in our experiments we do not find spurious patterns that do not influence downstream parts of the model, we restrict the examples in our dataset to sequences of maximum length of 64 tokens, which is the head dimension of BERT. Thus, the examples in our dataset have sequence lengths ranging between 6 and 64 tokens, with a median length of 34 tokens. In total, this subset contains 63,456 tokens.

6 Attention: Local Validation

The ability of attention distributions to provide explanations has been the target of a number of research studies (Wiegreffe and Pinter, 2019; Serrano and Smith, 2019; Pruthi et al., 2019). In particular, (Jain and Wallace, 2019) shows that attention distributions do not explain the model output and do not correlate well with attribution methods. However, if we are exclusively interested in how attention heads behave locally, i.e., without considering their impact to the model’s decisions, and given that self-attention is the only operation performed by the heads, we hypothesize that it is sound to use attention distributions to interpret the model. To verify this, we compare attention distributions to previous layer contribution by computing the correlation between attention maps and the contribution \( C(e^{l-1}_i, o^l_{h,j}) \) for each head.

A high correlation value would validate attention distributions as providing valuable insights about the local behavior of attention heads. To calculate the correlation, first, we extract the attention maps for all the heads of BERT for each of the tokens in the examples of our dataset. Then, we pair each attention map to the corresponding contribution. Note, that both attention maps and contributions are distributions that lay in the probability simplex, i.e., all the values are between 0 and 1 and their sum is 1. Next, we calculate Pearson’s correlation coefficient for each attention-contribution pair and we aggregate the results into one value per head by

![Figure 1](https://example.com/figure1.png)

Figure 1: (Upper) Pearson and (Lower) Spearman correlation between attention and previous layer contribution.
computing the mean of the correlation values.

Figure 5 (Upper) shows the mean correlation value per head. For all heads except for two, Pearson’s correlation coefficient is larger than 0.7. Furthermore, 89.6% of the heads show a correlation between attention and Hidden Token Attribution of over 0.85. Similarly, we calculate Spearman’s rank correlation coefficient \( r \) for each head. The results, displayed in Figure 5 (Lower), show that only four heads have a Spearman’s \( r \) smaller than 0.9 and that 75% of the heads have a correlation coefficient larger than 0.95.

These high correlation values empirically demonstrate that attention distributions do indeed represent the flow of information within attention heads with respect to the head inputs. Therefore, despite the fact that attention distributions may fail to accurately represent the global aggregation of information, they are informative about the local behavior of attention heads. Now that we have demonstrated that attention distributions are locally sound, we can investigate the behavior of the heads in more detail: examining the local patterns revealed by attention, the global patterns revealed by HTA, and the discrepancies between both.

7 Local Head Analysis

In this section we take a closer look into the local behaviour of attention heads. Here, local means that we analyze how the intermediate tokens fed into the heads are processed, as opposed to how the model input propagates. To this end, we study attention distributions, but rather than studying each individual example, we aggregate the attention distributions, thus obtaining a general picture of how each head behaves. In particular, we study how much attention is paid to tokens in each relative position with respect to the attending token.

For each head, we extract the attention maps for each token. Then, we define the position of the attending token in the sentence as the origin \((x = 0)\), thereby generating a histogram where the horizontal axis represents the position of the neighbours and the vertical axis the amount of attention paid to a token. We sum the histograms of all tokens and then normalize the result. To normalize, we divide the value of attention at each position by the number of times that a token is at that relative position with respect to the attending token; given that the median length of the examples is 36, distant positions are not penalized for having fewer occurrences.

Figure 2 presents the histograms for the heads in layers 2, 5 and 10, the other layers can be found...
in Appendix A. From these histograms, a clear pattern is observable. In the first layers, heads tend to aggregate more information from past context than from future context. In fact, the attention of heads 2, 5 and 7 in Layer 2 to future tokens is negligible. However, this trend progressively reverses with increasing depth, and in the last layers the aggregation of future context dominates for most heads. This suggests that despite its bidirectional training, BERT tends to process language like humans, from left to right. This is also inline with the sequential nature of language, i.e., the past context needs to be known to understand the future context.

8 Global Head Analysis

Although we have shown that attention maps are an effective tool to understand the local behavior of attention heads, drawing conclusions that refer to the input words can be misleading. Transformers are complex models that mix information from the entire input sequence at each layer. Recent work (Brunner et al., 2020; Pruthi et al., 2019) has raised concerns about the interpretability of attention maps as representative of global context aggregation. In this section, we look into the individual heads and study what we call global patterns, i.e., aggregation patterns that refer to the model’s input.

To this end, we follow the same procedure as in the previous section to generate input contribution $C(e^o_i, o^l_{h,j})$ histograms. In Figure 3 we show the histograms for layers 2, 5 and 10, i.e., the same layers as in Figure 2, the histograms for the whole model can be found in Appendix B. These histograms show that the global pattern of aggregation of information is much more uniform than shown by the attention maps. This is intuitive: given that in the first layers the heads are attending mostly to the past context, on average, all the hidden tokens have a larger amount of past context. Therefore, when in later layers the attention shifts to the future context, the past context already contained in these “future” tokens balances the contribution, resulting in a uniform pattern of context aggregation.

