RETHINKING POSITIONAL ENCODING IN LANGUAGE PRE-TRAINING

Guolin Ke, Di He & Tie-Yan Liu
Microsoft Research
{guolin.ke, dihe, tyliu}@microsoft.com

ABSTRACT

How to explicitly encode positional information into neural networks is important in learning the representation of natural languages, such as BERT. Based on the Transformer architecture, the positional information is simply encoded as embedding vectors, which are used in the input layer, or encoded as a bias term in the self-attention module. In this work, we investigate the problems in the previous formulations and propose a new positional encoding method for BERT called Transformer with Untied Positional Encoding (TUPE). Different from all other works, TUPE only uses the word embedding as input. In the self-attention module, the word contextual correlation and positional correlation are computed separately with different parameterizations and then added together. This design removes the addition over heterogeneous embeddings in the input, which may potentially bring randomness, and gives more expressiveness to characterize the relationship between words/positions by using different projection matrices. Furthermore, TUPE unties the [CLS] symbol from other positions to provide it with a more specific role to capture the global representation of the sentence. Extensive experiments and ablation studies on GLUE benchmark demonstrate the effectiveness and efficiency of the proposed method: TUPE outperforms several baselines on almost all tasks by a large margin. In particular, it can achieve a higher score than baselines while only using 30% pre-training computational costs. We release our code at https://github.com/guolinke/TUPE.

1 INTRODUCTION

The Transformer model (Vaswani et al., 2017) is the most widely used neural network architecture in language representation learning (Liu et al., 2019; Devlin et al., 2018; Radford et al., 2019; Bao et al., 2020), and positional encoding is essential for Transformer since the main components of the model are entirely invariant to sequence order. The original Transformer uses the absolute positional encoding, which provides each position an embedding vector. The positional embedding is added to the word embedding, and significantly helps the Transformer model learn the contextual representation of the words at different positions. Besides using the absolute positional encoding, Shaw et al. (2018); Raffel et al. (2019) further propose the relative positional encoding, which incorporates some carefully designed bias term inside the self-attention module to encode the distance between any two positions.

In this work, we revisit and study the formulation of the widely used absolute/relative positional encoding. First, we question the reasonability of adding the word embedding with the absolute positional embedding in the input layer. Since the two kinds of embeddings are apparently heterogeneous, this addition operation brings mixed correlations between the positional information and word semantics. For example, by expanding the self-attention module in the first layer, we find that there are explicit terms that use “word” to query “positions” and vice versa. However, without knowing any specific context, there is little evidence that a word has a strong correlation to where it appears in the sentence, especially for low-frequency words (Kohler et al., 2008). Our empirical analysis also supports this by showing that in a well-trained model, such correlation is noisy.

1The term “correlation” in this paper mainly refers to the dot product between Key and Query in the self-attention module.
Second, we notice that the BERT model does not only handle natural language words. A special symbol [CLS] is usually attached to the sentence. It is widely acknowledged that this symbol receives and summarizes useful information from all the positions, and the contextual representation of [CLS] will be used as the representation of the sentence in the downstream tasks. As the role of the [CLS] symbol is different from regular words that naturally contain semantics, we argue that it will be ineffective if we treat its position the same as word positions in the sentence. For example, if we apply the relative positional encoding to this symbol, the attention distribution of some heads will likely be biased to the first several words, which hurts the understanding of the whole sentence.

Based on the investigation above, we propose several simple, yet effective modifications to the current methods, which lead to a new positional encoding called Transformer with Untied Positional Encoding (TUPE) for language pre-training, see Figure 1. In TUPE, the Transformer only uses the word embedding as input. In the self-attention module, different types of correlations are separately computed to reflect different aspects of information, including word contextual correlation and absolute (and relative) positional correlation. Each kind of correlation has its own parameters and will be added together to generate the attention distribution. A specialized positional correlation is further set to the [CLS] symbol, aiming to capture the global representation of the sentence correctly. First, we can see that in TUPE, the positional correlation and word contextual correlation are de-coupled and computed using different parameters (Figure 3). This design successfully removes the randomness in word-to-position (or position-to-word) correlations and gives more expressiveness to characterize the relationship between a pair of words or positions. Second, TUPE uses a different function to compute the correlations between the [CLS] symbol and other positions. This flexibility can help the model learn an accurate representation of the whole sentence (Figure 4).

We provide an efficient implementation of TUPE. To validate the method, we conduct extensive experiments and ablation studies on the GLUE benchmark dataset. Empirical results confirm that our proposed TUPE consistently improves the model performance on almost all tasks. In particular, we observe that by imposing this inductive bias to encode the positional information, the model can be trained more effectively, and the training time of the pre-training stage can be largely improved.

2 Preliminary

2.1 Attention Module

Attention is one of the key components in the Transformer model (Vaswani et al., 2017). The attention module can be formulated as querying a dictionary with key-value pairs, e.g., Attention(Q, K, V) = softmax(QK^T/√d)V, where d is the dimensionality of the hidden representations, and Q (Query),...
We focus on the self-attention module in the BERT encoder (Devlin et al., 2018). For simplicity, where the self-attention module generally does not make use of the order of the sequence, but has the ability to distinguish the words at different positions. However, as pointed out in Shaw et al. (2018), the absolute positional encoding is not effective for the model to capture the relative word orders. Therefore, we need to modify the computation of using positional information in the self-attention module, the absolute positional encoding, and the relative positional encoding.

