SIMPLETRON: SIMPLE TRANSFORMER WITH O(N) COMPLEXITY

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ABSTRACT

In this paper, we propose that the dot product pairwise matching attention layer, which is widely used in Transformer-based models, is redundant for the model performance. Attention, in its original formulation, has to be seen rather as a human-level tool to explore and/or visualize relevancy scores in sequential data. However, the way how it is constructed leads to a significant computational complexity. Instead, we present SimpleTRON: Simple Transformer with O(N) Complexity, a simple and fast alternative without any approximation that, to the best of our knowledge, outperforms existing sub-quadratic attention approximation models on several tasks from the Long-Range Arena benchmark. Moreover, unlike other approximation models, SimpleTRON does not have any architecture-related overhead therefore can be seen as a purely linear Transformer-like model.

1 Introduction

Initially designed for natural language processing, the Transformer architecture [1] emerged in a wide range of other domains and quickly became a state-of-the-art in language modeling [2] as well as in generative tasks [3, 4], image processing [5, 6], speech recognition [7], reinforcement learning [8], and others. From the original paper named "Attention is All You Need" [1] on, it seems to be widely considered that the query-key-value framework, which implies a global pairwise comparison between query and key tokens, is a necessary condition for the model performance. Even though such a mechanism allows a human-comprehensible visualization of interactions between the tokens, unveiling the interpretability up to some extent, an element-wise token comparison leads to a quadratic complexity both in terms of time and space. Therefore, even though the original Transformer architecture virtually can handle arbitrarily long range dependencies given the infinite compute, which is in opposite to most recurrent neural networks [9], the complexity of regular full-rank attention limits Transformer applications when long sequences are required.
In this paper we present a SimpleTRON model with a SimpleAttention mechanism as an extremely simple yet efficient solution to replace the original quadratic complexity softmax attention. The proposed mechanism not only possesses linear time and memory complexity, but outperforms the current state-of-the-art Transformers on the text classification, matching and ListOps tasks from the LRA [10] benchmark, which became a widely applied test for sequence processing models. Moreover, since the SimpleAttention has analogous building blocks as the original attention it is suitable for transfer learning as one can use pre-trained weights from the existing transformer models.

2 Related Work

As a restrictive limitation, the computational complexity of the original model motivated the community to quest for the solution in order to approximate the architecture with asymptotically faster models [11]. Thus, recently, a dizzying number of so-called "Efficient Transformers" appeared. Each of these implementations applied some notion of sparsity to the otherwise dense attention mechanism and reached a sub-quadratic complexity with comparable performance.

Among the solutions to rationalize the Transformer complexity, there were engineering approaches such as sparse attention [12, 13], graph attention [14] or compressive attention [15] that maps past hidden activations to a smaller set of compressed representations, allowed to use longer sequences at comparable compute. Further engineering methods include Longformer [16], where attention mechanism is a combination of a windowed local-context self-attention and a global attention that encodes inductive bias. Coformer [17] and Attention Augmented CNN [18] which are hybrid architectures of CNN augmented Transformers. Imputer [19] – the model that generates output sequences iteratively via imputations and dynamic programming, Reformer [20] using dot-product attention and reversible residual layers, N-gram Masked Self-Attention [21] etc.

Another branch of research to reduce Transformer complexity is dedicated to matrix and kernel approximations based on strong mathematical basis. That includes Performer [22], which uses kernel approximation, factorized attention [23], random feature attention [24] or, for example, Nyströmformer [25] using Nyström matrix approximation. Finally, learnable kernel approximation was presented by Chowdhury et al. [26], where the authors reported trainable kernel by learning the spectral distribution and approximation of the Transformer kernel as a dot product between spectral feature maps.

Additionally there are several studies that changed the whole concept of attention and replaced it with Fast Fourier Transform (FFT) which does not require any training [27], or used dense layers to mix the tokens along both axes [28]. Another work [29] reported vision transformer-inspired [5] model that independently mixes the spatial and channel locations of image patches using depth-wise convolutions, outperforming existing Transformer-based solutions for image recognition.

