# SparseBERT: Rethinking the Importance Analysis in Self-attention

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# **Abstract**

Transformer-based models are popular for natural language processing (NLP) tasks due to its powerful capacity. As the core component, selfattention module has aroused widespread interests. Attention map visualization of a pre-trained model is one direct method for understanding selfattention mechanism and some common patterns are observed in visualization. Based on these patterns, a series of efficient transformers are proposed with corresponding sparse attention masks. Besides above empirical results, universal approximability of Transformer-based models is also discovered from a theoretical perspective. However, above understanding and analysis of self-attention is based on a pre-trained model. To rethink the importance analysis in self-attention, we delve into dynamics of attention matrix importance during pre-training. One of surprising results is that the diagonal elements in the attention map are the most unimportant compared with other attention positions and we also provide a proof to show these elements can be removed without damaging the model performance. Furthermore, we propose a Differentiable Attention Mask (DAM) algorithm, which can be also applied in guidance of SparseBERT design further. The extensive experiments verify our interesting findings and illustrate the effect of our proposed algorithm.

## 1. Introduction

The transformer (Vaswani et al., 2017) has been commonly used in various natural language processing (NLP) tasks such as text classification (Wang et al., 2018a), text translation (Ott et al., 2018), and question answering (Mohamed et al., 2019). The recent use of transformer for object detection (Carion et al., 2020) also demonstrates its potential

in computer vision. Two notable descendants from the transformer include the BERT (Devlin et al., 2019), which achieves state-of-the-art performance on a wide range of NLP tasks, and GPT-3 (Brown et al., 2020) which applies the transformer's decoder on generative downstream tasks.

Self-attention is a core component in transformer-based architectures. Recently, its interpretation has aroused a lot of interest. Visualization has been commonly used to understand the attention map during inference (Park et al., 2019; Gong et al., 2019; Kovaleva et al., 2019). For example, Park et al. (2019) and Gong et al. (2019) randomly select a sentence from the corpus and visualize the attention maps of different heads in a pre-trained transformer model. Kovaleva et al. (2019) summarizes five attention patterns and estimates their ratios in different tasks. A common observation from these studies is that local attention and global attention are both important for token understanding.

While self-attention is powerful, a main concern is its efficiency bottleneck. As each token has to attend to all n tokens in the sequence, the complexity scales as  $\mathcal{O}(n^2)$ . This can be expensive on long sequences. To alleviate this problem, sparse self-attention allows each token to attend to only a token subset. A series of transformer variants have been proposed along this direction (Guo et al., 2019; Child et al., 2019; Li et al., 2019; Beltagy et al., 2020). For example, the Star-Transformer (Guo et al., 2019) uses a star-shaped attention structure. However, these sparse attention schemes are designed manually. It is still an open issue on how to find a suitable attention scheme for general tasks.

Recently, there is growing interest in understanding self-attention from a theoretical perspective. Results show that the transformer and its variants are universal approximators of arbitrary continuous sequence-to-sequence functions (Yun et al., 2019; 2020; Zaheer et al., 2020). A key part of their proofs is that self-attention layers implement contextual mappings of the input sequences. Yun et al. (2019) constructs the self-attention model as a selective shift operation such that the contextual mapping can be implemented. Zaheer et al. (2020) shows that universal approximation holds for their sparse transformer Big Bird if it contains the star graph. Yun et al. (2020) provide a unifying framework for universal approximation of sparse transformers. Note that they all emphasize the importance of diagonal elements

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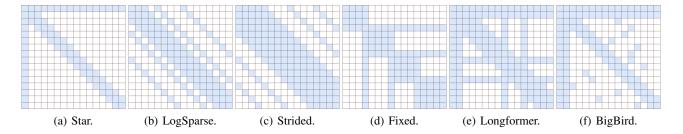


Figure 1. Examples of existing attention masks (with n = 16).

in the attention map.

To guide the design of an efficient transformer, it is useful to investigate the importance of different positions in self-attention. In this paper, we study this using differentiable search (Liu et al., 2019; Xie et al., 2018). A learnable attention distribution is constructed and the score of each position is learned in an end-to-end manner during pre-training. While existing theoretical and empirical findings suggest the importance of diagonal elements in the self-attention matrix, we observe that they are indeed least important compared to the other entries. Furthermore, neighborhood tokens and special tokens (such as the first token [CLS] and last token [SEP]) are also prominent, which is consistent with previous observations in (Park et al., 2019; Gong et al., 2019; Kovaleva et al., 2019; Clark et al., 2019). Besides, using the Gumbel-sigmoid function (Maddison et al., 2017), we propose the Differentiable Attention Mask (DAM) algorithm to learn the attention mask in an end-to-end manner. Extensive experiments using masks with different sparsities on various NLP tasks demonstrate the effect of the proposed algorithm. Specifically, highly sparse structured attention masks (with 91.3% sparsity) can already achieve 80.9% average score on the GLUE development set (Wang et al., 2018a).

## 2. Related Work

# 2.1. Transformer Block and Self-Attention

The transformer block is a basic component in the transformer (Vaswani et al., 2017) and BERT (Devlin et al., 2019) architectures. Let  $X \in \mathbb{R}^{n \times d}$  be the input to a transformer block, where n is the number of input tokens and d is the embedding size. Each block consists of a self-attention layer and a feed-forward layer.

The self-attention layer output can be written as:

$$Attn(X) = X + \sum_{k=1}^{H} \sigma(XW_{Q}^{k}(XW_{K}^{k})^{\top})XW_{V}^{k}W_{Q}^{k\top}, \quad (1)$$

where H is the number of heads,  $\sigma$  is the softmax function, and  $W_Q^k, W_K^k, W_V^k, W_Q^k \in \mathbb{R}^{d \times d_h}$  (where  $d_h = d/H$  is the dimension of a single-head output) are weight matrices for

the query, key, value, and output, respectively of the kth head. In particular, the self-attention matrix

$$A(X) = \sigma(XW_Q(XW_K)^\top) \tag{2}$$

in (1) plays a key role in the self-attention layer (Park et al., 2019; Gong et al., 2019; Kovaleva et al., 2019).

The fully-connected layer usually has two layers with residual connection:

$$FF(X) = Attn(X) + W_2 ReLU(W_1 Attn(X) + b_1) + b_2,$$

where  $W_1 \in \mathbb{R}^{d \times d_{\mathrm{ff}}}$ ,  $W_2 \in \mathbb{R}^{d_{\mathrm{ff}} \times d}$  ( $d_{\mathrm{ff}}$  is the size of the intermediate layer) are the weight matrices, and  $b_1, b_2$  are the biases. As in (Yun et al., 2019; Zaheer et al., 2020; Yun et al., 2020), we drop the scale product and layer-normalization layer to simplify analysis.

### 2.2. Sparse Transformers

To reduce the quadratic complexity in self-attention, a number of sparse transformers have been recently proposed. In these models, each token can attend to only a subset of fixed positions (Guo et al., 2019; Child et al., 2019; Li et al., 2019; Beltagy et al., 2020). This can be seen as being controlled by an attention mask  $M = [0, 1]^{n \times n}$ , where  $M_{i,j} = 1$  indicates that token i can attend to token j, and 0 otherwise. For example, Figure 1(a) shows the attention mask of the Star-Transformer (Guo et al., 2019). It uses ring connections for local attention, and radical connections to an auxiliary relay node (the first token in the figure) to represent global attention. Li et al. (2019) proposes the LogSparse self-attention, in which each token only attends to itself and its previous tokens with an exponential stepsize (Figure 1(b)), resulting in  $\mathcal{O}(n \log n)$  complexity. Child et al. (2019) performs sparse factorization on the attention matrix, and reduces its complexity to  $\mathcal{O}(n\sqrt{n})$  with the use of two attention masks. The strided mask (Figure 1(c)) attends to every lth location (where l is the stride step), while the fixed mask (Figure 1(d)) allows specific positions to be attended to. The very recent Longformer (Beltagy et al., 2020) (Figure 1(e)) and BigBird (Zaheer et al., 2020) (Figure 1(f)) models use a number of attention patterns, and reduce their complexities

to  $\mathcal{O}(n)$ . With these sparse transformers, BERT is shown to be more efficient for long document understanding (Child et al., 2019; Qiu et al., 2020).