2.2 Positional Encoding

The key to leveraging positional information in the self-attention module is to modify the computation of $\alpha_{ij}$ in Eq. (2) to reflect the positional relationship in a sentence. Generally, there are two categories of using positional information in the self-attention module, the absolute positional encoding, and the relative positional encoding.

Absolute Positional Encoding. The original Transformer (Vaswani et al., 2017) proposed to use absolute positional encoding to represent positions. In particular, a real-valued vector $p_i \in \mathbb{R}^d$ is assigned to each position $i$. Given a sentence, $p_i$ will be added to the word embedding $w_i$ at position $i$, and $w_i + p_i$ will be used as the input to the Transformer, e.g., $x_i^1 = w_i + p_i$. In such a way, the Transformer model can differentiate the word coming from different positions. For example, in the first self-attention layer, we have

$$\alpha_{ij}^{\text{Abs}} = \frac{1}{\sqrt{d}}((w_i + p_i)W^{Q,1})(w_j + p_j)W^{K,1})^T. \quad (3)$$

In Vaswani et al. (2017), a hand-craft positional encoding based on sinusoid function is proposed. But learnable positional encoding, i.e., treating $p_i$ as parameters, is often used in the recent works (He et al., 2020; Liu et al., 2019; Devlin et al., 2018; Clark et al., 2019b).

Relative Positional Encoding. Using different $p_i$ for different position $i$ helps the Transformer distinguish the words at different positions. However, as pointed out in Shaw et al. (2018), the absolute positional encoding is not effective for the model to capture the relative word orders. Therefore, besides using the absolute positional encoding, Shaw et al. (2018) proposes a relative positional encoding as an inductive bias to help the learning of the self-attention module.

$$\alpha_{ij}^{\text{Rel}} = \frac{1}{\sqrt{d}}((x_i^1W^{Q,1})(x_j^1W^{K,1} + a_{j-i}^{l-1}))^T, \quad (4)$$

where $a_{j-i}^{l-1} \in \mathbb{R}^d$ is learnable parameter and can be viewed as the embedding of the relative position $j - i$ in layer $l$. In this way, embedding $a_{j-i}^{l-1}$ explicitly models the relative word orders. T5 (Raffel et al., 2019) further simplifies it by eliminating $a_{j-i}^{l-1}$ in Query-Key product.

$$\alpha_{ij}^{\text{T5}} = \frac{1}{\sqrt{d}}((x_i^1W^{Q,1})(x_j^1W^{K,1})^T + b_{j-i}). \quad (5)$$
Figure 2: Visualizations of the four correlations (Eq. (6)) on a pretrained BERT model for a sampled batch of sentences. From left to right: word-to-word, word-to-position, position-to-word, and position-to-position correlation matrices. In each matrix, the \((i\text{-th, } j\text{-th})\) element is the correlation between \(i\)-th word/position and \(j\)-th word/position. We can find that the correlations between a word and a position are not strong as the values in the second and third matrices look uniform.

For each \(j - i\), \(b_{j-i}\) is a learnable scalar and shared in all layers.

3 Transformer with Untied Positional Encoding

3.1 Untie the Correlations between Positions and Words

In the absolute positional encoding, the positional embedding is added together with the word embedding and serves as the input to the neural networks. However, these two kinds of information are heterogeneous. It is well known that the word embedding encodes the semantic meanings of words, and word analogy tasks can be solved using simple linear arithmetic on word embeddings (Mikolov et al., 2013; Pennington et al., 2014; Joulin et al., 2016). On the other hand, the absolute positional embedding encodes the indices in a sequence, which is not semantic and far different from word meanings. We question the rationality of the linear operation between the word embedding and the positional embedding. To check clearly, we take a look at the expansion of Eq. (3).

\[
\alpha_{ij}^{\text{Abs}} = \frac{(w_i + p_i)WQ,1((w_j + p_j)WK,1)^T}{\sqrt{d}} + \frac{w_iWQ,1(p_jWK,1)^T}{\sqrt{d}} + \frac{(p_iWQ,1)(w_jWK,1)^T}{\sqrt{d}} + \frac{(p_iWQ,1)(p_jWK,1)^T}{\sqrt{d}}
\]

(6)

The above expansion shows how the word embedding and the positional embedding are projected and queried in the attention module. We can see that there are four terms after the expansion: word-to-word, word-to-position, position-to-word, and position-to-position correlations.

We have several concerns regarding this formulation. It is easy to see that the first and the last term characterize the homogeneous relationships between a pair of words or positions. However, the second and the third term use the position (word) as the query to get keys composed of words (positions). As far as we know, without knowing the contexts, there is little evidence that the word and where it appears in a sentence has a strong correlation. In Köhler et al. (2008), the authors even suggest that word with lower frequencies may occur anywhere. To further investigate this, we visualize the four correlations in Eq. (6) on a pre-trained BERT model, and find that the second and the third term looks uniform across positions, as shown in Figure 2. This phenomenon suggests that there are no strong correlations between the word and the absolute position and using such noisy correlation may be inefficient for model training.

