RETHINKING POSITIONAL ENCODING IN LANGUAGE PRE-TRAINING

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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 **T**ransformer with **U**ntied **P**ositional **E**ncoding (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[1] 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 (Köhler et al., 2008). Our empirical analysis also supports this by showing that in a well-trained model, such correlation is noisy.

[1]The term “correlation” in this paper mainly refers to the dot product between Key and Query in the self-attention module.

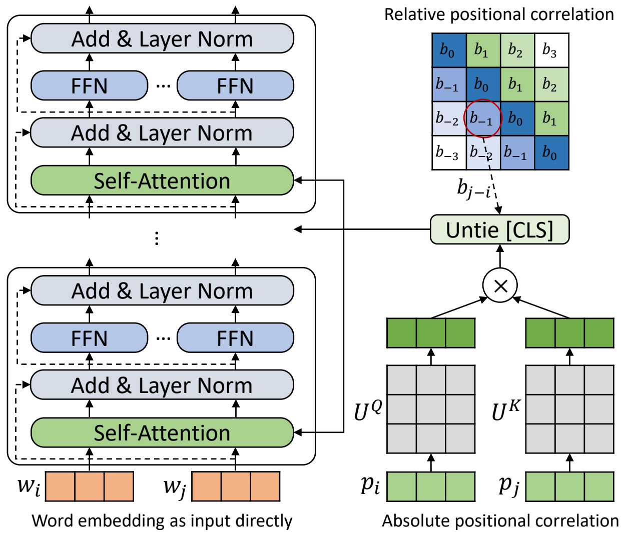


Figure 1: The architecture of TUPE.

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 **T**ransformer with **U**ntied **P**ositional **E**ncoding (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., $\text{Attention}(Q, K, V) = \text{softmax}(\frac{QK^T}{\sqrt{d}})V$, where d is the dimensionality of the hidden representations, and Q (Query),

K (Key), V (Value) are specified as the hidden representations of the previous layer. The multi-head variant of the attention module is popularly used which allows the model to jointly attend to information from different representation sub-spaces, and is defined as

$$\begin{aligned}\text{Multi-head}(Q, K, V) &= \text{Concat}(\text{head}_1, \cdots, \text{head}_H)W^O \\ \text{head}_k &= \text{Attention}(QW_k^Q, KW_k^K, VW_k^V),\end{aligned} \tag{1}$$

where $W_k^Q \in \mathbb{R}^{d\times d_K}, W_k^K \in \mathbb{R}^{d\times d_K}, W_k^V \in \mathbb{R}^{d\times d_V}$, and $W^O \in \mathbb{R}^{Hd_V\times d}$ are learnable project matrices, H is the number of heads. d_K and d_V are the dimensionalities of Key and Value.

We focus on the self-attention module in the BERT encoder (Devlin et al., 2018). For simplicity, we use the single-head self-attention module and set $d_K = d_V = d$ for the demonstration of our proposal. Denote $x^l = (x_1^l, x_2^l \cdots, x_n^l)$ as the input to the self-attention module in the l-th layer, where n is the length of the sequence and each vector $x_i^l \in \mathbb{R}^d$ is the contextual representation of the token at position i. Denote $z^l = (z_1^l, z_2^l \cdots, z_n^l)$ as the output. It is easy to check that in the single-head self-attention module, W^O is redundant. Then Eq. (1) can be rewritten as

$$z_i^l = \sum_{j=1}^{n} \frac{\exp(\alpha_{ij})}{\sum_{j'=1}^{n}\exp(\alpha_{ij'})}(x_j^l W^{V,l}), \text{where } \alpha_{ij} = \frac{1}{\sqrt{d}}(x_i^l W^{Q,l})(x_j^l W^{K,l})^T. \tag{2}$$

As we can see, the self-attention module generally does not make use of the order of the sequence, i.e., is permutation-invariant. However, natural language is well-structured, and the word order is important for natural language understanding (Sutskever et al., 2014). In the next section, we show several previous works that proposed different ways of incorporating positional information into the self-attention module.

2.2 Positional Encoding

The key to leveraging positional information in the self-attention module is to modify the computation of α_{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

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

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. proposes a relative positional encoding as an inductive bias to help the learning of the self-attention module.