# 3. Which Attention Positions are Important?

Previous works on sparse transformers only provide a crude understanding of the self-attention module that local attention and global attention are both important. In this section, we study the self-attention matrix  $A \in \mathbb{R}^{n \times n}$  in (2) in more detail. To emphasize its role, we write the output of the self-attention layer as Attn(X, A(X, M)), where M is a fixed attention mask. Since the nonzero elements of the attention matrix are fixed, one only needs to perform computations related to these positions. We define the sparsity of an attention mask as  $\rho = 1 - |M|/n^2$ . The complexity of the self-attention layer is thus reduced to  $\mathcal{O}(\rho n^2)$ .

With a low self-attention sparsity, a token can attend to more tokens given the same amount of computational cost, and is thus expected to have better performance. On the other hand, at high self-attention sparsity, model performance may drop. It is natural to ask which positions in self-attention are more important. In other words, which attention mask is better for a given sparsity. We formulate this problem as the search for a mask in  $[0,1]^{n\times n}$  such that the balance between performance and efficiency is optimized.

### 3.1. Continuous Relaxation

In this section, we investigate the importance of different positions in self-attention. A similar study on the importance of different heads in the transformer is recently performed in (Michel et al., 2019). However, while Michel et al. (2019) performs the ablation study with only 16 heads, there are  $2^{n \times n}$  possible attention distributions here. This huge search space makes the study very challenging.

In neural architecture search (NAS) (Elsken et al., 2019), one has to find a good architecture from a huge search space. Inspired by the similiarity with our problem, we propose to use continuous relaxation as in differentiable architecture search (DARTS) (Liu et al., 2019). Specifically, we associate an  $\alpha_{i,j}$  with each position (i,j) in the self-attention matrix A(X), and define the attention probability as

$$P_{i,j} = \sigma(\alpha_{i,j}) \in [0,1],\tag{3}$$

where  $\sigma(\cdot)$  is the sigmoid function. For symmetry, we enforce  $\alpha_{i,j} = \alpha_{j,i}$ . Analogous to (1), the soft-masked self-attention is then

$$Attn(X) = X + \sum_{k=1}^{H} (P^k \odot A^k)(X) V^k(X) W_O^{k \top},$$
 (4)

where  $\odot$  is the element-wise product. Obviously, when  $P_{i,j} = 1$  for all (i, j)'s, this reduces to Eq. (1).

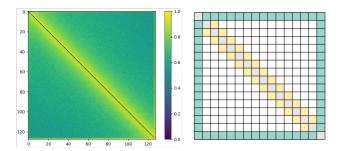


Figure 2. Visualization of the attention distribution. In the figure on the right, the dark entries are for diag-attention, yellow for neighborhood attention and green for special attention.

As in DARTS, there are two sets of learnable parameters: parameter w of the transformer model, and the attention parameter  $\alpha = \{\alpha_{i,j}\}$ . They can be learned by using either one-level optimization (Xie et al., 2018) or bi-level optimization (Liu et al., 2019) formulations. Recently, Bi et al. (2020) shows that the limitations of one-level optimization can be alleviated when a large data set is used. In our context, as a large data set is often available during pre-training, we apply the simpler one-level optimization here.

### 3.1.1. EXPERIMENTAL SETUP

In this experiment, we empirically study the effect of different positions in the self-attention module using the BERTbase. This model is stacked with 12 transformer blocks (Section 2.1) with the following hyper-parameters: number of tokens n = 128, number of self-attention heads h = 12, and hidden layer size d = 768. The parameters of P are shared among blocks, leading to a total of 12 P's (one for each selfattention head). As for the feed-forward layer, we set the number of filter size  $d_{\rm ff}=3072$  as in (Devlin et al., 2019). We follow the standard pre-training experiment setting in (Devlin et al., 2019), and take Masked Language Modeling (MLM) and Next Sentence Prediction (NSP) as our pretraining tasks. Data sets BooksCorpus (with 800M words) (Zhu et al., 2015) and English Wikipedia (with 2,500M words) (Devlin et al., 2019) are used. We use the WordPiece embedding (Wu et al., 2016), and 30,000 tokens are contained in the dictionary. The special token [CLS] is used as the first token of each sequence. Another special token [SEP] is used to separate sentences in a sequence. The pre-training is performed for 40 epochs. All experiments are performed on NVIDIA Tesla V100 GPUs.

### 3.1.2. RESULTS

Figure 2 shows the attention distribution P averaged over the 12 heads. The following can be observed: (i) Diagonal elements (denoted "diag-attention" in the sequel) are the least important compared to the other positions. Surprisingly, this conflicts with existing observations in (Park et al.,

2019; Gong et al., 2019; Kovaleva et al., 2019), which emphasize the importance of diagonal attention. We believe this is because the self-attention layer already has a skip connection (the term X in (1)). Influence of diag-attention can thus be conveyed in the skip connection instead of via the self-attention matrix; (ii) Neighborhood positions are the most significant in the attention distribution matrix; (iii) The special tokens ([CLS] and [SEP]) are important, which is also observed in (Clark et al., 2019); (iv) Importance of the other positions are similar.

# 3.2. Universal Approximability

Recall that the transformer and its variants are universal approximators of arbitrary continuous sequence-to-sequence functions (Yun et al., 2019; 2020; Zaheer et al., 2020). In their proofs, diagonal positions in the self-attention matrix play a key role. As Section 3.1 has shown that the diagonal elements are empirically the least important, an interesting question is whether universal approximability will still hold when these diagonal elements (diag-attention) are dropped.

Without diag-attention, the *i*th token output of the self-attention layer becomes:

$$Attn(X)_i = X_i + \sum_{k=1}^{H} \sum_{j \neq i} A_{i,j}^k(X) V_j^k(X) W_O^{k \top}.$$

Let  $\mathcal{T}^{H,d_h,d}$  be a class of transformers without diagattention stacks, and  $F_{CD}$  be the set of continuous functions  $f:[0,1]^{n\times d}\mapsto\mathbb{R}^{n\times d}$ . For any  $p\geq 1$ , the  $\ell_p$ -distance between  $f_1,f_2\in F_{CD}$  is defined as  $d_p(f_1,f_2)=(\int\|f_1(X)-f_2(X)\|_p^pdX)^{1/p}$ . The following Theorem shows that the self-attention mechanism without diagattention is also an universal approximator:

**Theorem 1.** Given  $1 , <math>\epsilon > 0$  and n > 2, for any  $f \in F_{CD}$ , there exists a transformer network without diag-attention  $g \in T^{2,1,4}$ , such that  $d_p(f,g) < \epsilon$ .

The following shows the proof outline, which is similar to that in (Yun et al., 2019). The main difference is in the contextual mapping step since each token cannot attend to itself in our scenario.