\[^{2}\text{Specifically, in Shaw et al. (2018); Raffel et al. (2019), the relative position } j - i \text{ will be first clipped to a pre-defined range clip}(j - i, t, t) \text{, e.g. } t = 128. \text{ The embedding is defined over the possible values of the clipped range, i.e., } [-t, t]. \text{ Besides, Shaw et al. also tried to add vector } a_{V,l}^{j-i} \text{ to the value } V \text{ in the output of self-attention, but the experiment results indicate that it did not improve much.}^{3}\]

\[^{3}\text{Some recent works (Yang et al., 2019; He et al., 2020) show that correlations between relative positions and words can improve the performance. Our results have no contradiction with theirs as our study is on the correlations between words and absolute positions.}\]
\[ \alpha_{ij} = \frac{1}{\sqrt{2d}} (x_i^Q W^{Q,i}) (x_j^K W^{K,j})^T + \frac{1}{\sqrt{2d}} (p_i U^Q) (p_j U^K)^T, \]  

(7)

where \( U^Q, U^K \in \mathbb{R}^{d \times d} \) are the projection matrices for the positional embedding, and scaling term \( \frac{1}{\sqrt{2d}} \) is used to retain the magnitude of \( \alpha_{ij} \). Our proposed method can be well combined with the relative positional encoding in Raffel et al. (2019) by simply changing Eq. (2) to

\[ \alpha_{ij} = \frac{1}{\sqrt{2d}} (x_i^Q W^{Q,i}) (x_j^K W^{K,j})^T + \frac{1}{\sqrt{2d}} (p_i U^Q) (p_j U^K)^T + b_{j-i}. \]  

(8)

We can see that the obtained coefficient \( \alpha_{ij} \) considers both absolute positional encoding and relative positional encoding.

3.2 Untie the [CLS] Symbol from Positions

Note that in language representation learning, the input sequence to the Transformer model is not always a natural sentence. In BERT, a special symbol [CLS] is attached to the beginning of the input sentence. The symbol is designed to capture the global information of the whole sentence, and its contextual representation will be used to make predictions in the sentence-level downstream tasks after pre-training (Devlin et al. 2018; Liu et al. 2019).
However, different from the artificially designed [CLS] symbol, the regular words usually have strong local dependencies in the sentence, which is reflected in the attention distributions. For example, many visualizations (Clark et al., 2019; Gong et al., 2019) show that the attention distributions of some heads concentrate locally. If we process the position of [CLS] the same as the position of natural language words using the same attention distribution, the symbol will be likely biased to focus on the first several words instead of the whole sentence, which will hurt the performance of the downstream tasks.

**Our modification.** To untie the [CLS] symbol from other positions, we propose to reset the positional correlations corresponding to [CLS]. For better demonstration, we denote $v_{ij}$ as the content-free (position-only) correlation between position $i$ and $j$. For example, when using the absolute positional encoding in Eq. (7), $v_{ij} = \frac{1}{\sqrt{d}} (p_i U^Q)(p_j U^K)^T$; when using relative positional encoding in Eq. (8), $v_{ij} = \frac{1}{\sqrt{d}} (p_i U^Q)(p_j U^K)^T + b_{j-i}$. We reset the values of $v_{ij}$ by the following equation:

$$\text{reset}_\theta (v, i, j) = \begin{cases} v_{ij} & i \neq 1, j \neq 1, (\text{no [CLS]}) \\ \theta_1 & i = 1, (\text{from [CLS] to others}) \\ \theta_2 & i \neq 1, j = 1, (\text{from others to [CLS]}) \end{cases}$$

(9)

where $\theta = \{\theta_1, \theta_2\}$ is a learnable parameter. Note that, this modification can be widely applied to any position-only correlations, including our proposed positional encoding in Sec.3.1 and previous relative positional encoding. A visualization is provided in Figure 4.

### 3.3 Implementation Details and Discussions

In the two subsections above, we propose several modifications to untie the correlations between positions and words (Eq. 7 and Eq. 8), and untie the [CLS] symbol from other positions (Eq. 9). By combining them, we obtain a new positional encoding method and call it TUPE (Transformer with Untied Positional Encoding). There are two versions of TUPE. The first version is to use the untied absolute positional encoding with the untied absolute positional encoding in Eq. (7), and the second version is to use an additional relative positional encoding (Eq. 8 + Eq. 9). We call them TUPE-A and TUPE-R respectively and list the mathematical formulations as below.

$$\alpha_{ij}^{\text{TUPE-A}} = \frac{1}{\sqrt{d}} (x_i^l W^Q)(x_j^l W^K)^T + \text{reset}_\theta (\frac{1}{\sqrt{d}} (p_i U^Q)(p_j U^K)^T, i, j)$$

(10)

$$\alpha_{ij}^{\text{TUPE-R}} = \frac{1}{\sqrt{d}} (x_i^l W^Q)(x_j^l W^K)^T + \text{reset}_\theta (\frac{1}{\sqrt{d}} (p_i U^Q)(p_j U^K)^T + b_{j-i}, i, j)$$

(11)

We provide the implementation details and several discussions as below.

**The multi-head version, parameter sharing, and efficiency.** TUPE can be easily extended to the multi-head version. In our implementation, the absolute positional embedding $p_i$ for position $i$ is shared across different heads, while for each head, the projection matrices $U^Q$ and $U^K$ are different. For the relative positional encoding, $b_{j-i}$ is different for different heads. The parameter $\theta$ is also not shared across heads.

