Abstract

The highly popular Transformer architecture, based on self-attention, is the foundation of large pretrained models such as BERT, that have become an enduring paradigm in NLP. While powerful, the computational resources and time required to pretrain such models can be prohibitive. In this work, we present an alternative self-attention architecture, Shatter, that more efficiently encodes sequence information by softly partitioning the space of relative positions and applying different value matrices to different parts of the sequence. This mechanism further allows us to simplify the multi-headed attention in Transformer to single-headed. We conduct extensive experiments showing that Shatter achieves better performance than BERT, with pretraining being faster per step (15% on TPU), converging in fewer steps, and offering considerable memory savings (>50%). Put together, Shatter can be pretrained on 8 V100 GPUs in 7 days, and match the performance of BERT Base – making the cost of pretraining much more affordable.

1 Introduction

Large pretrained models such as BERT (Devlin et al., 2019) have become a mainstay of natural language processing (NLP), enabling the transfer of knowledge learned from large amounts of unsupervised data to downstream tasks with a small number of labeled examples. Due to the size of both the unsupervised data and model architecture, pretraining is computationally very expensive, requiring either TPUs or a substantial number of GPUs (Liu et al., 2019), which can make experimentation cumbersome. As a result, many have attempted to improve pretraining efficiency from largely two aspects: the model architecture (Ke et al., 2020; Shaw et al., 2018; He et al., 2020) or pretraining objective (Yang et al., 2019; Clark et al., 2020).

In this work, we focus on developing a more efficient architecture, inspired by the recent literature of modeling sequence attention with relative position embeddings (Shaw et al., 2018). Similar techniques have been integrated in many Transformer variants (Yang et al., 2019; Raffel et al., 2019; He et al., 2020; Ke et al., 2020), and as we show in this work, relative position embeddings not only achieve better finetuned performance with fewer pretraining steps (§5.2), but also hold the potential of being pretrained on shorter sequences than used in finetuning, which could considerably reduce the memory requirements and accelerate pretraining.

Unfortunately, training with relative position embeddings is much slower per step: While Shaw et al. (2018) reported 7% more training time on GPUs, we found it 3.9 times slower than BERT on TPUs\(^1\) (§5.1). Consequently, the cost in speed hinders the adoption of this model.

In this work, we develop an alternative that captures the advantages of relative position embeddings (i.e. better finetuning performance with fewer pretraining steps, pretraining on shorter sequence length) without the associated speed overhead. Instead of using (absolute or relative) position embeddings, we propose to incorporate sequence order information by softly partitioning the space of relative positions into parts, which can be implemented by a TPU-efficient operation of multiplying the attention matrix with a constant mask.

Subsequently, we can replace multi-headed attention with a single-headed variant, by changing the activation function from softmax (i.e. L1-normalized $\exp$ which favors sparse positions of the top attention score) to L2-normalized sigmoid (which favors dense weighting of positions). This single-headed formulation simplifies the concept of self-attention, and leads to further efficiency gains.

\(^1\)TPUs are much faster than GPUs in matrix multiplication, but are not optimized for the operations that convert between relative and absolute positions as we explain in §2.
We exhaustively evaluate our model, Shatter, across several datasets: The GLUE Benchmark (Wang et al., 2018), SQuAD (Rajpurkar et al., 2016), BoolQ (Clark et al., 2019) and MultiRC (Khashabi et al., 2018). We show that our model is 15% faster per pretraining step than BERT on TPU (§5.1), and achieves better finetuned performance across the datasets, for both base and large size, with fewer pretraining steps (§5.2.3). Furthermore, we show that our approach generalizes better to longer sequences, and can pretrained on half the sequence length required in finetuning, which reduces the memory footprint by more than 50% (§5.2.2). Put together, we can pretrain the base-size (Wang et al., 2018), SQuAD (Rajpurkar et al., 2016), TPU (§5.1), and achieves better finetuned performance across several datasets: The GLUE Benchmark, SQuAD (Rajpurkar et al., 2016), BoolQ (Clark et al., 2019) and MultiRC (Khashabi et al., 2018). We show that our model is 15% faster per pretraining step than BERT on TPU (§5.1), and achieves better finetuned performance across the datasets, for both base and large size, with fewer pretraining steps (§5.2.3). Furthermore, we show that our approach generalizes better to longer sequences, and can pretrained on half the sequence length required in finetuning, which reduces the memory footprint by more than 50% (§5.2.2). Put together, we can pretrain the base-size Shatter on 8 V100 GPUs in 7 days and match or outperform BERTBase, significantly reducing the computational requirements for pretraining.