**Step 1**: Approximate  $F_{CD}$  with the set of piecewise-constant functions  $\bar{F}_{CD}$ . We split input  $[0,1]^{n\times d}$  into a set of grids  $\mathcal{G}_{\delta} \in \{0,\delta,\ldots,1\}^{n\times d}$ . We then approximate any input belonging to the same cube  $\mathcal{G}_{\delta} + [0,\delta]^{n\times d}$  by the same value, resulting in a piecewise-constant function  $\bar{f}$ . With  $\delta$  small enough, we have  $d_n(f,\bar{f}) \leq \epsilon/3$ .

**Step 2**: Approximate  $\bar{F}_{CD}$  with the modified transformer blocks  $\bar{\mathcal{T}}^{H,d_h,d}$ , which replace the softmax operator and ReLU with the hardmax operator and a piece-wise linear functions (at most three pieces). For each above  $\bar{f}$ , there exists a closely approximate function  $\bar{g} \in \bar{\mathcal{T}}^{2,1,1}$  such that

$$d_n(\bar{f}, \bar{q}) = O(\delta^{d/p}).$$

This is the key step related to the contextual mapping. A selective shift operation is proposed to construct an approximation in (Yun et al., 2019). Here, we consider a simple scenario where d=1 and n=3 and let  $L=[l_1\quad l_2\quad l_3]\in\mathcal{G}_\delta$ . Without loss of generality, we assume that  $l_1< l_2< l_3$ . For a transformer without diag-attention, the selective shift operation, consisting of 2 attention heads of size 1, is constrained as follows:

$$\begin{split} \Psi(Z;b_1,b_2)_{i,1} &= \left\{ \begin{array}{ll} \max_{j \neq i} Z_{j,1} - \min_{j \neq i} Z_{j,1} & b_1 < Z_{i,1} < b_2 \\ 0 & \text{otherwise} \end{array} \right. . \end{split}$$

We stack  $1/\delta$  self-attention layers, with attention parts  $\delta^{-1}\Psi(\cdot;l-\delta/2,l+\delta/2)$  for each  $l\in\{0,\delta,\ldots,1-\delta\}$  in increasing order of l. The shift operation is first applied to  $l_1$ , resulting in  $l_1 = l_1 + \delta^{-1}(l_3 - l_2) > l_3$ . The second shift operation is then applied to  $\widetilde{l_2} = l_2 + \delta^{-1}(\widetilde{l_1} - l_3) = l_2 + \delta^{-1}(\widetilde{l_2} - l_3) = l_2 + \delta^{-1}(\widetilde{l_1} - l_3) = l_2 + \delta^{-1}(\widetilde{l_2} - l_3) = l_2 + \delta^{-1}(\widetilde{l_1} - l_3) = l_2 + \delta^{-1}(\widetilde{l_2} - l_3) = l_2 + \delta^{-1}(\widetilde{l_1} - l_3) = l_2 + \delta^{-1}(\widetilde{l_2} - l_3) = l_2 + \delta^{-1}(\widetilde{l_1} - l_3) = l_2 + \delta^{-1}(\widetilde{l_2} - l_3) = l_2 + \delta^{-1}(\widetilde{l_1} - l_3) = l_2 + \delta^{-1}(\widetilde{l_2} - l_3) = l_2 + \delta^{-1}(\widetilde{l_1} - l_3) = l_2 + \delta^{-1}(\widetilde{l_2} - l_3) = l_3 + \delta^{-1}(\widetilde{l_3} - l_3) = l_3 +$  $\delta^{-1}(l_1-l_3)+\delta^{-2}(l_3-l_2)>\widetilde{l_1}$ . Finally, a similar operation is applied to  $l_3$ , and the shifted result is  $l_3 = l_3 + \delta^{-1}(l_2 - l_3)$  $\widetilde{l_1}$ ) =  $l_3 + \delta^{-1}(l_2 - l_1) + \delta^{-2}(l_1 + l_2 - 2l_3) + \delta^{-3}(l_3 - l_2)$ . It is easy to check that the map from the original L to  $\tilde{l_3}$  is one-to-one and that  $0 < \tilde{l}_1 < \tilde{l}_2 < \tilde{l}_3 < \delta^{-3}$ . We then add two additional layers shifting all positive elements, resulting in  $[\widetilde{l_1} + \Delta(\widetilde{l_2} + \widetilde{\widetilde{l_3}}) + \Delta^2 \widetilde{l_3} \quad \widetilde{l_2} + \Delta(\widetilde{l_1} + \widetilde{l_3}) + \Delta^2 \widetilde{l_3} \quad \widetilde{l_3} + 2\Delta \widetilde{l_2} + \Delta^2 \widetilde{l_3}]$ , where  $\Delta = (\delta^{-1} - 1)(\delta^{-3} + \delta^{-1} + 1)$ . Note that all elements are in the disjoint interval for different L's because  $L \to l_3$  is bijective. Thus, the self-attention layer without diag-attention is a contextual mapping as defined in (Yun et al., 2019).

**Step 3**: Approximate the modified transformer blocks  $\bar{g} \in \bar{\mathcal{T}}^{2,1,1}$  with standard transformer blocks  $g \in \mathcal{T}^{2,1,4}$  such that we have  $d_n(\bar{g},g) \leq \epsilon/3$ .

By Summarizing above three steps, we have:

$$d_p(f,g) \leq d_p(f,\bar{f}) + d_p(\bar{f},\bar{g}) + d_p(\bar{g},g) \leq 2\epsilon/3 + O(\delta^{d/p}).$$

With enough small  $\delta$ , we have  $d_p(f,g) \leq \epsilon$ . Thus, transformers without diag-attention are also universal approximators. The detailed proof is in Appendix A.

### 3.3. Emperical Verification

In this section, we study the effect of dropping diag-attention from the self-attention mechanism empirically. The fine-tuning experiments are performed on the GLUE benchmark (Wang et al., 2018a), SWAG (Zellers et al., 2018) and SQuAD (Rajpurkar et al., 2016) data sets.

## 3.3.1. DATA

The GLUE benchmark includes three categories of natural language understanding tasks: (i) single-sentence tasks

Table 1. Performance (in %) of the various BERT-base	se variants	s on the GLUE data set	
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	MNLI (m/mm)	QQP	QNLI	SST-2	COLA	STS-B	MRPC	RTE	average
Development Set									
BERT-base (ours)	85.4/85.8	88.2	91.5	92.9	62.1	88.8	90.4	69.0	83.8
BERT-base (randomly dropped)	84.6/85.2	87.7	91.1	92.7	62.0	88.9	89.3	68.9	83.4
BERT-base (no diag-attention)	85.6/85.9	88.2	92.0	93.8	63.1	89.2	91.2	67.9	83.9
Test Set									
BERT-base (Devlin et al., 2019)	84.6/83.4	71.2	90.5	93.5	52.1	85.8	88.9	66.4	79.6
BERT-base (ours)	84.8/84.1	71.3	90.9	93.4	52.3	85.3	88.3	66.9	79.7
BERT-base (randomly dropped)	84.5/83.5	70.3	91.1	93.4	52.0	85.8	87.4	66.7	79.4
BERT-base (no diag-attention)	85.5/84.9	71.3	91.1	93.4	53.3	86.3	88.9	67.9	80.3

Table 2. Performance (in %) of the various BERT-base variants on the SWAG and SQuAD development sets.