The difference in the patterns revealed by this global analysis and the local head analysis from the previous section shows that there is a strong mismatch between attention distributions and global context aggregation in attention heads. In Section 9, we study this difference quantitatively.

9 Local Attention vs. Global Attribution Distributions

To quantify the discrepancy between attention distributions and input contribution, i.e., local and global patterns of context aggregation, we calculate the correlation between attention maps and in-
input contribution $C(\epsilon^0_i, \sigma^h_{h,j})$. We follow the same methodology as in Section 6 and report Pearson’s and Spearman’s correlation coefficient in Figure 4. In line with the mismatch between attention and contribution histograms (Figures 2 and 3), we observe how the correlation between attention and input contribution quickly decreases in deeper layers. Particularly, after only four layers Pearson’s correlation coefficient for most heads is smaller than 0.5 and in the last four layers the median head correlation value is smaller than 0.25. Furthermore, Spearman’s correlation value falls monotonically from approximately 0.95 in the first layer to approximately 0.80 in the last layer, which indicates that also the ordering of the most contributing tokens progressively diverges from the most attended tokens. Although steadily decreasing, Spearman’s correlation is still high, which may be related the preservation of token identity reported by (Brunner et al., 2020).

The results from this section point at the importance of information mixing: attention maps show how the heads behave locally, i.e., how they aggregate context, but not what context is in fact aggregated. Knowing how the heads behave locally can give us a better understanding of transformer models that could be leveraged to further improve the performance of these models. However, attention maps are misleading when drawing conclusions about what input words are being aggregated into the contextual embeddings.

### 9.1 Specific examples

The histograms studied in the previous sections give us a high level picture of what is happening inside the model. However, we averaged across examples with different sequence length and with different token types in different positions. To gain a more detailed understanding of the model’s behaviour, we now look into specific input sequences randomly selected from our dataset.

(Kovaleva et al., 2019) study attention maps generated by BERT for many different examples and divide the attention patterns into five types: vertical, diagonal, vertical-diagonal, block and heterogeneous. When looking at the attention maps, we immediately observe the same five attention patterns. Nevertheless, as empirically demonstrated above, to understand what input information these heads are actually aggregating, we need to look at the contribution from the input tokens.

In Figure 5, we compare the five patterns observed by (Kovaleva et al., 2019) with the corresponding patterns produced by Hidden Token Attribution with respect to the input, $C(\epsilon^0_i, \sigma^h_{h,j})$, a comparison for all heads is available in Appendix C. Remarkably, heads with the vertical pattern pay the most attention to the SEP and CLS tokens. Nevertheless, the input contribution reveals that SEP tokens are used by the model to store general context, and by extracting information from the SEP token at intermediate layers, the model is in fact aggregating global context. Therefore, with respect to the input, heads with vertical, diagonal and vertical-diagonal patterns have a similar behavior to heterogeneous heads. However, tokens around the diagonal tend to contribute the most given the prevalent aggregation of local context.

On the other hand, as shown in the first column of Figure 5, we observe that the block patterns prevail when we apply Hidden Token Attribution to the input. It is noteworthy that while vertical and diagonal patterns fade, the blocks are still visible. The fact that attending to tokens inside a block results in aggregation of context from that block implies that up to that point, the context was aggregated within the blocks separated by SEP. We do not observe block patterns in deeper layers than layer 4, which suggests that the first layers aggre-
gate context within blocks and later on the context aggregated is more global.

10 Conclusion

We provide justification for interpreting attention distributions with respect to analyzing the local behaviour of attention heads. We uncover an interesting pattern in the attention distributions of heads: In earlier layers, heads attend mostly to earlier tokens, whereas this trend gradually reverses with increasing depth. This is surprising, since BERT is trained using bi-directional language modeling. A problem with local attention patterns is that they do not reveal how the attention heads are affected by the input tokens. We thus use hidden token attribution to effectively compute per-head “attention” distributions over the input words. Our results show that the mismatch between attention and attribution distributions increases with depth. This confirms the importance of accounting for information mixing when analyzing attention heads with respect to the model input. Finally, we show how five different attention head patterns (block, vertical, diagonal, vertical-diagonal, heterogeneous) compare to their token attribution equivalents.

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A Attention Histograms

Figure 6: Attention histograms for layers 1 to 6
Figure 7: Attention histograms for layers 7 to 12
Figure 8: Input contribution histograms for layers 1 to 6
Figure 9: Input contribution histograms for layers 7 to 12
C Comparison of Local vs. Global Head Patterns

Figure 10: Layer 1

Figure 11: Layer 2
Figure 12: Layer 3

Figure 13: Layer 4
Figure 14: Layer 5

Figure 15: Layer 6
Figure 16: Layer 7

Figure 17: Layer 8
Figure 18: Layer 9

Figure 19: Layer 10