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

where $a_{j-i}^l \in \mathbb{R}^d$ 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 explicitly models the relative word orders. T5 (Raffel et al., 2019) further simplifies it by eliminating a_{j-1}^l in Query-Key product.

$$\alpha_{ij}^{T5} = \frac{1}{\sqrt{d}}(x_i^l W^{Q,l})(x_j^l W^{K,l})^T + b_{j-i}. \tag{5}$$

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-th, j-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 $j - i$[2] , 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).

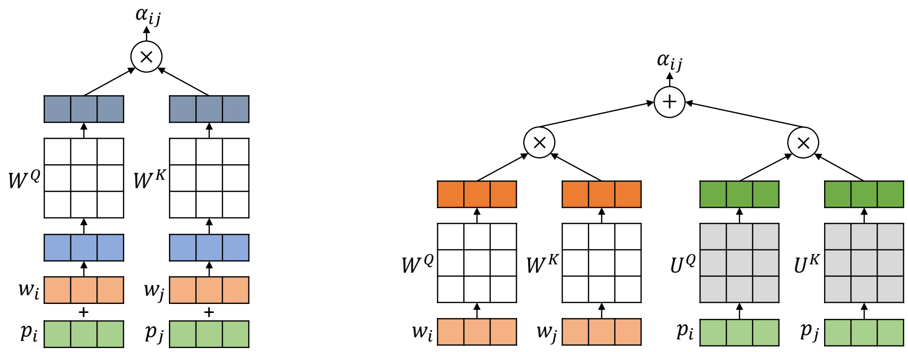
$$\begin{aligned}\alpha_{ij}^{Abs} &= \frac{((w_i+p_i)W^{Q,1})((w_j+p_j)W^{K,1})^T}{\sqrt{d}} \\ &= \frac{(w_iW^{Q,1})(w_jW^{K,1})^T}{\sqrt{d}} + \frac{(w_iW^{Q,1})(p_jW^{K,1})^T}{\sqrt{d}} \\ &+ \frac{(p_iW^{Q,1})(w_jW^{K,1})^T}{\sqrt{d}} + \frac{(p_iW^{Q,1})(p_jW^{K,1})^T}{\sqrt{d}} \end{aligned} \tag{6}$$

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[3] between the word and the absolute position and using such noisy correlation may be inefficient for model training.

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

[3]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.



(a) Absolute positional encoding.

(b) Untied absolute positional encoding.

Figure 3: Instead of adding the absolute positional embedding to the word embedding in the input (left), we compute the positional correlation and word correlation separately with different projection matrices, and add them together in the self-attention module (right).

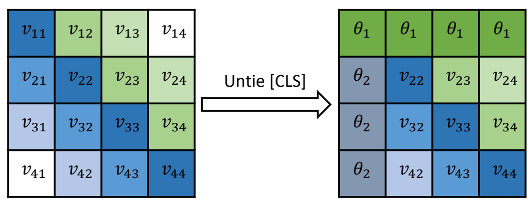


Figure 4: Illustration of untying [CLS]. v_{ij} denotes the positional correlation of pair (i, j). The first row and first column are set to the same values respectively.

Furthermore, although the first and the last term characterize the relationship between homogeneous information, the projection matrices $W^{Q,l}$ and $W^{K,l}$ are shared in both terms. As a common knowledge, the projection is served as a way to map contextual vectors to a different semantic space (Vaswani et al., 2017) to increase the expressiveness of the model. It is not reasonable to apply the (semantic) projection to the positional information.

Our modification. To overcome these problems, we propose to directly model the relationships between a pair of words or positions by using different projection matrices and remove the two terms in the middle. That is, we use

$$\alpha_{ij} = \frac{1}{\sqrt{2d}}(x_i^l W^{Q,l})(x_j^l W^{K,l})^T + \frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T, \tag{7}$$

where $U^Q, U^K \in \mathbb{R}^{d\times d}$ are the projection matrice for the positional embedding, and scaling term $\frac{1}{\sqrt{2d}}$ is used to retain the magnitude of α_{ij} . Our proposed method can be well combined with the relative positional encoding in Raffel et al. (2019) by simply changing Eq. (5) to

$$\alpha_{ij} = \frac{1}{\sqrt{2d}}(x_i^l W^{Q,l})(x_j^l W^{K,l})^T + \frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T + b_{j-i}. \tag{8}$$