For efficiency, we share the (multi-head) projection matrices $U^Q$ and $U^K$ in different layers. Therefore, in TUPE, the number of total parameters does not change much. Taking BERT-Base as an example, we introduce about 1.18M ($2 \times 768 \times 768$) new parameters, which is only about 1% of the 110M parameters in BERT-Base. Besides, as the positional correlation term $\frac{1}{\sqrt{d}} (p_i U^Q)(p_j U^K)^T$ is shared in all layers, we only need to compute it in the first layer, and reuse its outputs in other layers. Therefore, TUPE almost does not introduce additional computational costs.

**Normalization and rescaling.** Layer normalization (Ba et al., 2016; Xiong et al., 2020) is a key component in Transformer. In TUPE, we also apply layer normalization on $p_i$ whenever it is used. The $\frac{1}{\sqrt{d}}$ in Eq. (10) is used in the Transformer (Vaswani et al., 2017) to rescale the dot product outputs into a standard range. In a similarly way, we use $\frac{1}{\sqrt{d}}$ in the Eq. (7) to both terms to keep the scale after the summation. Furthermore, in order to directly obtain similar scales for every term, we parameterize $\theta_1$ and $\theta_2$ by using $\theta_1 = \frac{1}{\sqrt{d}} (p_0 U^Q)(p_0 U^K)^T$ and $\theta_2 = \frac{1}{\sqrt{d}} (p_{\theta_2} U^Q)(p_{\theta_2} U^K)^T$, where $p_{\theta_1}, p_{\theta_2} \in \mathbb{R}^d$ are learnable vectors.
Are absolute/relative positional encoding redundant to each other? One may think that both the absolute positional encoding and relative positional encoding in Eq. (11) describe the content-free correlation, and thus one of them is redundant. To formally study this, we denote \( B \) as an \( n \times n \) matrix where each element \( B_{i,j} = b_{j-i} \). By definition, \( B \) is a Toeplitz matrix [Gray, 2006]. We also denote \( P \) as an \( n \times n \) matrix where the \( i \)-th row is \( p_i \), and thus the absolute positional correlation in matrix form is \( \frac{1}{\sqrt{2d}}(PU^Q)(PU^K)^T \). We study the expressiveness of \( B \) and \( \frac{1}{\sqrt{2d}}(PU^Q)(PU^K)^T \) by first showing \( B \) can be factorized similarly from the following proposition.

**Proposition 1.** Any Toeplitz matrix \( B \in C^{n \times n} \) can be factorized into \( B = GDG^* \), where \( D \) is a \( 2n \times 2n \) diagonal matrix. \( G \) is a \( n \times 2n \) Vandermonde matrix\(^4\) in the complex space, where each element \( G_{j,k} = \frac{1}{\sqrt{2n}}e^{\pi j(k+1)/n} \).\(^{4}\) and \( G^* \) is the conjugate transpose of \( G \).

**Proof.** We first construct a circulant matrix \( \hat{B} \) of shape \( 2n \times 2n \) using \( B \). Note that \( B \) is a Toeplitz matrix consisting of \( 2n - 1 \) values \( \{b_{-(n-1)}, b_{-(n-2)}, \ldots, b_{0}, \ldots, b_{(n-2)}, b_{(n-1)}\} \). For ease of reference, we further define \( b_{-n} = b_0 \). Then \( \hat{B} \) is constructed as

\[
\hat{B}_{j,k} = \begin{cases} 
    b_{k-j} & -n \leq k - j \leq n \\
    b_{k-j-2n} & n < k - j < 2n \\
    b_{k-j+2n} & -2n < k - j < -n
\end{cases}
\]

(12)

To avoid any confusion, we use \( k \) and \( j \) in the subscription for positions and use \( j \) as the imaginary unit. It is easy to check that \( \hat{B} \) is a circulant matrix by showing that \( \hat{B}_{j,k} = \hat{B}_{j+1,k+1} \) and \( \hat{B}_{j,2n-1} = \hat{B}_{j+1,0} \) for any \( 0 \leq j, k < 2n - 1 \). Using Theorem 7 in [Gray, 2006], the matrix \( B \) can be factorized into \( \hat{B} = QDQ^* \). \( Q \) is an \( 2n \times 2n \) Vandermonde matrix, where \( Q_{k,j} = \frac{1}{\sqrt{2n}}e^{\pi j(k+1)/n} \) and \( D \) is a \( 2n \times 2n \) diagonal matrix. Since the top-left \( n \times n \) submatrix of \( \hat{B} \) is \( B \), we can rewrite \( B = \frac{1}{\sqrt{2d}}(PU^Q)(PU^K)^T \), where \( G \) is defined in the theorem. Then we have

\[
QDQ^* = \begin{bmatrix} G & C_1 \\ C_2 & C_3 \end{bmatrix} \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} \begin{bmatrix} G^* & C_4 \end{bmatrix}.
\]

Considering that \( D \) is a diagonal matrix, we can obtain \( B = GDG^* \) using block matrix multiplication.