2 Background
A Transformer encoder (Vaswani et al., 2017) is a stack of self-attention (Cheng et al., 2016; Parikh et al., 2016) and feed-forward layers. In the following, we briefly review the self-attention mechanism and some variants to model relative position. Vectors are denoted by lowercase bold letters, matrices by uppercase bold, and tensors of higher ranks by bold sans-serif. We use Numpy indexing 2 for tensors, and matrices are row-major.

At each layer $k$, the hidden state of a Transformer is represented by an $l \times d$ matrix $X^k$, where $l$ is the sequence length and $d$ the hidden size. For simplicity of notation, we omit the $k$ superscript unless the layer index is critical. The hidden vector $x_i = X[i, :]$ $(0 \leq i < l)$ encodes context around position $i$ in the sequence.

From the hidden state, self-attention calculates the query $Q$, key $K$, and value $V$ matrices as trainable linear transformations of $X$:

\[ Q = XW^Q, \quad K = XW^K, \quad V = XW^V \]

Then, it uses query and key to compute attention scores and construct a weighted average of the value:

\[ A = \text{softmax} \left( \frac{QQ^T}{\sqrt{d}} \right) \]
\[ \bar{X} = AV \]

Here, $A$ is an $l \times l$ matrix, with $A[i, j]$ representing the attention score from position $i$ to position $j$.

The input to the next layer $X^{k+1}$ is computed as $F^k(X^k, X^k)$, where $F^k$ is a feed forward network with layer normalization (Ba et al., 2016).

**Multi-headed Attention** In practice, it performs better to divide the inner dimension of $Q$, $K$ and $V$ into $n$ blocks, and run the self-attention mechanism $n$ times in parallel. This is calculated formally by converting $Q$ into a rank 3 tensor $Q$ such that:

\[ Q[h, :, :] = Q[:, :, h \times d : h \times d + 1] \quad (0 < h < n) \]

and similarly $K$, $V$ into $K$, $V$, respectively. Then, multi-headed attention is computed by:

\[ A = \text{softmax} \left( \frac{QK^T}{\sqrt{d/n}} \right) \]
\[ \bar{X} = AV \]

where multiplication of tensors means batched matrix multiplication. The tensor $\bar{X}$ is converted back to a matrix $\bar{X}$ by setting

\[ \bar{X}[:, h \times d: h \times d + 1] = \bar{X}[h, :, :] \quad (0 < h < n). \]

Here, $A$ is a $n \times l \times l$ tensor, where each “attention head” $A[h, :, :]$ is expected to weight sequence positions from different aspects, and the model more efficiently encodes context information.

**Position Embeddings** Self-attention does not recognize sequence order; i.e., a permutation of rows in $X$ leads to the same permutation of rows in $\bar{X}$. To inject order information, Transformer learns an $l \times d$ matrix $P$ as “position embeddings”, besides the word embeddings $E$. Namely, given a word sequence $w_0w_1\ldots$ of length $l$, the input vector $x^0_i$ of the first layer is calculated by:

\[ x^0_i = \text{LayerNormalize}(E(w_i) + P[i]). \]

Thus, a permutation of the word sequence $w_0w_1\ldots$ does not lead to a permutation of rows in $X^0$, thanks to position embeddings.

**Relative Position Embeddings** Although being simple, position embeddings only inject order information to the first layer, and the solution is not shift-invariant (e.g., if we shift $w_0w_1\ldots$ one position to the right, the input sequence $<\text{pad}>w_0w_1\ldots$ will be encoded into completely different hidden states, not the shift of hidden states of $w_0w_1\ldots$, which is unintuitive of a sequence encoder). As an alternative, the Relative Position Embeddings (RPE)

2https://numpy.org/doc/stable/reference/arrays.indexing.html
model (Shaw et al., 2018) aims to inject stronger notion of position at each self-attention layer, with shift-invariance. The model learns a $$(2l - 1) \times d$$ matrix $$R^k$$ at each layer $$k$$, which contributes to both attention scores and values, as below:

$$S = QK^\top, \quad S_{rel}[i, j - i] = S[i, j]$$

$$K_{rel} = RW^K, \quad V_{rel} = RW^V$$

$$A_{rel} = \text{softmax} \left( S_{rel} + QK_{rel}^\top \right) \sqrt{d}$$

$$A[i, j] = A_{rel}[i, j - i]$$

$$X = AV + A_{rel}V_{rel}$$

Here, $$S_{rel}$$ and $$A_{rel}$$ are $$l \times (2l - 1)$$ matrices with inner index ranging from $$-l + 1$$ to $$l - 1$$, representing attention to relative positions. Intuitively, the calculation corresponds to using $$x_j + R[j - i]$$ to obtain key and value, while using $$x_i$$ to obtain query. The multi-headed case is defined similarly.