	SWAG	SQuAD v1.1		SQuAD v2.0	
	acc	EM	F1	EM	F1
BERT-base (Devlin et al., 2019)	81.6	80.8	88.5	-	-
BERT-base (ours)	82.5	79.7	87.1	72.9	75.5
BERT-base (randomly dropped)	81.6	79.7	87.0	71.5	74.2
BERT-base (no diag-attention)	83.5	80.3	87.9	73.2	75.9

(CoLA and SST-2); (ii) similarity and paraphrase tasks (MRPC, QQP and STS-B); (iii) inference tasks (MNLI, QNLI and RTE). For MNLI task, we experiment on both the matched (MNLI-m) and mismatched (MNLI-mm) sections. The SWAG data set is for grounded commonsense inference, while the SQuAD data set is for question answering. In SQuAD v1.1, the answers are included in the context; while in SQuAD v2.0, some answers are not included. Detailed descriptions of the data sets are in Appendix B.

### 3.3.2. METRIC

Following BERT (Devlin et al., 2019), we report different metrics for different GLUE sub-tasks. Specifically, we use accuracy for the MNLI, QNLI, RTE, SST-2 tasks, F1 score for QQP and MRPC, Spearman correlation for STS-B, and Matthews correlation for CoLA. For the SWAG task, we use accuracy for evaluation. For SQuAD v1.1 and v2.0, we use the Exact Match (EM) and F1 scores.

# 3.3.3. DETAILS

We perform pre-training and fine-tuning. The experiment settings are the same as (Devlin et al., 2019). We take the BERT-base model in Section 3.1 as baseline, and verify the effect of diagonal elements in the self-attention matrix. In the variant "BERT-base (no diag-attention)", the diagattention in each self-attention layer is removed, dropping a total of 128 elements (as n=128). In "BERT-base (randomly dropped)", we remove the same number (128) of entries randomly. To reduce statistical variability, the results are averaged over three random repetitions. Details of the other hyper-parameter settings are in Appendix C.

We choose the best hyper-parameter combination on the development set and test on the evaluation server.

### 3.3.4. RESULTS

Results on the GLUE benchmark are shown in Table 1. For comparison, we also show the BERT-base results reported in (Devlin et al., 2019). As can be seen, even by constraining the self-attention mechanism such that each token cannot attend to itself, the performance of this constrained model "BERT-base (no diag-attention)" is still comparable with the original BERT or even better. On the other hand, when the sparse attention masks are randomly chosen, the performance has a drop. Table 2 shows the results on SWAG and SQuAD, and the observations are similar. This inspires us the attentions in diagonal position are not necessary. Without attending to self-token, the model performance will not be damaged.

# 3.4. Progressive Pruning of Self-attention

To further investigate the effectiveness of our searched mask, we perform progressive pruning of self-attention according to the results in Section 3.1.2. Experiments are again performed on the GLUE benchmark. We threshold P to binary attention mask M so that the small entries in P are pruned. We study the performance with different mask sparsities. Specifically, for each head, we remove the smallest  $10\%/20\%/\ldots/90\%$  entries from P. For comparison, we include a random baseline that randomly removes the same number of entries.

As can be seen from Figure 3, pruning by the attention distri-

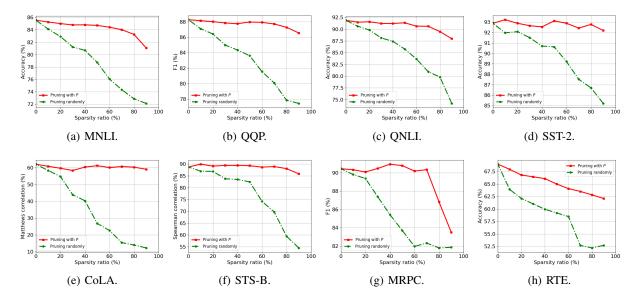


Figure 3. Performance of the BERT-base at different attention mask sparsities on the GLUE development set. MNLI is the average performance on the MNLI-m and MNLI-mm sections.

bution matrix P consistently outperforms random pruning on all GLUE tasks. This verifies the importance analysis in Section 3.1.2. Moreover, models from different GLUE sub-tasks can have different degrees of redundancy. For instance, performance on the CoLA sub-task remains stable when sparsity gets higher. In contrast, the RTE sub-task performance shows a significant drop as the model is sparsified, illustrating the need for a denser self-attention computation.

# 4. SparseBERT

As discussed in Section 2.2, vanilla self-attention suffers from quadratical complexity, and a number of sparse transformers have been proposed (Guo et al., 2019; Child et al., 2019; Li et al., 2019; Beltagy et al., 2020; Zaheer et al., 2020). However, their attention masks are manually designed. In this section, we use the observations in the previous sections to help develop a series of sparse attention masks with different sparsities.

### 4.1. Differentiable Attention Mask

A straightforward method to generate sparse transformers is by pruning the attention distribution P as is performed in Section 3.4. However, this involves two separate stages. The resultant performance maybe sub-optimal as the whole model is not trained end-to-end. And the discretization of continuous attention distribution P may mislead the final attention mask.

To enable end-to-end training, we propose to use the Gumbel relaxation (Maddison et al., 2017). Instead of using the

# **Algorithm 1** Differentiable Attention Mask (DAM).

- 1: initialize model parameter w and attention mask parameter  $\alpha$ .
- 2: repeat
- 3: generate mask  $M_{i,j} \leftarrow \text{gumbel-sigmiod}(\alpha_{i,j})$ ;
- 4: obtain the loss with attention mask  $\mathcal{L}$ ;
- 5: update parameter w and  $\alpha$  simultaneously;
- 6: until convergence.
- 7: **return** attention mask M.

sigmoid function to output the attention probability as in (3), we use the Gumbel-sigmoid:

$$M_{i,j} = \operatorname{gumbel-sigmoid}(\alpha_{i,j}) = \operatorname{sigmoid}(\alpha_{i,j} + G_1 - G_2),$$

where  $G_1$ ,  $G_2$  are independent Gumbel noises generated from the uniform distribution U as:

$$G_k = -\log(-\log(U_k)), U_k \sim U(0, 1),$$

and  $\tau$  is a temperature hyperparameter. As  $\tau$  approaches zero, the Gumbel-sigmoid output becomes a discrete distribution in  $\{0,1\}$ . Thus, we can train the attention mask in an end-to-end manner with the Gumbel-sigmoid variant. To balance mask sparsity with performance, we add the sum absolute values of the attention mask to the loss, as:

$$\mathcal{L} = l(BERT(X, A(X) \odot M(\alpha); w)) + \lambda ||M(\alpha)||_1, (5)$$

where l(BERT(X, A(X); w)) is the pre-training loss, and  $\lambda$  is a trade-off hyperparameter. When  $\lambda$  is large, we pay more emphasis on efficiency and the learned attention mask

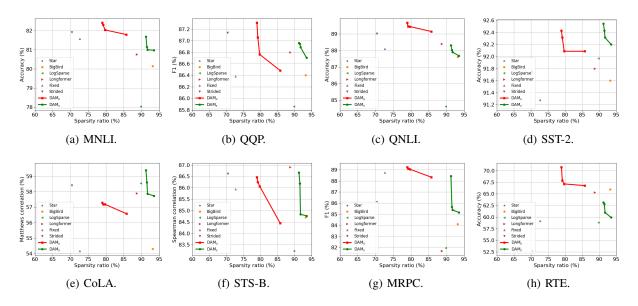


Figure 4. Performance of the BERT-base for different attention masks on the GLUE development set. MNLI shows the average performance on the MNLI-m and MNLI-mm sections.