3 The Model

The original multi-head attention layer utilizes the softmax-normalization of a head-wise product of query and transposed key matrices combined with the value matrix as:

$$\text{Attention}(Q_h, K_h, V_h) = \text{softmax} \left( \frac{Q_h K_h^T}{\sqrt{d}} \right) V_h,$$

where $Q_h$, $K_h$, and $V_h \in \mathbb{R}^{L, d}$ are the query, key, and value, respectively, corresponding to the $h$-th head, $d$ is the query dimensionality, and $L$ is the length of the input sequence. The head-wise inputs to the operation are obtained by splitting the $Q$, $K$, $V \in \mathbb{R}^{L, D_h \times N_h}$ matrices across the hidden dimension axis $D_h \times N_h$ into $N_h$ pieces of size $d = D_h / N_h$ corresponding to $N_h$ heads. The input $X \in \mathbb{R}^{L, D_h}$ is transformed to the query $Q$, key $K$, and value $V$ matrices by a linear transformation using matrices $Q^*$, $K^*$, $V^* \in \mathbb{R}^{D_h, D_h \times N_h}$ and biases $q^*$, $k^*$, $v^* \in \mathbb{R}^{D_h, N_h}$ as parameters:

$$Q = XQ^* + q^*, \quad K = XK^* + k^*, \quad V = XV^* + v^*.$$

The final output of the attention layer is then produced by applying another linear layer on a concatenation of all heads and adding the duplicated input $X$ that corresponds to a skip connection:

$$\text{SelfAttention}(X) = X + (\text{Attention}(Q_1, K_1, V_1), \ldots, \text{Attention}(Q_{N_h}, K_{N_h}, V_{N_h})) W + w,$$

where $W \in \mathbb{R}^{D_h \times D_k}$ and $w \in \mathbb{R}^{L, D_k}$ are the parameters of the linear layer.

The $Q_h$, $K_h$, and $V_h$ are rectangular matrices with the first dimension typically dominating the second one. Thus, the quadratic complexity appears upon the $Q_h K_h^T$ operation with respect to the sequence length. Swapping matrix multiplication order (first $K_h^T V_h$, then multiply with $Q_h$) would reduce complexity to linear. However, softmax
non-linearity forbids such shuffling. Here, we applied several major tweaks to the model in order to reach linear complexity and to improve performance:

- Reject the softmax nonlinearity.
- Change the order of matrix multiplication to avoid quadratic complexity.
- (Optionally) Remove the linear layer producing the final output of the attention layer.

Therefore we obtain a no-softmax attention with the direct q-k-v product, which could be described by the following simple formula for an attention operation on a single head:

$$\text{SimpleAttention}(Q_h, K_h, V_h) = \frac{1}{\sqrt{L}} Q_h (K_T h V_h).$$

When the linear layer is not used to produced the final output, then the q-k-v product concatenated for all heads goes directly to the residual sum with duplicated input from skip connection.

Unlike the linear mixing models such as [27], this transformation is not linear in terms of input X. To see this just note that

$$Q_h = Q I_h = X Q^* I_h + q^* I_h$$

and analogously for K_h and V_h, where I_h ∈ R^{D_{hid} × d} is a matrix with all entries zero except identity matrix d × d on rows from d(h − 1) + 1 to dh, i.e. the multiplication Q I_h takes exactly those columns from matrix Q that correspond to the h-th head. Hence, we obtain

$$\text{SimpleAttention}(X) = \frac{1}{\sqrt{L}} (X Q^* I_h + q^* I_h) ((X K^* I_h + k^* I_h)^T (X V^* I_h + v^* I_h)).$$

This equation resembles the quadratic form multiplied again by the input.

We further refer the above-mentioned mechanism as SimpleAttention, and the model as SimpleTRON which stands for Simple Transformer with O(N) Complexity. The matrix operations within a single head of SimpleAttention is illustrated in Figure 1.

4 Experiments

4.1 LRA benchmark

Even though numerous sub-quadratic complexity approximations of the vanilla Transformer claimed comparable or even superior performance to the original model, it is fair to express that each model can be task-dependent and
possess strikingly different results upon modality. Moreover, some benchmark test can be parameter-dependent, thus bigger models can perform better. Therefore up to some point effective evaluation of the Transformer-like models was uncertain, due to the absence of a unified and systematic benchmark. In this regard, Tay et al. [10] published the benchmark for efficient Transformer models called "Long Range Arena" (LRA), that consists of task of various data types and modalities, where data is presented in sequences ranging from 1K to 16K tokens.