In the above calculation, RPE requires conversion between $$S, A$$ and $$S_{rel}, A_{rel}$$, respectively, which changes the memory configuration of these tensors in the accelerator in a less optimized manner, and increases computational cost. This is especially a bottleneck on TPUs, making the model difficult to scale up to larger size.

Nevertheless, RPE consistently performs better in our experiments (§5.2), and the model can be naturally extended to longer sequences by copying the learnt embeddings $$R[-l + 1]$$ and $$R[l - 1]$$ to farther relative positions. It serves as a strong motivation for us to design a fast alternative for relative position modeling.

**Relative Attention Bias** Several Transformer variants (Raffel et al., 2019; He et al., 2020; Ke et al., 2020) have simplified the relative position modeling, in addition to the (absolute) position embeddings. For example, instead of Eq.1, the T5 model (Raffel et al., 2019) learns an attention bias $$B$$ according to relative positions:

$$B[:, i, j] = W^B[g, :] \quad (b_g \leq j - i < b_{g+1})$$

$$A = \text{softmax} \left( QK^\top + B \right)$$

In which, $$B$$ is an $$n \times l \times l$$ tensor obtained from a trainable $$m \times n$$ matrix $$W^B$$, with the relative position $$j - i$$ put into one of $$m$$ fixed buckets: $$b_0 = -\infty < \ldots b_g \ldots < b_m = \infty$$. The computation of this Relative Attention Bias (RAB) model is much simpler than RPE, but still adds extra cost. In our experiments, using the T5 default $$m = 32$$, pre-training RAB is 20% more costly than the vanilla Transformer on TPU. Performance is improved on some tasks, but not all (§5.2.1).

### 3 Our Approach

In this section, we describe the components of our more efficient self-attention architecture, *Shatter*, by steps. First, we partition the space of relative positions to softly bias each attention head to focus on a different part of the sequence (§3.1). Then, we can simplify the multi-head attention to single-headed (§3.2). Finally, we show how to incorporate partition embeddings for improved performance with minimal additional cost (§3.3).

A demonstrating experiment is shown in **Figure 1**: We progressively develop our model variants and show their Masked Language Modeling (MLM) loss (Devlin et al., 2019) on a validation corpus during pretraining. Detailed settings are given in §A.2. The baseline is BERT*Base*, and we note its learning curve converging to $$\approx 2$$ (Figure 1, “BERT*Base*”). We start from removing the position embeddings in Eq.4, and the valid loss drastically increases to > 6 (Figure 1, “No_Position”), which suggests that the sequence order information is crucial for a Transformer encoder.
3.1 Soft Relative Partition of Sequence

Instead of position embeddings, we explore an alternative way of integrating sequence order, by restricting different attention heads to different parts of a sequence. This is achieved by multiplying a mask \(N\) to the attention score:

\[
A = \text{softmax} \left( \frac{QK^\top}{\sqrt{d/n}} \right) \odot N. \tag{5}
\]

Here, \(\odot\) denotes element-wise multiplication, and \(N\) is an \(n \times l \times l\) constant tensor up to model design. Intuitively, the attention head \(h\) at position \(i\) is more sensitive to position \(j\) if \(N[h, i, j]\) is larger. We set \(N\) to be dependent only on the relative position \(j - i\), which makes the model shift-invariant:

\[
N[h, i, j] = f_h(j - i).
\]

In order to recognize sequence order, \(f_h\) should not be constant; we use a partition of unity to evenly concentrate different \(f_h\) to different parts of the relative position space.

A partition of unity is a group of functions \(\{f_h\}\) \((0 \leq h < n)\) such that: (i) \(f_h(x) \geq 0\) and (ii) \(\sum_{h=0}^{n-1} f_h(x) = 1\), for any \(x \in (-\infty, \infty)\). For example, consider the four functions in Figure 2: \(f_0\) concentrates at relative position \(j - i = x = 1\) and \(f_2\) peaks around \(j - i = x = 4\), while \(f_0 + f_1 + f_2 + f_3\) constantly equals 1 at all positions.

The partition of unity is a generalization of T5’s idea of putting relative positions into buckets: Dividing \((-\infty, \infty)\) into \(n\) buckets, \(b_0 = -\infty < \ldots < b_h \ldots < b_n = \infty\), is equivalent to setting

\[
f_h(x) = \begin{cases} 
1 & \text{if } b_h \leq x < b_{h+1} \\
0 & \text{otherwise}
\end{cases}.
\]

In our case, instead of a hard division into buckets, we adopt a soft division to avoid discontinuity at bucket boundaries. Specifically, we use Bernstein polynomials to construct the partition of unity, and the detailed definition is given in §4.1.