\( \square \)

We show here that the two terms \((B \text{ and } \frac{1}{\sqrt{2d}}(PU^Q)(PU^K)^T)\) form different subspaces in \( R^{n \times n} \). In the multi-head version, the shape of the matrix \( U^Q \) and \( U^K \) are \( d \times \frac{d}{2} \). Therefore, the rank of \( \frac{1}{\sqrt{2d}}(PU^Q)(PU^K)^T \) is no more than \( \frac{d}{2} \), and the absolute positional correlations in matrix form can characterize low-rank matrices in \( R^{n \times n} \). But from the factorization, we can see that \( B \) forms a linear subspace in \( R^{n \times n} \) with only \( 2n - 1 \) freedoms, which is quite different from the space of \( \frac{1}{\sqrt{2d}}(PU^Q)(PU^K)^T \). There are also some practical reasons which make using both terms together essential. As discussed previously, in [Raffel et al., 2019], the range of the relative distance \( j - i \) will be clipped up to an offset beyond which all relative positions will be assigned the same value. In such a situation, the relative positional encoding may not be able to differentiate words far away and \( \frac{1}{\sqrt{2d}}(p_iU^Q)(p_jU^K)^T \) can be used to encode complementary information.

4 EXPERIMENT

To verify the performance of the proposed TUPE, we conduct extensive experiments and demonstrate the results in this section. All codes are implemented based on fairseq [Ott et al., 2019] in PyTorch [ Paszke et al., 2017] and available at https://github.com/guolinke/TUPE. All models are run on 16 NVIDIA Tesla V100 GPUs with mixed-precision [Micikevicius et al., 2017].

4.1 EXPERIMENTAL DESIGN

We mainly follow the BERT [Devlin et al., 2018], but TUPE could be easily applied to any Transformer-based models such as RoBERTa [Liu et al., 2019] and ELECTRA [Clark et al., 2019]. The detailed setting of the experiment is shown below.

\(^{4}\) The matrix \( G \) can be viewed as some kind of fixed absolute positional encoding using sinusoidal functions, which is quite similar to the absolute positional encoding in the original Transformer [Vaswani et al., 2017].
Table 1: Hyperparameters for the pre-training and fine-tuning.

|                     | Pre-training | Fine-tuning |
|---------------------|--------------|-------------|
| **Max Steps**       | 1M           | -           |
| **Max Epochs**      | -            | 5 or 10 \(^a\) |
| **Learning Rate**   | 1e-4         | (2e-5, 3e-5, 4e-5, 5e-5) |
| **Batch Size**      | 256          | 32          |
| **Warm-up Ratio**   | 0.01         | 0.06        |
| **Sequence Length** | 512          | 512         |
| **Learning Rate Decay** | Linear       | Linear     |
| **Adam \(\epsilon\)** | 1e-6         | 1e-6        |
| **Adam \((\beta_1, \beta_2)\)** | (0.9, 0.999) | (0.9, 0.999) |
| **Clip Norm**       | 1.0          | 1.0         |
| **Dropout**         | 0.1          | 0.1         |
| **Weight Decay**    | 0.01         | 0.01        |

\(^a\) we use five for the top four high-resource tasks, MNLI-m/-mm, QQP, and QNLI, to save the fine-tuning costs. Ten is used for other tasks.

Model architecture and baselines. We use BERT-Base (110M parameters) architecture for all experiments. Specifically, BERT-Base is consist of 12 Transformer layers. For each layer, the hidden size is set to 768 and the number of attention head is set to 12. To compare with TUPE-A and TUPE-R, we set up two baselines correspondingly: BERT-A, which is the standard BERT-Base with absolute positional encoding (Devlin et al., 2018); BERT-R, which uses both absolute positional encoding and relative positional encoding (Raffel et al., 2019) (Eq. (5)).

Pre-training. Following BERT (Devlin et al., 2018), we use the English Wikipedia corpus and BookCorpus (Zhu et al., 2015) for pre-training. By concatenating these two datasets, we obtain a corpus with roughly 16GB in size. We follow a couple of consecutive pre-processing steps: segmenting documents into sentences by Spacy\(^5\), normalizing, lower-casing, and tokenizing the texts by Moses decoder (Koehn et al., 2007), and finally, applying byte pair encoding (BPE) (Sennrich et al., 2015) with setting the vocabulary size as 32,678.

We use masked language modeling as the objective of pre-training. We remove the next sentence prediction task and use FULL-SENTENCES mode to pack sentences as suggested in RoBERTa (Liu et al., 2019). We train the models for 1000k steps where the batch size is 256 and the maximum sequence length is 512. The masked probability is set to 0.15, with replacing 80% of the masked positions by [MASK], 10% by randomly sampled words, and keep the remaining 10% unchanged. We use Adam (Kingma & Ba, 2014) as the optimizer, and set the its hyperparameter \(\epsilon\) to 1e-6 and \((\beta_1, \beta_2)\) to (0.9, 0.999). The peak learning rate is set to 1e-4 with a 10k-step warm-up stage. After the warm-up stage, the learning rate decays linearly to zero. We set the dropout probability to 0.1, gradient clip norm to 1.0, and weight decay to 0.01. Besides the final checkpoint, we also save intermediate checkpoints (100k, 300k, 600k) steps) and fine-tune them on downstream tasks, to check the efficiency of different methods.