We use LRA [10] as the standardised benchmark for efficient Transformer evaluation:

- Following the recommendations from [10], we replicate the learning schedule and all the hyperparameters that relate to our model architecture, while keeping additional parametrization below 10%.
- To reproduce the experimental setup from [10], we used the gradient accumulation in order to simulate larger batch sizes.
- Given the stochastic weight initialization and sampling, each model was trained for 5 times to observe model behavior, accuracy variance and to avoid so-called black swans – random seeds that give radically different results [30]. Best results are reported in Table 1.
- As we focus on NLP domain in the present work, we test out model on three LRA tasks – BPE text classification, information retrieval and ListOps.
- Since our models tend to converge slower in terms of number of iterations, we prolonged the training on matching and ListOps tasks to 15 k steps.

The model was implemented in PyTorch library [NEURIPS2019_9015].

4.2 SimpleTRON transfer learning

In the beginning of the paper, we raised a question, whether we need a pairwise matching attention layer or any of its approximations. To find the answer we performed a simple experiment:

First, the SimpleTRON model was trained regularly, reaching its top accuracy. As q-k-v matrices are of the same dimensions in both SimpleAttention and original SoftmaxAttention, thus the weights are interchangeable. Therefore, we transferred the trained weights from SimpleAttention to SoftmaxAttention, froze q-k-v layers and retrained the rest of the model. The logic behind such experiment was quite simple: if we need a pairwise comparison in q-k product, then the model won’t be able to reach the efficiency of a vanilla Transformer as q-k-v layers are frozen and not trained optimally.

Moreover, as we know the community performed an immense effort to pretrain large language models on comprehensive datasets, allowing many researchers and companies reap all the benefits of transfer learning by fine-tuning pretrained models on specific tasks from various domains [sun2019fine, zhang2021revisiting, GPT-2_2021]. Lately it was proposed, that learning abilities of the Transformer models trained on a extensive language dataset can overcome NLP modality and used as a universal computational engines [lu2021pretrained]. On the other hand, such training is an extremely resource demanding process [dale2021gpt] with a considerable carbon footprint [patterson2021carbon]. Therefore, simply of of curiosity, we tried to apply fine tuning for text classification on our SimpleTRON model using weight from pretrained BERT [2]. This operation of weight transfer is applicable to SimpleTRON architecture as the size and dimensionality of the model layers can be fully identical and, therefore, transferable.

5 Results and Discussion

5.1 LRA

Number of parameters  By removing a linear layer following the q-k-v product, our model in fact had less parameters than its counterparts given the restrictions reported in [10]. Which is only a small margin, however worth mentioning as the authors placed parametrization restrictions in their paper.

Training speed  By swapping the q-k-v product matrices and avoiding any kind of approximation we’ve reached a truly linear complexity with a respect to the input length. It has to be emphasized, that the most of linear attention approximations reporting linear complexity, in fact omitting high architecture-dependent multiplier, which should be taken into account in practice.

Memory efficiency  The current model, given the above-mentioned LRA tasks, was found to be an order of magnitude more memory efficient in comparison with the vanilla transformer.
| Model                  | Complexity         | Classification | Matching | ListOps |
|------------------------|--------------------|----------------|----------|---------|
| Random                 | $O(1)$            | 50.00          | 50.00    | 10.00   |
| Transformer            | $O(L^2)$          | 64.27          | 57.46    | 36.37   |
| Synthesizer            | $O(L^2)$          | 61.68          | 54.67    | 36.99   |
| Sinkhorn Trans.        | $O(B^2 + (N/B)^2)$| 61.20          | 53.83    | 33.67   |
| Sparse Trans.          | $O(L \sqrt{L})$  | 63.58          | 59.59    | 17.07   |
| Reformer               | $O(L \log L)$    | 56.10          | 53.90    | 37.27   |
| Local Attention        | $O(LK)$           | 52.98          | 53.39    | 15.82   |
| Longformer             | $O(LK)$           | 62.85          | 56.98    | 35.63   |
| Linformer              | $O(L)$            | 53.94          | 52.27    | 35.70   |
| BigBird                | $O(L)$            | 64.02          | 59.29    | 36.05   |
| Linear ELU             | $O(L)$            | 65.90          | 53.09    | 16.13   |
| Performer              | $O(L)$            | 65.40          | 53.82    | 18.01   |
| GMM-RKS                | $O(L)$            | 66.20          | 58.74    | 18.15   |
| FastFood-RKS           | $O(L)$            | 65.91          | 57.47    | 18.20   |
| Generative-RKS         | $O(L)$            | 66.37          | 59.02    | 17.80   |
| GMM-PRF                | $O(L)$            | 62.70          | 59.64    | 36.95   |
| FastFood-PRF           | $O(L)$            | 64.69          | 67.90    | 37.25   |
| Generative-PRF         | $O(L)$            | 62.39          | 67.18    | 37.10   |
| Simple (ours)          | $O(L)$            | 66.75          | 73.92    | 37.45   |
| Simple-Res (ours)      | $O(L)$            | 66.65          | 74.83    | 37.10   |
| Simple-ResL (ours)     | $O(L)$            | 66.71          | 73.59    | 37.55   |