Compared to Eq.1, the extra computation cost of Eq.5 is negligible, because \(N\) is constant without any trainable components. Figure 1 (“Part_Mask”) shows that multiplying \(N\) largely closes the gap between BERT\textsubscript{Base} and “No_Position”.

3.2 One-Head Sigmoid Attention

The partition mask \(N\) makes different attention heads focus on different parts of the sequence, limiting the overlap between parts. It suggests a possibility to neatly combine all the attention scores over the whole sequence into one \(l \times l\) matrix, without the multi-headed redundancy. Formally, it suggests that we may replace the tensor \(QK^\top\) with the matrix version \(QK^\top\), without loss of model expressivity. For the matrix version, linear algebra suggests that we may further replace \(K = XW^K\) by \(X\), which reduces one matrix multiplication for the self-attention layer. It leads to 5% reduction of training time on GPU and 15% on TPU, in our experiments (§5.1).

One issue with the matrix version (i.e. single-headed attention), is that attention scores are calculated by softmax (i.e. L1-Normalized exp), which favors sparse positions of the top attention score; it might still be better to attend to more positions, as in multi-headed attention. Thus, we propose to use L2-Normalized sigmoid instead of softmax, which favors a dense weighting of positions:

\[
A = \text{L2-Normalize} \left( \sigma \left( \frac{QX^\top}{\sqrt{d}} \right) \right) \odot N. \tag{6}
\]

Figure 1 shows the effect of single-headed attention: If we use softmax scores (“1H_Sigmoid”), the validation loss gets slightly worse; however, it is significantly improved by using L2-Normalized sigmoid (“1H_Sigmoid”).

It is noteworthy that in Eq.6, although \(QX^\top\) is a matrix, we still get an \(n \times l \times l\) tensor \(A\) by multiplying to \(N\) through Numpy broadcasting. We use Eq.6 to replace Eq.1, then the tensor \(X = AV\) is calculated the same as in Eq.2. It is crucial to keep \(V\) as a rank 3 tensor to make the model aware of different parts of the sequence. We have confirmed in preliminary experiments, that reducing \(V\) to matrix would hurt valid loss, even with sigmoid attention score.

3.3 Partition Embeddings

Besides injecting sequence order, (absolute or relative) position embeddings enable a model to attend to a position no matter what the token is. To achieve a similar role, we further add partition embeddings to our final model, named Shatter (Single-headed attention with relative partition).
At each layer, \textit{Shatter} learns an \( n \times d \) matrix \( R \) to represent partition, in analogue to the relative position embeddings. It uses the query \( Q \), partition embeddings \( R \), and the partition mask \( N \) to calculate an attention bias \( B \) as the following:
\[
B[i,:]=\sum_{h=0}^{n-1}(QR^T)[i,h]\cdot N[h,i,:]
\]
\[
A=L2\text{-Normalize}\left(\sigma\left(\frac{QX^T}{\sqrt{d}}+B\right)\right)\odot N
\]
In addition, \( R \) contributes to the value as below:
\[
A_{\text{part}}^T=\sum_{j=0}^{l-1}A[:,j],
\]
\[
\bar{X} = \tilde{X} + A_{\text{part}}V_{\text{part}}
\]
where \( \tilde{X} \) is defined the same as in Eq.3. Then, \( \tilde{X} \) is used in the feed-forward network instead of \( X \).

In Figure 1, “Part Bias” shows the effect of adding the bias term \( B \), and “Shatter” shows the result adding value contribution. Our final model now matches the valid loss of BERT\textsubscript{Base}.

The computation cost of partition embeddings is small, because \( n \ll l \), and the part-wise bias for the attention score is converted to absolute positions via matrix multiplication by a constant tensor \( N \), without memory rearrangement.

### 3.4 Sequence Classification with Relative Position Modeling

For sequence classification tasks, BERT adds [CLS] and [SEP] tokens to the input sequence(s) and feeds the final hidden state at [CLS] to a classifier. As pointed out by Ke et al. (2020), this strategy might hurt models using relative position, since the hidden state at [CLS] might be affected by its position relative to other tokens, which is irrelevant to [CLS]’s role of capturing the semantics of the whole sequence(s). Therefore, Ke et al. (2020) propose a mechanism to “reset” relative positions regarding [CLS], but this mechanism is model specific. Related to the issue, He et al. (2020) propose to model relative positions but add absolute position embeddings to the last few layers.