Fine-tuning. We use the GLUE (General Language Understanding Evaluation) dataset (Wang et al., 2018) as the downstream tasks to evaluate the performance of the pre-trained models. Particularly, we use nine tasks in GLUE, including CoLA, RTE, MRPC, STS, SST, QNLI, QQP, and MNLI-m/mm. For the evaluation metrics, we report Matthews correlation for CoLA, Pearson correlation for STS-B, and accuracy for other tasks. We use the same optimizer (Adam) with the same hyperparameters as in pre-training. Following previous works, we search the learning rates during the fine-tuning for each downstream task. The setting details are listed in Table 1. For a fair comparison, we do not apply any tricks for fine-tuning. Each configuration will be run five times with different random seeds, and the median of these five results on the development set will be used as the performance of one configuration. We will ultimately report the best number over all configurations.
Table 2: GLUE scores. All settings are pre-trained by BERT-Base (110M) model with 16GB data. TUPE-A\textsuperscript{mid} (TUPE-R\textsuperscript{mid}) is the intermediate 300\textsuperscript{k}-step checkpoint of TUPE-A (TUPE-R). TUPE-A\textsubscript{tie-cls} removes the reset function from TUPE-A. BERT-A\textsuperscript{d} uses different projection matrices for words and positions, based on BERT-A.

| Steps | MNLI-m/mm | QNLI | QQP | SST | CoLA | MRPC | RTE | STS | Avg. |
|-------|-----------|------|-----|-----|------|------|-----|-----|------|
| BERT-A | 1M | 84.93/84.91 | 91.34 | 91.04 | 92.88 | 55.19 | 88.29 | 68.61 | 89.43 | 82.96 |
| BERT-R | 1M | 85.81/85.84 | 92.16 | 91.12 | 92.90 | 55.43 | 89.26 | 71.46 | 88.94 | 83.66 |
| TUPE-A | 1M | 86.05/85.99 | 91.92 | 91.16 | 93.19 | 63.09 | 88.37 | 71.61 | 88.88 | 84.47 |
| TUPE-R | 1M | **86.21/86.19** | **92.17** | **91.30** | **93.26** | **63.56** | **89.89** | **73.56** | **89.23** | **85.04** |
| TUPE-A\textsuperscript{mid} | 300\textsuperscript{k} | 84.76/84.83 | 90.96 | 91.00 | 92.25 | 62.13 | 87.1 | 68.79 | 88.16 | 83.33 |
| TUPE-R\textsuperscript{mid} | 300\textsuperscript{k} | 84.86/85.21 | 91.23 | 91.14 | 92.41 | 62.47 | 87.29 | 69.85 | 88.63 | 83.68 |
| TUPE-A\textsubscript{tie-cls} | 1M | 85.91/85.73 | 91.90 | 91.05 | 93.17 | 59.46 | 88.53 | 69.54 | 88.97 | 83.81 |
| BERT-A\textsuperscript{d} | 1M | 85.26/85.28 | 91.56 | 91.02 | 92.70 | 59.73 | 88.46 | 71.31 | 87.47 | 83.64 |

(a) Validation loss in pre-training. (b) MNLI-m score. (c) GLUE average score.

Figure 5: Both TUPE-A and TUPE-R convergence much faster than baselines, and achieve the better performance in downstream tasks while using much fewer pre-training steps.

### 4.2 Overall Comparison

The overall comparison results are shown in Table 2. Firstly, it is easy to find that both TUPE-A and TUPE-R outperform baselines significantly. In particular, TUPE-R outperforms the best baseline BERT-R by 1.38 points in terms of GLUE average score and is consistently better on almost all tasks, especially on MNLI-m/mm, CoLA and MRPC. We can also see that TUPE-R outperforms TUPE-A by 0.57 points. As discussed in Sec 3.3, although using the absolute/relative positional encoding together seems to be redundant, they capture complement information to each other.

Besides the final performance, we also examine the efficiency of different methods. As shown in Figure 5a, TUPE-A (TUPE-R) achieves smaller validation loss than the baselines during pre-training. As shown in Table 2 and Figure 5c, TUPE-A (TUPE-R) can even achieve a better GLUE average score than the baselines while only using 30% pre-training steps.

To summarize, the comparisons show the effectiveness and efficiency of the proposed TUPE. As the only difference between TUPE and baselines is the positional encoding, these results indicate TUPE can better utilize the positional information in sequence. In the following subsection, we will examine each modification in TUPE to check whether it is useful.

### 4.3 Ablation Study

**Untie the [CLS] symbol from other positions.** To study the improvement brought by untying [CLS], we evaluate a positional encoding method which removes the reset function in Eq. 10. We call it TUPE-A\textsubscript{tie-cls} and train this model using the same configuration. We also list the performance
Untie the correlations between positions and words. Firstly, from Table 2 it is easy to find that TUPE-A\textsuperscript{tie-cls} outperforms BERT-A. Since the only difference between TUPE-A\textsuperscript{tie-cls} and BERT-A is the way of dealing with the absolution positional encoding, we can get a conclusion that untying the correlations between positions and words helps the model training.

To further investigate this, we design another encoding method, BERT-A\textsuperscript{d}, which is based on BERT-A and uses different projection matrices for words and positions. Formally, $\alpha_{ij} = \frac{1}{\sqrt{d}} \left( (x^l_i W^Q,l)(x^l_j W^K,l)^T + (p_i U^Q)(p_j U^K)^T + (p_i U^Q)(p_j U^K)^T \right)$ in BERT-A\textsuperscript{d}. Therefore, we can check whether the improvement is brought by using different projection matrices (BERT-A vs. BERT-A\textsuperscript{d}) or the removal of word-to-position and position-to-word correlations (BERT-A\textsuperscript{d} vs. TUPE-A\textsuperscript{tie-cls}). From the summarized results in Table 2 we find that TUPE-A\textsuperscript{tie-cls} is the best of them, and BERT-A\textsuperscript{d} is better than BERT-A. These results indicate that using different projection matrix and the removal of correlations between words and positions both contribute to the final improvement.