Table 1: Baseline and proposed models on the three LRA tasks. We denote sequence length as $L$, attention span as $K$ and Sinkhorn model block size as $B$. The notation for our models is: **Simple** - SimpleAttention without both skip connection and linear layer, **Simple-Res** - SimpleAttention with skip connection and without linear layer, and **Simple-ResL** - SimpleAttention with skip connection and linear layer behind the q-k-v multiplication.

**Classification accuracy** To observe the model behaviour and accuracy variance, we train our models for 5 times to avoid the so-called black swans – random seeds that give radically different results [30]. As a result, our model had shown 66.75/73.92/37.45% top accuracy on the test classification/matching/ListOps splits and 66.61/73.74/37.15% mean test accuracy respectively, outperforming other known linear approximation of attention mechanism.

**Normalization** The original Transformer model uses the $1/\sqrt{d}$ normalization term of the $Q_hK_h^T$ product to counteract the vector magnitude explosion and the following decreased gradient flow through the Softmax. Since we don’t use any saturating function in the attention module, our model works without any normalization terms. However, we have found the $1/\sqrt{L}$ term to be useful for a more stable convergence.

**Convergence** We have found our model to be converging slower than competitors in terms of number of iterations, but this is being counteracted by faster computation. Furthermore, we argue that according to the validation loss and accuracy behavior on some tasks better results could be obtained by further training of our model, see Figure 2a and 2b.

**Compressed representation** The $Q_hK_h^TV_h$ product in SimpleAttention may be interpreted as a comparison of an uncompressed input projection $Q_h$ with its compressed representation $K_h^TV_h$.

**Attention transfer** Transferred weights from, SimpleAttention model to the original SoftmaxAttention model has shown an interesting behaviour: having about 30% less trainable parameters and in fact no ability to learn pairwise
As shown above, our architecture is superior on long text classification from the LRA benchmarks, which is unified test for efficient Transformer models. However, the true power of Transformer architecture is its ability to capture patterns from the large scale comprehensive datasets (often natural language datasets). Therefore, we performed preliminary experiment on comparing BERT [2] language model with SimpleTRON of the similar architecture. Training from scratch of AG News Corpus dataset [Zhang2015CharacterlevelCN], showed that SimpleTRON (with skip connections and linear layer) model with the architecture mimicking BERT possessed 89.9% of accuracy, while training vanilla Transformer with BERT-base architecture we obtained 1.2% higher accuracy.
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**Table 2:** Model’s performance with respect to the number of layers in the model. Training on AG News Corpus dataset.

| N_{blocks} | BERT  | SimpleTRON |
|------------|-------|------------|
| 1          | 89.12 | 90.90      |
| 2          | 90.38 | 90.32      |
| 3          | 90.28 | 90.44      |
| 4          | 90.66 | 90.41      |
| 5          | 90.11 | 90.35      |
| 6          | 90.30 | 90.22      |
| 7          | 90.68 | 90.19      |
| 8          | 90.68 | 89.98      |
| 9          | 91.13 | 89.95      |
| 10         | 91.21 | 89.94      |
| 11         | 90.78 | 89.43      |
| 12         | 90.10 | 89.90      |
| 6*         | 92.70 | 92.30      |
| 12*        | 94.20 | 92.70      |

* fine-tuning

However, while SimpleTRON model in this experiment contained linear layer, the weights from BERT are fully transferable to the proposed architecture. Therefore, using weights from pretrained BERT model, we were able to perform fine-tuning on SimpleTRON architecture. Interestingly, even though SimpleTRON is in fact a different model we could obtain an inference gain using the weights from pretrained model, with the accuracy of 92.7%, which was, however, still 1.5% lower than pre-trained BERT model fine tuned on AG News dataset.