In this work, we adopt a modified strategy for sequence classification, and apply it to all sequence encoders in our experiments for fair comparison. We first encode [CLS]- and [SEP]- augmented input sequence(s) and record the hidden state \( X^k \) at each layer \( 0 \leq k \leq L \). Then, instead of using [CLS]’s final hidden state \( X^L[0,:] \), we newly start from a learnt vector \( y^0 \) and recalculate a weighted average of the hidden states at each layer:
\[
q=yW^Q, \ K=XW^K, \ V=XW^V
\]
\[
a=\text{softmax}\left(\frac{qK^T}{\sqrt{d}}\right), \ \tilde{y}=aV
\]
Finally, the result \( y^L \) is used for classification. In the above, the attention mechanism is replaced with either multi-headed or single-headed sigmoid, according to the sequence encoder model.

Our experiments suggest that the strategy does not affect the performance of BERT, but improves others that model relative positions (§A.4).

### 4 Related Work

The original Transformer (Vaswani et al., 2017) uses fixed sinusoid functions to encode positions, justified by the existence of linear transformations between vectors of different positions. This idea is conveyed further by XLNet (Yang et al., 2019), which models relative positions (hence shift-invariant) and can accumulate context information of arbitrary length. Our relative sequence partitioning method differs by directly affecting the attention score, and the coarse partition imposes more regularization than position-wise vectors. We will further compare with XLNet in our evaluation.

BERT (Devlin et al., 2019) learns the position embeddings, and Shaw et al. (2018) model relative positions. Many (Raffel et al., 2019; He et al., 2020; Ke et al., 2020; Wennberg and Henter, 2021; Chen et al., 2021) combine the techniques with different approaches, while we point out that modeling relative positions with learnt components often increases pretraining cost, and will clearly evaluate the cost-performance trade-off.

Many ideas are explored to reduce the training cost (Lan et al., 2019; Jiang et al., 2020; Chen et al., 2020; Lee-Thorp et al., 2021), some specifically for very long (\( \geq 4096 \)) sequences (Child et al., 2019; Kitaev et al., 2020; Choromanski et al., 2020; Beltagy et al., 2020), but we are not aware of previous work that can pretrain with 8 V100 GPUs within 1 week and match BERT\textsubscript{Base}.

Previous works have found that multiple attention heads are redundant and can be pruned (Michel et al., 2019; Voita et al., 2019), but incorporating this insight into training is more challenging, as naively reducing the number of heads will reduce performance. Our single-headed self-attention both simplified the concept and improved performance.
| Model       | Size                  | # Params | Hardware      | Batch | Length | # Steps | Time  |
|------------|-----------------------|----------|---------------|-------|--------|---------|-------|
| BERT<sub>GPU</sub> | 12-layers 12-heads 768-hidden | 84.9M     | GPU V100×8    | 128   | 256    | 1.6M    | 170 hrs|
| Shatter<sub>GPU</sub> | 12-layers 12-parts 768-hidden | 78.0M     | GPU V100×8    | 128   | 256    | 1.6M    | 161 hrs|
| BERT<sub>Base</sub> | 12-layers 12-heads 768-hidden | 84.9M     | TPUv3 4x4     | 256   | 512    | 1M      | 53 hrs |
| Shatter<sub>Base</sub> | 12-layers 12-parts 768-hidden | 78.0M     | TPUv3 4x4     | 256   | 512    | 1M      | 45 hrs |
| BERT-RPE | 12-layers 12-heads 768-hidden | 87.3M     | TPUv3 4x4     | 256   | 512    | 1M      | 206 hrs|
| BERT-RAB | 12-layers 12-heads 768-hidden | 84.9M     | TPUv3 4x4     | 256   | 512    | 1M      | 64 hrs |
| XLNet<sub>base</sub> | 12-layers 12-heads 768-hidden | 92.0M     | TPUv3 4x4     | 256   | 512    | 1M      | 123 hrs|
| BERT<sub>Large</sub> | 24-layers 16-heads 1024-hidden | 151.0M    | TPUv3 8x8     | 1024  | 512    | 1M      | 180 hrs|
| Shatter<sub>Large</sub> | 24-layers 16-parts 1024-hidden | 138.6M    | TPUv3 8x8     | 1024  | 512    | 1M      | 151 hrs|

Table 1: Number of trainable parameters (excluding word embeddings), pretraining settings and pretraining speed.

5 Experiments

For evaluation, we implemented and compared the following models:

**BERT** (Devlin et al., 2019) is a Transformer encoder (Vaswani et al., 2017) with model parameters trained on large amounts of unsupervised data (i.e. pretraining). The Masked Language Modeling (MLM) pretraining objective attempts to recover the original tokens when 15% tokens in an input sequence are masked out. We pretrain three models, BERT<sub>GPU</sub>, BERT<sub>Base</sub> and BERT<sub>Large</sub>, using different model size (Base or Large), sequence length (256- or 512-) and hardware (GPU or TPU).