We can see that the obtained coefficient α_{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., 2019a; 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), $v_{ij} = \frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T$; when using relative positional encoding in Eq. (8), $v_{ij} = \frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T + b_{j-i}$. We reset the values of v_{ij} by the following equation:

$$\mathrm{reset}_\theta(v, i, j) = \begin{cases} v_{ij} & i \neq 1, j \neq 1, (\text{no } \texttt{[CLS]}) \\ \theta_1 & i = 1, (\text{from } \texttt{[CLS]} \text{ to others}) \\ \theta_2 & i \neq 1, j = 1, (\text{from others to } \texttt{[CLS]}) \end{cases}, \tag{9}$$

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 `[CLS]` symbol (Eq. (7) + Eq. (9)), 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.

$$\alpha_{ij}^{\text{TUPE-A}} = \frac{1}{\sqrt{2d}}(x_i^l W^{Q,l})(x_j^l W^{K,l})^T + \mathrm{reset}_\theta\left(\frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T, i, j\right) \tag{10}$$

$$\alpha_{ij}^{\text{TUPE-R}} = \frac{1}{\sqrt{2d}}(x_i^l W^{Q,l})(x_j^l W^{K,l})^T + \mathrm{reset}_\theta\left(\frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T + b_{j-i}, i, j\right), \tag{11}$$

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 θ 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 $\frac{1}{\sqrt{2d}}(p_i U^Q)(p_j U^K)^T$ 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. (2) 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 $\frac{1}{\sqrt{2d}}$ 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 θ_1 and θ_2 by using $\theta_1 = \frac{1}{\sqrt{2d}}(p_{\theta_1} U^Q)(p_{\theta_1} U^K)^T$ and $\theta_2 = \frac{1}{\sqrt{2d}}(p_{\theta_2} U^Q)(p_{\theta_2} U^K)^T$, 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 $G_{j,k} = \frac{1}{2n}e^{i\pi(j+1)k/n}$ 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 $\{b_{-(n-1)}, b_{-(n-2)}, \cdots, b_0, \cdots, b_{(n-2)}, b_{(n-1)}\}$. For ease of reference, we further define $b_{-n} = b_n = b_0$. Then $\hat{B}$ is constructed as

$$\hat{B}_{j,k} = \begin{cases} b_{k-j} & -n \leq k-j \leq n \\ b_{k-j-2n} & n < k-j < 2n \\ b_{k-j+2n} & -2n < k-j < -n \end{cases}. \tag{12}$$

To avoid any confusion, we use k and j in the subscription for positions and use i 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 $\hat{B}$ can be factorized into $\hat{B} = QDQ^*$. Q is an $2n \times 2n$ Vandermonde matrix, where $Q_{k,j} = \frac{1}{2n}e^{i\pi(j+1)k/n}$ 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 $\hat{B} = \begin{bmatrix} B & C_1 \\ C_2 & C_3 \end{bmatrix}$. We also rewrite $Q = \begin{bmatrix} G \\ C_4 \end{bmatrix}$, where G is defined in the theorem. Then we have $QDQ^* = \begin{bmatrix} G \\ C_4 \end{bmatrix} \begin{bmatrix} D_1 & 0 \\ 0 & D_2 \end{bmatrix} [G^* \quad C_4^*]$. Considering that D is a diagonal matrix, we can obtain $B = GDG^*$ using block matrix multiplication. □

We show here that the two terms (B 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 $d \times \frac{d}{H}$. Therefore, the rank of $\frac{1}{\sqrt{2d}}(PU^Q)(PU^K)^T$ is no more than $\frac{d}{H}$, 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 faraway 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., 2019b). 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 ϵ	1e-6	1e-6
Adam (β_1, β_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)).