As discussed above, SimpleTRON architecture works especially well, when there are limited number of stacked blocks, therefore we performed the experiments on the models with reduced depth both for fine-tuning and training from scratch. Indeed, SimpleTRON architecture was found to outperform BERT based model, when two models containing 6 blocks were trained from scratch. While transferring 6 blocks of pretrained BERT a notable increase of performance was observed, 6 blocks SimpleTRON model lags only a small margin behind the original BERT architecture. Overall, we found that even-though SimpleTRON blocks are able to outperform Transformer architecture, in case of larger models, the proposed architecture do not take advantage of a stacked blocks well. This is a subject for a further investigation of SimpleTRON architecture training and regularization. The performances of the models on depth from 1 to 12 blocks show that testing accuracy of our model saturates quickly with depth and may even decrease, when vanilla using vanilla self-attention mechanism inference accuracy increases with the model depth.

### 6 Conclusion and Future Work

To conclude, we raised the question, whether the attention or any of its approximation is needed for the model performance. We presented a simple alternative of a truly linear model with a respect to the input length, that outperformed existing models on the several LRA tasks, at the same time possessing an extremely fast and memory efficient training. The key point is to reject the $Q_hK_h^T$ product with the following Softmax normalization and the linear layer after. We showed that trained q-k-v in the SimpleAttention model can be effectively transferred to the classical...
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Multi-Head
Simple Self-Attention
Add & LayerNorm
Feed Forward Layer
Query
Key
Value
Add & LayerNorm
Linear Layer (optional)

Figure 4: Illustration of the SimpleAttention block with a double skip connection.

SoftmaxAttention, which allows fast model pre-training. Moreover as layers in the model are identical to the ones of transformer, weight transfer from pretrained large language models, such as BERT is possible with clear evidence of positive effect on the model performance. This is a valuable feature since training of large language models is a very resource demanding task. Nevertheless, there are several tasks yet to be done:

Different tasks Transformer architecture is known to be pervasive, however we are fully aware that performance of any model can be task-dependent. Here we show the results on text-classification task from LRA benchmark dataset and AG News. Therefore thus our goal in the near future is to expand SimpleTRON application to other modalities, such as computer vision, as well as looking for a more efficient way to utilize the model depth.

Interpretability Initially the attention mechanism allowed a human-comprehensible visualization of relevancy scores in the sequences, nevertheless many approximation models lost this feature. Therefore, our goal is to gain it back using our model.

q-k-v framework elimination In the present work we followed the original q-k-v framework in order to show the step further towards attentionless transformer architecture. However, we believe that there is a more efficient framework as long as q-k-v initially assumed global pairwise comparison.

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Appendix A  Hyperparameters

| Parameter          | Classification | Matching | ListOps |
|--------------------|----------------|----------|---------|
| Seq. Length        | 4000           | 4000     | 2000    |
| Batch Size         | 32             | 32       | 32      |
| Training Steps     | 20 000         | 15 000   | 15 000  |
| Optimizer          | AdamW ($\beta_1 = 0.9$, $\beta_2 = 0.999$) | | |
| Base LR            | 0.05           | 0.05     | 0.0005  |
| Weight Decay       | 0.1            | 0.1      | 0.1     |
| Warmup Steps       | 8000           | 8000     | 1000    |
| Schedule           | Base LR * Warmup * Sqrt Decay | | |
| Warmup Mul.        | $\min(1, \text{Current Step/Warmup Steps})$ | | |
| Sqrt Decay Mul.    | $1/\sqrt{\max(\text{Current Step, Warmup Steps})}$ | | |
| Loss               | CCE            | | |
| Blocks             | 4              | 4        | 6       |
| Heads              | 4              | 4        | 8       |
| Hidden dim.        | 256            | 128      | 512     |
| QKV dim.           | 256            | 128      | 512     |
| MLP dim.           | 1024           | 512      | 2048    |
| Dropout            | 0.1            | 0.1      | 0.1     |
| Activation         | GELU           | GELU     | GELU    |
| (ReLU in output)   | | | |
| Pooling            | CLS            | CLS      | CLS     |
| Pos. encoding      | Learnable      | Learnable| Learnable|

Table 3: Hyperparameters used for this experiment

Appendix B  Parameters’ Training Evolution
Figure 5: Training evolution of standard deviation of Attention output weights for vanilla transformer (softmax($\frac{QK^T}{\sqrt{d}}V$)) and SimpleTRON ($\frac{1}{\sqrt{L}}QK^TV$) model containing 8 blocks, on text classification task. In case of vanilla transformer Softmax normalization is omitted in standard deviation calculation.