Table 3. Comparison of BERT-base model with different attention masks on GLUE development set (%)	Table 3. Comparison of	of BERT-base m	nodel with differen	nt attention masks on	GLUE develo	pment set (	%).
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	Sparsity ratio	MNLI-(m/mm)	QQP	QNLI	SST-2	COLA	STS-B	MRPC	RTE	Average
Strided	70.4	81.9/81.9	87.1	89.0	91.7	58.4	86.6	86.1	52.7	79.5
Fixed	72.7	81.4/81.8	86.4	88.1	91.3	54.2	85.9	88.7	59.2	79.7
Longformer	88.7	80.5/81.0	86.8	88.4	91.8	57.9	86.9	81.7	65.3	80.1
LogSparse	89.8	77.9/78.2	85.9	84.6	92.0	58.5	83.2	82.0	58.8	77.9
BigBird	93.2	80.2/80.1	86.4	87.6	91.6	54.3	84.7	84.1	66.0	79.4
Star	96.1	79.1/79.0	86.2	86.4	91.2	59.6	84.7	83.9	60.3	78.9
$DAM_u (\lambda = 10^{-4})$	78.9	82.2/82.6	87.3	89.7	92.4	57.3	86.5	89.2	70.8	82.0
$\mathrm{DAM}_u \ (\lambda = 10^{-3})$	79.2	82.2/82.4	87.1	89.5	92.3	57.2	86.2	89.1	67.9	81.6
$\mathrm{DAM}_u \ (\lambda = 10^{-2})$	79.8	81.7/82.3	86.8	89.4	92.1	57.2	86.1	89.0	67.1	81.3
$\mathrm{DAM}_u \ (\lambda = 10^{-1})$	85.8	81.4/82.2	86.5	89.1	92.1	56.6	84.4	88.3	66.8	80.8
$DAM_s (\lambda = 10^{-4})$	91.2	81.7/81.7	87.0	88.3	92.5	59.4	86.7	88.4	63.2	80.9
$DAM_s (\lambda = 10^{-3})$	91.6	81.0/81.2	86.9	88.0	92.4	58.6	86.2	85.7	62.8	80.3
$DAM_s (\lambda = 10^{-2})$	91.7	81.1/80.9	86.9	87.9	92.3	57.9	84.8	85.4	61.0	79.8
$DAM_s (\lambda = 10^{-1})$	93.5	80.9/81.0	86.7	87.7	92.2	57.7	84.8	85.2	59.9	79.6

M is sparser, and vice versa. The obtained one-hot Gumbel sigmoid output can then be directly used as the attention mask. The whole algorithm is shown in Algorithm 1.

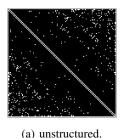
Note that the attention mask obtained in Algorithm 1 is unstructured, as the  $\alpha_{i,j}$ 's are all independent of each other. This irregular structure may affect the efficiency of the final CUDA implementation.

To alleviate this problem, we use the observed sparsity patterns in Figure 2 to constrain the structure of the attention mask. First, as the special tokens are important, we require the first and last row/column of the attention mask to be active. Second, for all positions on each line parallel to the diagonal line, we share their mask parameters including their two Gumbel noises such that the generated mask has  $M_{i,j} = M_{i+k,j+k}$  for integer k. Among previous proposed

attention masks, Sparse Transformer (strided) (Child et al., 2019) and LogSparse Transformer (Li et al., 2019) conform to our definition about structured attention masks and they can be implemented by custom CUDA kernels. Benefit from the above prior structure, there are only n-2 different attention mask parameters. Therefore, the search space is reduced to  $2^{n-2}$  for structured attention mask search. Since the sparsity ratio can represent the efficiency of the Sparse-BERT, we discover the performance of attention mask with respect to its sparsity ratio.

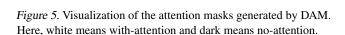
### 4.2. Experiments

As in previous sections, we evaluate the proposed DAM algorithm by using the BERT-base (Devlin et al., 2019) model on the GLUE data sets (Wang et al., 2018a) with pre-training





(b) structured.



and fine-tuning (Devlin et al., 2019). We use the same pretraining setting as in Section 3.1 with the dynamic attention mask. As for fine-tuning, the attention mask is fixed and other experiment setting is the same as Section 3.3. The DAM variant using unstructured attention mask is denoted DAM<sub>u</sub>, while the one using structured attention mask is denoted DAM<sub>s</sub>. The trade-off hyperparameter  $\lambda$  in (5) is varied in  $\{10^{-1}, 10^{-2}, 10^{-3}, 10^{-4}\}$  to generate masks with different sparsities.

For comparison, we consider the following baselines with different manually-designed attention masks (Figure 1): (i) Star (Guo et al., 2019); (ii) LogSparse (Li et al., 2019); (iii) Strided (Child et al., 2019); (iv) Fixed (Child et al., 2019); (v) Longformer (Beltagy et al., 2020); and (vi) BigBird (Zaheer et al., 2020). For the Longformer, we set the sliding window size to 2 and two input locations are randomly selected for global attention. For the BigBird, we neglect its block structure for fair comparison and set its random attention size to 2, window attention size to 1, and global attention size to 2. The sparsities of these fixed attention masks can be easily computed.

Results of performance on the GLUE sub-tasks used are shown in Figure 4 and Table 3. As can be seen, attention masks generated by our proposed method outperform manual-designed masks in almost all the cases and their sparsity ratio can be controlled by  $\lambda$ . For example, compared with BigBird, our DAM<sub>s</sub> ( $\lambda=10^{-1}$ ) achieve higher average performance while our attention mask is sparser.

Figure 5 shows two attention masks generated by DAM after pre-training with  $\lambda=10^{-1}$ . We also illustrate an assembly of attention masks in Appendix D. As can be seen, the diagonal entries are not attended, while their neighborhood positions are always attended. From the visualization of all attention masks in Figure 1 and Figure 5, we can summarize them into three categories: (i) Stride/Fixed/Logsparse, which only contain neighboring attention; (ii) BigBird/Longformer/Star, which contain both neighboring attention and attention from special tokens; (iii) our attention masks, replace diag-attention with other atten-

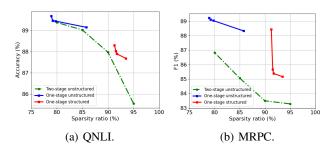


Figure 6. Comparison of one-stage and two-stage attention mask on QNLI and MRPC development set.

tion based on the second category. From the performance on GLUE, the first class is the worst, the second is competing while ours are the best, which agrees with our observations in Section 3.1.2.

# 4.3. Ablation Study

In this section, we compare Differentiable Attention Mask described in Algorithm 1, which generates the attention mask as part of the end-to-end training process (one-stage) with the pruning approach in Section 3.4, which first obtains the attention probabilities in P and then performs thresholding to obtain the binary attention mask (two-stage). For two-stage attention mask, we prune 80%/85%/90%/95% entries of self-attention for better comparison.

Due to space limitations, we only illustrate the performance comparison on the QNLI and MRPC development sets in Figure 6. As can be seen, the attention masks (unstructured and structured) generated by one-stage optimization achieve better performance. However, while the two-stage attention mask can easily adjust its sparsity to any desired value, the one-stage approach cannot set the sparsity directly as it is controlled by the hyper-parameter  $\lambda$  in Eq. (5).

## 5. Conclusion

In this paper, we investigate the importance of the different attention positions in the self-attention mechanism. By jointly optimizing a soft attention mask with the BERT model, we obtain several interesting findings. In particular, one surprising observation is that the diagonal elements in the attention matrix are the least important. We then show, both theoretically and experimentally, that these diagonal elements are indeed not useful for universal approximation and empirical performance. Besides, by using the Gumbelsigmoid function, we propose to optimize the attention mask in an end-to-end manner for efficient transformer design. Extensive experimental results on a number of NLP tasks demonstrate the usefulness of the proposed algorithm.