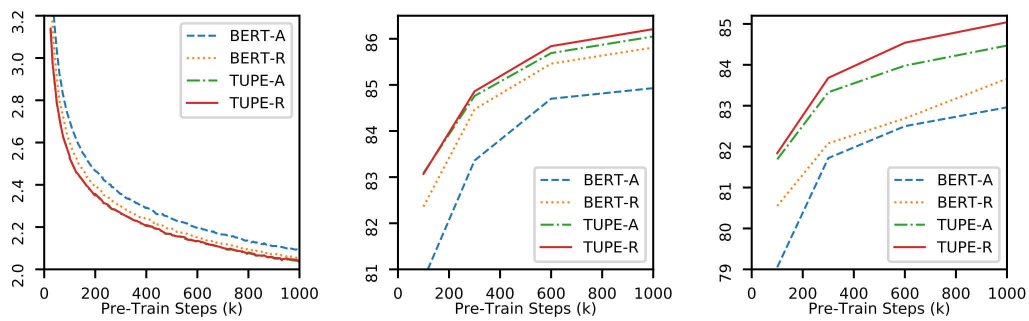
Pre-training. Following BERT (Devlin et al., 2018), we use the English Wikipedia corpus and BookCorpus (Zhu et al., 2015) for pre-training. By concatenating these two datasets, we obtain a corpus with roughly 16GB in size. We follow a couple of consecutive pre-processing steps: segmenting documents into 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 ϵ 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 (**G**eneral **L**anguage **U**nderstanding **E**valuation) 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$^{\text{mid}}$ (TUPE-R$^{\text{mid}}$) is the intermediate 300k-step checkpoint of TUPE-A (TUPE-R). TUPE-A$^{\text{tie-cls}}$ removes the reset function from TUPE-A. BERT-A^{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$^{\text{mid}}$	300k	84.76/84.83	90.96	91.00	92.25	62.13	87.1	68.79	88.16	83.33
TUPE-R$^{\text{mid}}$	300k	84.86/85.21	91.23	91.14	92.41	62.47	87.29	69.85	88.63	83.68
TUPE-A$^{\text{tie-cls}}$	$1M$	85.91/85.73	91.90	91.05	93.17	59.46	88.53	69.54	88.97	83.81
BERT-A^{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$^{\text{tie-cls}}$ and train this model using the same configuration. We also list the performance

[5] `https://spacy.io`

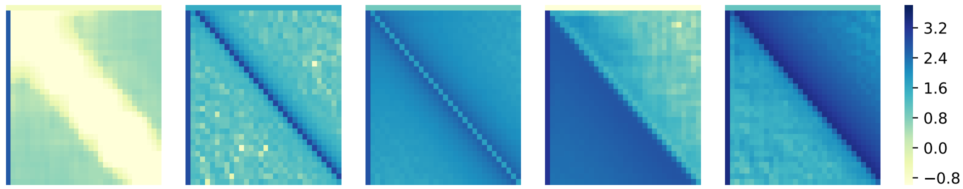


Figure 6: The visualization of learned positional correlations by TUPE-A.

of TUPE-A$^{\text{tie-cls}}$ in Table 2. From the table, we can see that TUPE-A works consistently better than TUPE-A$^{\text{tie-cls}}$, especially for low-resource tasks, such as CoLA and RTE.

Untie the correlations between positions and words. Firstly, from Table 2, it is easy to find that TUPE-A$^{\text{tie-cls}}$ outperforms BERT-A. Since the only difference between TUPE-A$^{\text{tie-cls}}$ 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^d, which is based on BERT-A and uses different projection matrices for words and positions. Formally, $\alpha_{ij} = \frac{1}{\sqrt{4d}}\left((x_i^l W^{Q,l})(x_j^l W^{K,l})^T + (x_i^l W^{Q,l})(p_j U^K)^T + (p_i U^Q)(x_j^l W^{K,l})^T + (p_i U^Q)(p_j U^K)^T\right)$ in BERT-A^d. Therefore, we can check whether the improvement is brought by using different projection matrices (BERT-A vs. BRET-A^d) or the removal of word-to-position and position-to-word correlations (BRET-A^d vs. TUPE-A$^{\text{tie-cls}}$). From the summarized results in Table 2, we find that TUPE-A$^{\text{tie-cls}}$ is the best of them, and BERT-A^d is better than BERT-A. These results indicate that using different projection matrice 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.

8 ACKNOWLEDGMENTS

We would like to thank Yatao Li for collecting and processing the pre-training data, and thank Benyou Wang, Tianle Cai, Yunzhen Feng, Chen Xing and Lingyuan Gong for offering quite a lot of suggestions to the draft.

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