**Shatter** is our proposed model architecture. We pretrain Shatter<sub>GPU</sub>, Shatter<sub>Base</sub> and Shatter<sub>Large</sub>, in correspondence to the BERT models.

**BERT-RPE** (Shaw et al., 2018) uses Relative Position Embeddings (RPE) at each layer, instead of (absolute) position embeddings. We set the vocab size of RPE to $2 \times 128 - 1 = 255$, so that relative positions farther than 128 are represented by the same embedding vector.

**BERT-RAB** adds a Relative Attention Bias (RAB) to the BERT model. Relative positions are put into buckets, and each bucket shares the same bias term. We copied code from the T5 model (Raffel et al., 2019) to implement bucketing, and the number of buckets is set to 32 (T5 default).

**XLNet** (Yang et al., 2019) uses fixed sinusoid encoding to represent relative positions, and has a memorization mechanism to accumulate context information of arbitrary length. It is also pretrained by an auto-regressive Permutation Language Modeling (PLM) objective instead of MLM. In this work, we pretrain XLNet with PLM but without memorization, in order to adopt the same input data pipeline as other models.

All the models were implemented by modifying the code of Huggingface Transformers package (Wolf et al., 2020), using TensorFlow 2<sup>4</sup>. We use the BooksCorpus (Zhu et al., 2015) and English Wikipedia to pretrain the models, the same as Devlin et al. (2019) (but not the same as RoBERTa (Liu et al., 2019)). More detailed settings for pretraining are given in §A.2.

5.1 Pretraining Cost

Table 1 shows the number of trainable parameters, and the time required to pretrain the models on different hardware. **Shatter** has a significant reduction in number of parameters than other models, due to the omission of a $d \times d$ matrix per layer (§3.2). It also leads to 5% faster pretraining speed than BERT on GPUs and 15% on TPUs.

Reducing the batch size to 128 and sequence length to 256 (the largest possible to fit in memory), we can pretrain **Shatter** on 8 V100 GPUs for 1.6M steps within 1 week. At step 1.6M, **Shatter**<sub>GPU</sub> sees the same amount of tokens as **Shatter**<sub>Base</sub> at step 400k; as we will show in §5.2.1, it is already close to converge and outperforms BERT<sub>Base</sub> on GLUE.

**BERT-RPE** has significantly more parameters than BERT<sub>Base</sub>, due to the relative position embeddings at each layer; which prevents the model from running on GPUs using the same settings as BERT<sub>GPU</sub>. It is also 3.9 times slower than BERT on TPUs, making it impractical to scale up to larger size. **BERT-RAB** has almost the same number of parameters as BERT, but still 20% slower on TPU; The most memory intensive model is XLNet, due to an extra trainable $d \times d$ matrix at each layer to transform the sinusoid encoding of relative positions. Pretraining of XLNet<sub>Base</sub> is also slow, probably due to the two-stream self-attention calculation for the PLM objective.

<sup>4</sup>https://www.tensorflow.org/overview
We finetune the models on GLUE (Wang et al., 2018) with learning rate \([1e^{-5}, 2e^{-5}, 3e^{-5}, 4e^{-5}, 5e^{-5}]\) and points on small datasets such as RTE or MRPC. With the findings of a reproduction study (Sellam et al., 2021), that it usually requires BERTBase to be pretrained for a larger number of steps in order to reproduce the performance on GLUE. As a reference, we also show the finetuned results of the “bert-base-uncased” checkpoint in the Huggingface Transformers package (row “Huggingface BERT” in Table 2), which reproduces Devlin et al. (2019).

Overall, Shatter\_CPU and Shatter\_Base match Huggingface BERT on the development set, and outperform BERT\_Base on test. It is noteworthy that, although Shatter\_Base is better than Shatter\_CPU on dev, the performance gap on test set is only marginal. It suggests that Shatter\_CPU is close to convergence, making the model favorable given its low pretraining cost. Shatter\_CPU achieves such cost-performance thanks to two ingredients: a shorter sequence length in pretraining and a faster convergence, making the model favorable given its low pretraining cost.

Table 2 shows the results.

For BERT\_Base, Devlin et al. (2019) finetuned with learning rate \([1e^{-5}, 2e^{-5}, 3e^{-5}, 4e^{-5}, 5e^{-5}]\) and took the best. We found smaller learning rates almost always give better results, but the numbers on development set can randomly vary \(\sim 0.25\) points on large datasets such as MNLI or QNLI, and up to 2 points on small datasets such as RTE or MRPC. Thus, we set the learning rate on CoLA and SST-2 to 5e-6, otherwise to 1e-5, and we conduct several runs to show one run better than average (i.e., if the number on some task is worse than average, we will re-run it and show a better one).