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# Appendix for

# SparseBERT: Rethinking the Importance Analysis in Self-attention

## A. Proof

# A.1. Proof for Step 1

**Lemma 2** (Lemma 8 (Yun et al., 2019)). For any  $f \in \mathcal{F}_{CD}$ , there exists a piece-wise constant function  $\bar{f}$  such that  $d_p(f,\bar{f}) < \epsilon/3$ .

*Proof.* f is uniformly continously since f is a continous function on  $[0,1]^{n\times d}$ , which implies:  $\forall \epsilon > 0, \exists \delta > 0$ , such that

$$\forall X, Y, ||X - Y||_{\infty} < \delta \Rightarrow ||f(X) - f(Y)||_{p} < \epsilon/3.$$

Then we split the compact domain  $[0,1]^{n\times d}$  into a grid of granularity  $\delta$ , such that  $G_{\delta} \in \{0, \delta, \dots, 1\}$ . By defining the following piece-wise constant function

$$\bar{f}(X) = \sum_{G \in G_{\delta}} f(G) * \mathbb{1}\{X \in G + [0, \delta]^{n \times d}\},$$

we have

$$||f(X) - \bar{f}(X)||_p = ||f(X) - f(G)||_p < \epsilon/3.$$

Thus,

$$d_p(f, \bar{f}) = (\int ||f(X) - \bar{f}(X)||_p^p dX)^{1/p} < \epsilon/3.$$

This proves the lemma.

### A.2. Proof for Step 2

### A.2.1. QUANTIZATION (FEED-FORWARD)

**Lemma 3** (lemma 5 (Yun et al., 2019)). Consider a quantization mapping  $g_a^{ent}$ :

$$g_q^{ent}(t) = \begin{cases} k\delta & k\delta \leq t < (k+1)\delta, k \in [1:1/\delta-1], \\ -\delta^{-nd} & \textit{otherwise}. \end{cases}$$

There exsits a function  $g_q$  composed of  $d/\delta + d$  token-wise feed-forward layers with r = 1 and piece-wise linear functions (at most three pieces), such that the quantization is performed on each entry of the input.

We first quantize the input X to their corresponding grid  $G_{\delta}$  by quantization function  $g_q$ .

# A.2.2. CONTEXUAL MAPPING (SELF-ATTENTION)

This is the main difference between ours and previous works, where self-attention without diag-attention adds additional constrains to attention matrix. We will illustrate the definition of contextual mapping first and then proof transformer blocks without diag-attention can also reach contexual mapping.

**Definition 1.** (Contextual Mapping) For a set  $G_{\delta} \in \mathbb{R}^{n \times d}$ , a contextual mapping is a function mapping  $q: G_{\delta} \to \mathbb{R}^n$  satisfying:

- For any  $G \in G_{\delta}$ , all entries in q(G) are distinct.
- For any  $G_1, G_2 \in G_\delta$  ( $G_1 \neq G_2$ ), all entries of  $q(G_1)$  and  $q(G_2)$  are distinct.

**Lemma 4.** There exists a function  $g_c$  composed of  $\delta^{-d} + 1$  self-attention layers without diag-attention, such that  $q(G) := g_c(G)u$  satisfies the contextual mapping definition.

*Proof.* Consider the function  $\psi$ , which can be implemented by a self-attention without diag-attention:

$$\psi(Z;b)_{i} = \sigma_{H}[(Z_{i,:}u - b)(Z_{j \neq i}u)^{\top}]Z_{j \neq i}ue^{(1)\top}$$

$$= \begin{cases} (\max_{j \neq i} Z_{j}u)e^{(1)\top} & Z_{i,:}u > b, \\ (\min_{j \neq i} Z_{j}u)e^{(1)\top} & Z_{i,:}u < b, \end{cases}$$

where  $e^{(1)} = [1, 0, \dots, 0] \in \mathbb{R}^d$  and  $u \in \mathbb{R}^d$  is an auxiliary vector, which will be selected later.

We can contrust a self-attention layer without diag-attention that consists of two such heads  $\Psi(Z;b_1,b_2)=\psi(Z;b_1)-\psi(Z;b_2)$ , such that

$$\begin{split} \Psi(Z;b_1,b_2)_{i,1} \\ &= \left\{ \begin{array}{ll} \max_{j\neq i} Z_{j,:} u - \min_{j\neq i} Z_{j,:} u & b_1 < Z_{i,:} u < b_2 \\ 0 & \text{otherwise} \end{array} \right. . \end{split}$$

Thus, if we define a self-attention layer without diagattention of the form  $Z \to Z + \delta^{-d} \Psi(Z;b_1,b_2)$ , then selective shift operation is performed.

Next, we select  $u=(1,\delta^{-1},\delta^{-2},\dots,\delta^{-d+1})$  and the following holds:

- If  $Z_{i,j} \neq -\delta^{-nd}$  for all j, then  $Z_{i,:}u \in [0:\delta:\delta:\delta^{-d+1}-\delta]$ . And the mapping from  $Z \in \{0,\delta,\ldots,1-\delta\}^d$  to  $[0:\delta:\delta^{-d+1}-\delta]$  is a bijective mapping.
- If  $Z_{i,j}=-\delta^{-nd}$  for some j, then  $Z_{i,:}u\leq -\delta^{-nd}+\delta^{-d+1}-\delta<0$ .

Thus, the mapping  $Z_{i,:} \to Z_{i,:}u$  is a bijective mapping for  $\{0, \delta, \dots, 1 - \delta\}^d$ . We define  $l_i = Z_{i,:}u$  and assume  $l_1 < l_2 < \dots < l_n$  without loss of generality.

For each  $l \in [0:\delta:\delta^{-d+1}-\delta]$ , we choose  $b_1=l-\delta/2, b_2=l+\delta/2$  and use  $\delta^{-d}$  self-atteniton layers without diag-attention. Only one row will be in the range  $(b_1,b_2)$  each time and no other row will be affected. After above operation,  $l_i$  becomes  $\widetilde{l_i}$  for better clarification.

For n rows, there are total n phases for column updation. After each i phases, we will maintain the following ordering:

$$l_{i+1} < l_{i+2} < \dots < l_n < \widetilde{l_1} < \widetilde{l_2} < \dots < \widetilde{l_i}$$
.

**Base Step** When i = 0, it's the trivial case as

$$l_1 < l_2 < \cdots < l_n$$
.