Summary. From the above analysis, we find that untying [CLS] helps a great deal for the low-resource tasks, such as CoLA and RTE. Untying the positional correlation and word correlation helps high-resource tasks, like MNLI-m/-mm. By combining them, TUPE can consistently perform better on all GLUE tasks.

4.4 Visualization

Since the correlations between words and positions are removed in TUPE, we can easily visualize the attention patterns over positions, without considering the variability of input sentences. We dump the learned positional correlations by TUPE-A and find there are mainly five patterns (from 12 heads). As illustrated in Figure 6, the patterns are: (1) attending globally and ignoring local positions; (2) attending locally; (3) attending broadly; (4) attending to the previous positions; (5) attending to the next positions. Interestingly, the model can automatically extract these patterns from random initialization. As there are some attention patterns indeed have strong local dependencies, our proposed method to untie [CLS] is necessary. Besides, we find the values of the first column (from others to [CLS]) are consistently relatively large in most heads. This indicates that the global information (on [CLS]) is quite important. Similar patterns could be found in TUPE-R as well.

5 Failed Attempts

We tried to replace the parametric form of the positional correlation ($\frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T$) to the non-parametric form. However, empirically we found that the training of this setting converges much slower than the baselines. We also tried to parameterize relative position bias $b_{j-i}$ by $(r_{j-i} F^Q)(r_{j-i} F^K)^T$. But the improvement is just marginal.

6 Related Work

Although the Transformer is widely used in natural language processing, there are very few works investigating the positional encoding methods. As introduced in Sec 2 [Shaw et al., 2018] was the
first work to leverage relative positional encoding to Transformer. Most of the other works are based on Shaw et al. (2018). For example, Transformer-XL (Dai et al., 2019) re-parameterize the self-attention to integrate relative positional encoding directly. T5 (Raffel et al., 2019) simplified the vector representation of relative positions in Shaw et al. (2018) to a scalar. He et al. (2020) extended Shaw et al. (2018) by adding the position-to-word correlation for relative position. Nevertheless, none of the above works focus on untying the correlations between positions and words or untying [CLS] from position encoding.

There are some other parallel works to enhance the absolute positional encoding in Transformer, but not directly related to our work. For example, Shiv & Quirk (2019) extended the sequence positional encoding to tree-based positional encoding in Transformer; Wang et al. (2019) extended positional encoding to complex-valued domain; Liu et al. (2020) modeled the positional encoding by dynamical systems.

7 CONCLUSION

We propose TUPE (Transformer with Untied Positional Encoding), which improves existing methods by two folds: untying the correlations between words and positions, and untying [CLS] from sequence positions. Specifically, we first remove the absolute positional encoding from the input of the Transformer and compute the positional correlation and word correlation separately with different projection matrices in the self-attention module. Then, we untie [CLS] by resetting the positional correlations related to [CLS]. Extensive experiments demonstrate that TUPE achieves much better performance on GLUE benchmark. Furthermore, with a better inductive bias over the positional information, TUPE can even outperform the baselines while only using 30% pre-training computational costs.

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REFERENCES

Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. Layer normalization. arXiv preprint arXiv:1607.06450, 2016.

Hangbo Bao, Li Dong, Furu Wei, Wenhui Wang, Nan Yang, Xiaodong Liu, Yu Wang, Songhao Piao, Jianfeng Gao, Ming Zhou, et al. Unilmv2: Pseudo-masked language models for unified language model pre-training. arXiv preprint arXiv:2002.12804, 2020.

Kevin Clark, Urvashi Khandelwal, Omer Levy, and Christopher D Manning. What does bert look at? an analysis of bert’s attention. ACL 2019, pp. 276, 2019a.

Kevin Clark, Minh-Thang Luong, Quoc V Le, and Christopher D Manning. Electra: Pre-training text encoders as discriminators rather than generators. In International Conference on Learning Representations, 2019b.

Zihang Dai, Zhilin Yang, Yiming Yang, Jaime Carbonell, Quoc V Le, and Ruslan Salakhutdinov. Transformer-xl: Attentive language models beyond a fixed-length context. arXiv preprint arXiv:1901.02860, 2019.

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

Linyuan Gong, Di He, Zhuohan Li, Tao Qin, Liwei Wang, and Tieyan Liu. Efficient training of bert by progressively stacking. In International Conference on Machine Learning, pp. 2337–2346, 2019.

Robert M Gray. Toeplitz and circulant matrices: A review. now publishers inc, 2006.
Pengcheng He, Xiaodong Liu, Jianfeng Gao, and Weizhu Chen. Deberta: Decoding-enhanced bert with disentangled attention. *arXiv preprint arXiv:2006.03654*, 2020.

Armand Joulin, Edouard Grave, Piotr Bojanowski, Matthijs Douze, Hérve Jégou, and Tomas Mikolov. Fasttext. zip: Compressing text classification models. *arXiv preprint arXiv:1612.03651*, 2016.