It is especially important to use the small learning rate 5e-6 on CoLA; our accuracy on CoLA dev is better than Devlin et al. (2019) and other papers. On the other hand, our BERT\_Base is \(\sim 1\) point worse on MNLI than Devlin et al. (2019), which agrees with the findings of a reproduction study (Sellam et al., 2021), that it usually requires BERT\_Base to be pretrained for a larger number of steps in order to reproduce the performance on GLUE. As a reference, we also show the finetuned results of the “bert-base-uncased” checkpoint in the Huggingface Transformers package (row “Huggingface BERT” in Table 2), which reproduces Devlin et al. (2019).

Overfitting position modeling. However, its high training cost on TPU becomes a burden, as one can outperform BERT-RPE with larger models. On the other hand, BERT-RAB and XLNet\_Base outperform BERT\_Base on some tasks, but not all.

Scaling up, Shatter\_large consistently outperforms BERT\_Large, showing the ability of our model. We also cite Jacob Devlin’s original BERT\_Large submission to GLUE leaderboard for better comparison.

### 5.2 Finetuning Results

We finetune the models on GLUE (Wang et al., 2018), SQuAD v1.1 (Rajpurkar et al., 2016), and MultiRC (Khashabi et al., 2018) and BoolQ (Clark et al., 2019) from SuperGLUE (Wang et al., 2019). For all tasks, we use the Adam optimizer (Kingma et al., 2014), set batch size to 16, evaluate the model in every 1k steps and choose the one that naturally extends longer. In order to demonstrate

Table 2: Results on GLUE. Test performance obtained by submitting to https://gluebenchmark.com/.
Table 3: Results on SQuAD v1.1 development set.

| Model          | Dev. | Test |
|----------------|------|------|
| BERT_GPU 256-l | 80.0 | 75.6 |
| BERT_GPU 512-l ext. | 79.7 | 87.3 |
| Shatter_GPU 256-l | 78.8 | 75.5 |
| Shatter_GPU 512-l ext. | 81.8 | 88.7 |
| BERT_Base 512-l | 83.3 | 90.0 |
| BERT_Base 1024-l ext. | 79.7 | 86.6 |
| Shatter_Base 512-l | 82.6 | 89.6 |
| Shatter_Base 1024-l ext. | 82.8 | 89.6 |
| BERT-RPE 512-l | 84.7 | 91.0 |
| BERT-RPE 1024-l ext. | 84.4 | 91.0 |
| BERT_Large 512-l | 86.5 | 92.8 |
| BERT_Large 1024-l ext. | 86.5 | 92.7 |
| Shatter_Large 512-l | 86.5 | 92.8 |
| Shatter_Large 1024-l ext. | 86.3 | 93.0 |

Table 4: Results on the MultiRC task.

| Model          | Dev. (Acc.) | Test (F1a) |
|----------------|-------------|------------|
| BERT_Large 512-l | 81.0 | 76.6 |
| BERT_Large 1024-l ext. | 79.6 | 75.8 |
| Shatter_Large 512-l | 79.4 | 77.1 |
| Shatter_Large 1024-l ext. | 81.7 | 78.9 |

Table 5: Results on the BoolQ task.

| Model          | Dev. | Test |
|----------------|------|------|
| BERT_Large 256-l | 84.5 | 82.6 |
| Shatter_Large 256-l | 84.3 | 82.7 |
| BERT_Large 400k | 81.8 | 80.2 |
| Shatter_Large 400k | 82.8 | 80.1 |

Figure 3: Plots showing finetuned performance on dev set (y-axis) as a function of pretrained steps (x-axis).

5.2.3 Convergence

Next, we investigate convergence, i.e. how many pretrained steps are required for a model to achieve certain performance. In Figure 3, we plot the fine-tuned performance of base-size models on MNLI dev sets, and large-size models on BoolQ dev, as a function of pretrained steps. Shatter achieves better performance with fewer pretrained steps than BERT, and Shatter_Base scores the second among all base-size models, next to BERT-RPE. The good convergence is a critical factor for Shatter_GPU, as Shatter_GPU only sees the same amount of tokens as Shatter_Base at pretrained step 400k.

For further comparison, we show performance of large-size models at pretrained step 400k in Table 2, and BoolQ in Table 5, where Shatter_Large outperforms BERT_Large as well. It is but noteworthy that dev and test performance do not always align; so pretraining longer seems a safe choice.

6 Conclusion

We have presented Shatter, an efficient Transformer encoder with a novel self-attention architecture. We expect broader applications in the future.
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A More Details for Shatter

In this appendix, we show more detailed settings of Shatter, as well as additional ablation experiments.