When i=1, we have  $\max_{j\neq 1} l_j = l_n$  and  $\min_{j\neq 1} l_j = l_2$ .  $\widetilde{l}_1 = \delta^{-d}(l_n - l_2) + l_1$ .

$$\widetilde{l}_{1} - l_{n} = \delta^{-d}(l_{n} - l_{2}) + (l_{1} - l_{n}) 
> \delta^{-d}(\delta) - (\delta^{-d+1} - \delta) 
= \delta^{-d+1} - \delta^{-d+1} + \delta 
= \delta > 0.$$

**Inductive Step** When 1 < i < n, we have  $\max_{j \neq i} l_j = \widetilde{l}_{i-1}$  and  $\min_{j \neq i} l_j = l_{i+1}$ . Thus,  $\widetilde{l}_i = \delta^{-d}(\widetilde{l}_{i-1} - l_{i+1}) + l_i$ . By expansion, we have:

$$\widetilde{l}_i = (l_n - l_2)\delta^{-id} + \sum_{i=1}^{i-1} (l_j - l_{j+2})\delta^{-(i-j)d} + l_i.$$

$$\begin{split} &\widetilde{l}_{i} - \widetilde{l}_{i-1} = (l_{n} - l_{2})(\delta^{-id} - \delta^{-(i-1)d}) \\ &+ \sum_{j=1}^{i-2} (l_{j} - l_{j+2})(\delta^{-(i-j)d} - \delta^{-(i-j-1)d}) \\ &+ \delta^{-d}(l_{i-1} - l_{i+1}) + l_{i} - l_{i-1} \\ &= (\delta^{-d} - 1)[(l_{n} - l_{2})\delta^{-(i-1)d} + \sum_{j=1}^{i-2} (l_{j} - l_{j+2})\delta^{-(i-j-1)d}] \\ &+ \delta^{-d}(l_{i-1} - l_{i+1}) + l_{i} - l_{i-1} \\ &> (\delta^{-d} - 1)[\delta \cdot \delta^{-(i-1)d} + \sum_{j=1}^{i-2} (\delta - \delta^{-d+1})\delta^{-(i-j-1)d}] \\ &- \delta^{-d}(\delta^{-d+1} - \delta) + \delta \\ &= (\delta^{-d} - 1)\delta[\delta^{-(i-1)d} + \sum_{j=1}^{i-2} (1 - \delta^{-d})\delta^{-(i-j-1)d}] \\ &- \delta^{-d}(\delta^{-d+1} - \delta) + \delta \\ &= (\delta^{-d} - 1)\delta \cdot \delta^{-d} - \delta^{-d}(\delta^{-d+1} - \delta) + \delta \\ &= \delta > 0. \end{split}$$

Therefore,  $\widetilde{l}_i > \widetilde{l}_{i-1}$  holds and the ordering after operation on row i is:

$$l_{i+1} < l_{i+2} < \dots < l_n < \widetilde{l}_1 < \widetilde{l}_2 < \dots < \widetilde{l}_i$$
.

When i=n, we have  $\max_{j\neq i}l_j=\widetilde{l}_{n-1}$  and  $\min_{j\neq i}l_j=\widetilde{l}_1$ , resulting in  $\widetilde{l}_n=\delta^{-d}(\widetilde{l}_{n-1}-\widetilde{l}_1)+l_n$ . Similarly,

$$\begin{split} &\widetilde{l}_{n} - \widetilde{l}_{n-1} = (l_{n} - l_{2})(\delta^{-nd} - \delta^{-(n-1)d}) \\ &+ \sum_{j=1}^{n-2} (l_{j} - l_{j+2})(\delta^{-(n-j)d} - \delta^{-(n-j-1)d}) \\ &- \delta^{-2d}(l_{n} - l_{2}) + \delta^{-d}(l_{n-1} - l_{1}) + l_{n} - l_{n-1} \\ &= (l_{n} - l_{2})(\delta^{-nd} - \delta^{-(n-1)d} - \delta^{-2d}) \\ &+ \sum_{j=1}^{n-2} (l_{j} - l_{j+2})(\delta^{-(n-j)d} - \delta^{-(n-j-1)d}) \\ &+ \delta^{-d}(l_{n-1} - l_{1}) + l_{n} - l_{n-1} \\ &> (\delta)(\delta^{-nd} - \delta^{-(n-1)d} - \delta^{-2d}) \\ &+ \sum_{j=1}^{n-2} (\delta - \delta^{-d+1})(\delta^{-(n-j)d} - \delta^{-(n-j-1)d}) \\ &+ \delta^{-d}(\delta) + \delta \\ &= \delta > 0. \end{split}$$

The last inequation holds when  $\delta^{-nd} - \delta^{-(n-1)d} - \delta^{-2d} > 0$ , which is correct for n > 2 and small enough  $\delta$ .

After n operations, we have  $\widetilde{l}_1 < \widetilde{l}_2 < \cdots < \widetilde{l}_n$ . Note that:

$$\begin{split} \widetilde{l}_n &= (l_n - l_2)\delta^{-nd} + \sum_{j=1}^{n-2} (l_j - l_{j+2})\delta^{-(n-j)d} \\ &- (l_n - l_2)\delta^{-2d} + (l_{n-1} - l_1)\delta^{-d} + l_n \\ &< (\delta^{-d+1} - \delta)\delta^{-nd} + (\delta^{-d+1} - \delta)\delta^{-d} + (\delta^{-d+1} - \delta) \\ &= \delta(\delta^{-d} - 1)(\delta^{-nd} + \delta^{-d} + 1). \end{split}$$

thus  $\widetilde{l}_i$  has the upper bound (denoted as  $\Delta_h$ ).

To ensure that all tokens are distinct, we will add two additional layers of the form  $Z \to Z + (\Delta_h/\delta)\psi(Z;0)$ .

First Global Shift Since  $0 < \widetilde{l}_1 < \widetilde{l}_2 < \cdots < \widetilde{l}_n < \Delta_h$ , the additional layer adds  $(\Delta_h/\delta)(\max_{j\neq i} Z_{j,:}u)e^{(1)^{\top}}$  for each i. Thus,

$$\widetilde{l}_{i}^{+} = \begin{cases}
\widetilde{l}_{i} + (\Delta_{h}/\delta)\widetilde{l}_{n} & i \neq n, \\
\widetilde{l}_{n} + (\Delta_{h}/\delta)\widetilde{l}_{n-1} & i = n.
\end{cases}$$

For any  $i, j \neq n$ , we have  $\widetilde{l}_i^+ < \widetilde{l}_j^+$  if i < j. Note that:

$$\widetilde{l}_{1}^{+} - \widetilde{l}_{n}^{+} = (\Delta_{h}/\delta)(\widetilde{l}_{n} - \widetilde{l}_{n-1}) + \widetilde{l}_{1} - \widetilde{l}_{n}$$

$$> (\Delta_{h}/\delta) \cdot \delta - \Delta_{h}$$

$$> 0,$$

the order after first global shift is

$$\widetilde{l}_n^+ < \widetilde{l}_1^+ < \widetilde{l}_2^+ < \dots < \widetilde{l}_{n-1}^+.$$

Second Global Shift At the second global shift, we have

$$\widetilde{l}_i^{++} = \begin{cases} \widetilde{l}_i^+ + (\Delta_h/\delta)\widetilde{l}_{n-1}^+ & i \neq n-1, \\ \widetilde{l}_{n-1}^+ + (\Delta_h/\delta)\widetilde{l}_{n-2}^+ & i = n-1. \end{cases}$$

By expansion,  $\widetilde{l}_i^{++}$  has a more clear form as follows.

$$\begin{split} &\widetilde{l}_{i}^{++} \\ &= \begin{cases} \widetilde{l}_{n-1} + (\Delta_{h}/\delta)(\widetilde{l}_{n-2} + \widetilde{l}_{n}) + (\Delta_{h}/\delta)^{2}\widetilde{l}_{n} & i = n-1, \\ \widetilde{l}_{n} + 2(\Delta_{h}/\delta)\widetilde{l}_{n-1} + (\Delta_{h}/\delta)^{2}\widetilde{l}_{n} & i = n, \\ \widetilde{l}_{i} + (\Delta_{h}/\delta)(\widetilde{l}_{n-1} + \widetilde{l}_{n}) + (\Delta_{h}/\delta)^{2}\widetilde{l}_{n} & others. \end{cases} \end{split}$$

The output of the second global shift is our  $g_c$  (i.e.,  $\widetilde{l}_i^{++} = g_c(G)_{i,:}u$ ). Finally, we verify two properties of contextual mapping in Definition 1.