Diederik P. Kingma and Jimmy Ba. Adam: A method for stochastic optimization. *CoRR*, abs/1412.6980, 2014. URL [http://arxiv.org/abs/1412.6980](http://arxiv.org/abs/1412.6980).

Philipp Koehn, Hieu Hoang, Alexandra Birch, Chris Callison-Burch, Marcello Federico, Nicola Bertoldi, Brooke Cowan, Wade Shen, Christine Moran, Richard Zens, Chris Dyer, Ondrej Bojar, Alexandra Constantin, and Evan Herbst. Moses: Open source toolkit for statistical machine translation. In *ACL*, 2007.

Reinhard Köhler, Gabriel Altmann, and Rajmund G Piotrowski. *Quantitative Linguistik/Quantitative Linguistics: Ein internationales Handbuch/An International Handbook*, volume 27. Walter de Gruyter, 2008.

Xuanqing Liu, Hsiang-Fu Yu, Inderjit Dhillon, and Cho-Jui Hsieh. Learning to encode position for transformer with continuous dynamical model. *arXiv preprint arXiv:2003.09229*, 2020.

Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. Roberta: A robustly optimized bert pretraining approach. *arXiv preprint arXiv:1907.11692*, 2019.

Paulius Micikevicius, Sharan Narang, Jonah Alben, Gregory Diamos, Erich Elsen, David Garcia, Boris Ginsburg, Michael Houston, Oleksii Kuchaiev, Ganesh Venkatesh, et al. Mixed precision training. *arXiv preprint arXiv:1710.03740*, 2017.

Tomas Mikolov, Ilya Sutskever, Kai Chen, Greg S Corrado, and Jeff Dean. Distributed representations of words and phrases and their compositionality. In *Advances in neural information processing systems*, pp. 3111–3119, 2013.

Myle Ott, Sergey Edunov, Alexei Baevski, Angela Fan, Sam Gross, Nathan Ng, David Grangier, and Michael Auli. fairseq: A fast, extensible toolkit for sequence modeling. *arXiv preprint arXiv:1904.01038*, 2019.

Adam Paszke, Sam Gross, Soumith Chintala, Gregory Chanan, Edward Yang, Zachary DeVito, Zeming Lin, Alban Desmaison, Luca Antiga, and Adam Lerer. Automatic differentiation in pytorch. 2017.

Jeffrey Pennington, Richard Socher, and Christopher D Manning. Glove: Global vectors for word representation. In *Proceedings of the 2014 conference on empirical methods in natural language processing (EMNLP)*, pp. 1532–1543, 2014.

Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language models are unsupervised multitask learners. *OpenAI Blog*, 1(8), 2019.

Colin Raffel, Noam Shazeer, Adam Roberts, Katherine Lee, Sharan Narang, Michael Matena, Yanqi Zhou, Wei Li, and Peter J Liu. Exploring the limits of transfer learning with a unified text-to-text transformer. *arXiv preprint arXiv:1910.10683*, 2019.

Rico Sennrich, Barry Haddow, and Alexandra Birch. Neural machine translation of rare words with subword units. *CoRR*, abs/1508.07909, 2015. URL [http://arxiv.org/abs/1508.07909](http://arxiv.org/abs/1508.07909).

Peter Shaw, Jakob Uszkoreit, and Ashish Vaswani. Self-attention with relative position representations. *arXiv preprint arXiv:1803.02155*, 2018.

Vighnesh Shiv and Chris Quirk. Novel positional encodings to enable tree-based transformers. In *Advances in Neural Information Processing Systems*, pp. 12058–12068, 2019.

Ilya Sutskever, Oriol Vinyals, and Quoc V Le. Sequence to sequence learning with neural networks. In *Advances in neural information processing systems*, pp. 3104–3112, 2014.
Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. In Advances in Neural Information Processing Systems, pp. 6000–6010, 2017.

Alex Wang, Amanpreet Singh, Julian Michael, Felix Hill, Omer Levy, and Samuel R. Bowman. GLUE: A multi-task benchmark and analysis platform for natural language understanding. CoRR, abs/1804.07461, 2018. URL http://arxiv.org/abs/1804.07461.

Benyou Wang, Donghao Zhao, Christina Lioma, Qiuchi Li, Peng Zhang, and Jakob Grue Simonsen. Encoding word order in complex embeddings. arXiv preprint arXiv:1912.12333, 2019.

Ruibin Xiong, Yunchang Yang, Di He, Kai Zheng, Shuxin Zheng, Chen Xing, Huishuai Zhang, Yanyan Lan, Liwei Wang, and Tie-Yan Liu. On layer normalization in the transformer architecture. arXiv preprint arXiv:2002.04745, 2020.

Zhilin Yang, Zihang Dai, Yiming Yang, Jaime Carbonell, Ruslan Salakhutdinov, and Quoc V Le. Xlnet: Generalized autoregressive pretraining for language understanding. arXiv preprint arXiv:1906.08237, 2019.

Yukun Zhu, Ryan Kiros, Richard Zemel, Ruslan Salakhutdinov, Raquel Urtasun, Antonio Torralba, and Sanja Fidler. Aligning books and movies: Towards story-like visual explanations by watching movies and reading books. In arXiv preprint arXiv:1506.06724, 2015.