A.1 Partition of Unity

Given the number of parts \( n \), the partition of unity \( \{ f_h \} (0 \leq h < n) \) consists of \( n \) functions. We use half of the functions to cover relative positions to the left (i.e. \( x < 0 \)), and the other half to the right (\( x > 0 \)).

Let \( D = n/2 - 1 \). The Bernstein polynomials of degree \( D \) consists of \( D + 1 = n/2 \) polynomials, \( B_\nu(u) \) \((0 \leq \nu \leq D)\), of the variable \( u \). They are defined by:

\[
B_\nu(u) = \binom{D}{\nu} u^\nu (1 - u)^{D-\nu}
\]

where \( \binom{D}{\nu} \) is the binomial coefficient. \( \{ B_\nu(u) \} \) is a partition of unity on the interval \( 0 \leq u \leq 1 \), and we transform the interval \( u \in [0, 1] \) to \( x \in [0, \infty] \), in order to obtain \( n/2 \) functions that cover the relative positions to the right. Then, we reflex the \( x \)-axis to obtain another \( n/2 \) functions to cover the relative positions to the left.

Formally, we transform \( u \in [0, 1] \) to \( x \in [0, \infty] \) by setting

\[
u = \frac{\ln \left( e^{\beta x} (1 - e^{\alpha}) + e^{\alpha} \right)}{\alpha}
\]

where \( \alpha < 0 \) and \( \beta < 0 \) are hyper-parameters. The above is an affine transformation of the softplus; it maps \( x = 0 \) to \( u = 0 \), and \( x = +\infty \) to \( u = 1 \).

As \( \alpha \to -\infty \), the limit of \( u \) converges to the hinge function \( \min(\frac{2}{\alpha} x, 1) \).

In this work, we set

\[
\alpha = -\frac{k + 1}{L} D
\]

\[
\beta = -\frac{1}{D} \left( \frac{D}{12} \right)^{k+1}
\]

where \( 0 \leq k < L \) is the layer index and \( L \) is the number of layers. Thus, the first layer (i.e. \( k = 0 \)) has more parts that concentrate to relative positions close to 0, while the last layer (i.e. \( k = L - 1 \)) has all parts more evenly distributed with interval \( \approx 12 \).

In our preliminary experiments, we have tried other settings (e.g. all layers using the same partition), and the pretraining loss and finetuned performance are sensitive to the choice of the partition of unity. The current setting is largely based on our intuition, but might not yet be optimal.

A.2 Pretraining Settings

Instead of the word-piece tokenizer (Wu et al., 2016) used in BERT, we use sentence-piece (Kudo and Richardson, 2018) for tokenization, on account of its easy usage and fast speed. The pretraining corpus is lower-cased and the vocabulary size set to 32k. This same tokenizer is used in all models in our experiments, for fair comparison.

To save pretraining time, we tokenize the corpus in advance and cache the results to files. The tokenization can be done with 20 parallel 4-core CPU machines in 2 hours. Following RoBERTa (Liu et al., 2019), we use Masked Language Modeling (MLM) as the pretraining objective, without Next Sentence Prediction.

For optimization we use Adam with 0.01 weight decay (Bentivogli et al., 2009). The learning rate is set to 1e-4, with 10k steps warmup then linear decay to 0.

For validation we use the Penn Tree Bank corpus (Marcus et al., 1994), and the valid loss is plotted in Figure 1 (for our model variants and BERT\_Base), Figure 4 (for base-size models) and Figure 5 (for large-size models). In Figure 4, BERT-RPE consistently outperforms other models, while Shatter\_Base shows faster convergence than BERT-RAB, which roughly aligns with the convergence of finetuned performance (Figure 3). In Figure 5, Shatter\_Large outperforms BERT\_Large. The valid loss for XLNet is not shown in the figures, since XLNet is pretrained with PLM instead of MLM.
A.3 Ablation on GLUE

In Table 6, we compare the finetuned performance of our model variants developed in §3. Mostly, the performance of ShatterBase $\geq$ Part_Bias $>$ 1H_Sigmoid $>$ Part_Mask, which aligns with the comparison of pretraining loss in Figure 1. The performance of ShatterBase and Part_Bias are close, but ShatterBase slightly outperforms Part_Bias on MNLI and QQP.

A.4 Sequence Classification Strategy

We further compare different sequence classification strategies in Table 7. The sequence classification method originally used in BERT (Devlin et al., 2019), which takes the hidden state at the [CLS] token, is indicated by a “[CLS]” suffix in the table. It is compared with our modified sequence classification method described in §3.4.

For BERTBase, the difference in sequence classification strategy does not affect finetuned performance; but for ShatterBase and BERT-RPE, our modified method is generally better, which suggests that our method can better cope with the relative position modeling of the [CLS] token.