• For any  $G \in G_{\delta}$ , we have  $g_c(G)_{i,:}u \mod (\Delta_h/\delta) = \widetilde{l}_i$ . All entries of q(G)u are distinct because  $\widetilde{l}_i$  is distinct with each other.

• For any  $G_1, G_2 \in G_\delta$   $(G_1 \neq G_2)$ , each entry of  $g_c(G_i)u$  lies in the interval  $[(\Delta_h/\delta)^2 \tilde{l}_n, (\Delta_h/\delta)^2 (\tilde{l}_n + \delta))$ . Since  $\tilde{l}_n$  is the unique identity for the input G, all entries of  $g(G_1)$  and  $g(G_2)$  are distinct.

Therefore,  $g_c(G)$  satisfies the definition of contextual mapping.  $\Box$ 

# A.2.3. VALUE MAPPING (FEED-FORWARD)

**Lemma 5** (Lemma 7 (Yun et al., 2019)). There exists a function  $g_v$  composed of  $n(1/\delta)^{dn}$  token-wise feed-forward layers with r=1 and piece-wise linear functions (at most three pieces), such that  $g_v$  is defined by a token-wise function  $q_v^{tkn}$ ,

$$g_v(Z) = [g_v^{tkn}(Z_1) \dots g_v^{tkn}(Z_n)],$$

where

$$g_v^{tkn}(Z_i) = g_v^{tkn}(g_c(G)_i) = f(G_i).$$

Therefore, we have  $\bar{g}(X) = g_v \circ g_c \circ g_q(X) = \bar{f}(X)$  expect for a set has measure  $O(\delta^d)$  (Yun et al., 2019), which implies that  $d_v(\bar{f}, \bar{g}) \leq O(\delta^{d/p})$ .

# A.3. Proof for Step 3

**Lemma 6** (Lemma 9 (Yun et al., 2019)). For each modified transformer blocks  $\bar{g} \in \bar{\mathcal{T}}^{2,1,1}$ , there exists the transformer without diag-attention blocks  $g \in \mathcal{T}^{2,1,4}$  such that  $d_p(\bar{g},g) \leq \epsilon/3$ .

Since the modification is only the softmax function and ReLU activation function (not related with self-attention matrix *A*), the lemma is still holds.

By Summarizing above three steps, we have:

$$d_p(f,g) \le d_p(f,\bar{f}) + d_p(\bar{f},\bar{g}) + d_p(\bar{g},g) \le 2\epsilon/3 + O(\delta^{d/p}).$$

With enough small  $\delta$ , we have  $d_p(f,g) \leq \epsilon$ . Thus, transformers without diag-attention are also universal approximators.

### B. Data Set

# B.1. MNLI

The Multi-Genre Natural Language Inference (Williams et al., 2018) is a crowdsourced ternary classification task. Given a premise sentence and a hypothesis sentence, the target is to predict whether the last sentence is an [entailment], [contradiction], or [neutral] relationships with respect to the first one.

## B.2. QQP

The Quora Question Pairs (Chen et al., 2018) is a binary classification task. Given two questions on Quora, the tar-

get is to determine whether these two asked questions are semantically equivalent or not.

# **B.3. QNLI**

The Question Natural Language Inference (Wang et al., 2018b) is a binary classification task derived from the Stanford Question Answering Dataset (Rajpurkar et al., 2016). Given a sentence pairs (question, sentence), the target is to predict whether the last sentence contains the correct answer of the question.

### **B.4. SST-2**

The Stanford Sentiment Treebank (Socher et al., 2013) is a binary sentiment classification task for a single-sentence. All sentences are extracted from movie reviews with human annotations of their sentiment.

### B.5. CoLA

The Corpus of Linguistic Acceptability (Warstadt et al., 2019) is a binary classification task consisting of English acceptability judgments extracted from books and journal articles. Given a single-sentence, the target is to determine whether the sentence is linguistically acceptable or not.

### B.6. STS-B

The Semantic Textual Similarity Benchmark (Cer et al., 2017) is a regression task for predicting the similarity score (from 1 to 5) between a given sentence pair, whose sentence pairs are drawn from news headlines and other sources.

### B.7. MRPC

The Microsoft Research Paraphrase Corpus (Dolan & Brockett, 2005) is a binary classification task. Given a sentence pair extracted from online news sources, the target is to determine whether the sentences in the pair are semantically equivalent.

### **B.8. RTE**

Recognizing Textual Entailment (Bentivogli et al., 2009) is a binary entailment classification task similar to MNLI, where [neutral] and [contradiction] relationships are classified into [not entailment].

## B.9. SWAG

The Situations with Adversarial Generations (Zellers et al., 2018) is a multiple choice task consisting of 113k questions about grounded situations. Given a source sentence, the task is to select the most possible one among four choices for sentence continuity.

### **B.10. SQuAD v1.1**

The Stanford Question Answering Dataset (SQuAD v1.1) (Rajpurkar et al., 2016) is a large-scale question and answer task consisting of 100k question and answer pairs from more than 500 articles. Given a passage and the question from Wikipedia, the goal is to determine the start and the end token of the answer text.

### **B.11. SQuAD v2.0**

The SQuAD v2.0 task is the extension of above SQuAD v1.1, which contains the 100k questions in SQuAD v1.1 and 50k unanswerable questions. The existence of unanswerable question makes this task more realistic and challenging.

# C. Implementation Details

The hyper-parameters of various downstream tasks are shown in Table 4.

Table 4. Hyper-parameters for different downstream tasks.

	GLUE	SWAG	SQuAD v1.1	SQuAD v2.0			
Batch size	32	16	32	48			
Weight decay	[0.1, 0.01]	[0.1, 0.01]	[0.1, 0.01]	[0.1, 0.01]			
Warmup proportion	0.1	0.1	0.1	0.1			
Learning rate decay	linear	linear	linear	linear			
Training Epochs	3	3	3	2			
Learning rate	[2e-5, 1e-5, 1.5e-5, 3e-5, 4e-5, 5e-5]						

## D. Searched Attention Mask

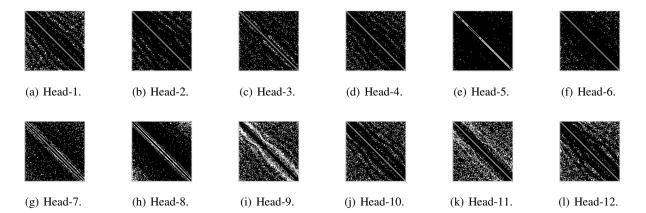


Figure 7. Visualization of the attention masks generated by  $DAM_u$  ( $\lambda = 10^{-1}$ ). Here, white means with-attention and dark means no-attention.

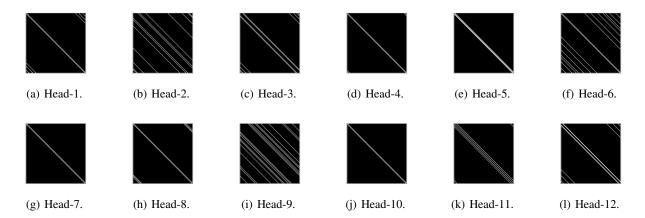


Figure 8. Visualization of the attention masks generated by  $DAM_s$  ( $\lambda=10^{-1}$ ). Here, white means with-attention and dark means no-attention.