Skyformer: Remodel Self-Attention with Gaussian Kernel and Nyström Method

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Abstract

Transformers are expensive to train due to the quadratic time and space complexity in the self-attention mechanism. On the other hand, although kernel machines suffer from the same computation bottleneck in pairwise dot products, several approximation schemes have been successfully incorporated to considerably reduce their computational cost without sacrificing too much accuracy. In this work, we leverage the computation methods for kernel machines to alleviate the high computational cost and introduce Skyformer, which replaces the softmax structure with a Gaussian kernel to stabilize the model training and adapts the Nyström method to a non-positive semidefinite matrix to accelerate the computation. We further conduct theoretical analysis by showing that the matrix approximation error of our proposed method is small in the spectral norm. Experiments on Long Range Arena benchmark show that the proposed method is sufficient in getting comparable or even better performance than the full self-attention while requiring fewer computation resources and improving the stability in training.

1 Introduction

The cost of language model training increases exponentially. Among different models, Transformer-based language models [Vaswani et al., 2017, Devlin et al., 2019, Liu et al., 2019, Lewis et al., 2020] are shown to enjoy state-of-the-art (SOTA) performances on many Natural Language Processing (NLP) tasks despite of their enormous training cost that was unthinkable years ago. For example, it may theoretically take around 355 years to train GPT-3 [Brown et al., 2020] on a Tesla V100. One of the computation bottlenecks lies in the self-attention mechanism, which is known to be resource-intensive with quadratic time and space complexity ($O(n)$ where n is the input sequence length). Consequently Transformers cannot support long sequence processing and large batch size.

The challenge of improving computational efficiency of Transformers has motivated several recent studies on attention acceleration, using either sparse attention pattern [Qiu et al., 2020, Child et al., 2019, Zaheer et al., 2020, Beltagy et al., 2020] or low-rank approximation [Choromanski et al., 2020, Wang et al., 2020, Kitaev et al., 2020]. However, there is usually a lack of theoretical analysis on the approximation error of these methods due to the complex softmax structure, which makes the theoretical comparison between the efficiency of each method infeasible. It is also unclear in theory how to set the hyper-parameters of those methods to attain a desired level of approximation accuracy.

Another issue of Transformers is the training instability that small perturbations in parameter updates tend to be amplified, resulting in significant disturbances in the model output [Liu et al., 2020a]. Transformers on some Natural Language Processing tasks have shown to be sensitive to hyper-parameters, learning schedulers or even random seeds, which usually demands a time costly grid search for the best configuration in real world applications. It has also been observed in our experiments that a slight change in the learning rate may cause the failure of convergence for some models. We conjecture

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that the instability in Transformer training comes from the softmax structure, as the un-normalized attention score matrices before softmax tend to have extremely large condition numbers due to its fast singular value decay.

To alleviate the instability issue, an extra factor of $1/\sqrt{p}$ in the softmax kernel SM is suggested by Vaswani et al. [2017] to restrain the scale variation; Liu et al. [2020a] instead proposes a new scheme to control the magnitude of output change and stabilize the training in early stages. In practice, we also need to consider the lower numerical precision of GPU implementation in model training, which further deteriorates the stability.

Kernel methods may be the answer to both challenges. As pointed out by Choromanski et al. [2020], the softmax structure is closely related to Gaussian kernels up to diagonal matrix multiplications, as the pairwise dot products naturally appears when expanding the squared ℓ_2 distance. We further notice some important connections between self-attention and Gaussian kernels. First, the un-normalized attention score matrix can be formed via basic matrix operations on an empirical Gaussian kernel matrix. Moreover, the form of Gaussian kernels has the natural interpretation of assigning "attention" to different tokens. Compared to the softmax function, Gaussian kernels automatically perform the normalization as softmax does (c.f. Section 4.1). These observations motivate us to replace the softmax structure with Gaussian kernels. As we demonstrated in this paper, the new attention model, **Kernelized Attention**, empirically stabilizes of the model training while being comparable to self-attention in model accuracy.

To further improve the efficiency, we propose **Skyformer** to accelerate Kernelized Attention. Skyformer adapts the Nyström method [Williams and Seeger, 2001, Drineas et al., 2005] to the non-PSD empirical Gaussian kernel matrix (query matrices in general do not equal to key matrices), by instead lifting the kernelized attention score matrix into a large PSD matrix that contains the un-normalized attention score matrix as the off-diagonal block. We further conduct theoretical analysis by showing that Skyformer has a small matrix approximation error on Kernelized Attention in the spectral norm. Our experiments on the LRA benchmark show that Skyformer consistently use less space and time while achieving better accuracy than other baseline methods.

In summary, our main contributions are:

(1) We revisit the intrinsic connection between self-attention and kernel methods, and explore a new kernel-based structure to stabilize the training of Transformers.

(2) We approximate the Kernelized Attention via low dimensional randomized sketches by adapting the Nyström method to a non-PSD matrix. We provide theoretical guarantee that the matrix multiplication error is small in term of spectral norm.

(3) We conduct extensive experiments showing that Skyformer achieves comparable performance to the original self-attention with fewer computational costs.

2 Related Work

Among the transformer acceleration methods, such as attention layer simplification by pruning redundant attention heads [Voita et al., 2019, Michel et al., 2019] and model size reduction with knowledge distillation [Jiao et al., 2020, Tang et al., 2019, Liu et al., 2020b], we focus on attention approximation models, which are closely related to kernel methods.

By reduce the time and space complexity by avoiding exhaustive computation over the attention metric, recent studies propose to apply sparse attention patterns to limit the numbers of elements participating in matrix multiplications [Qiu et al., 2020, Child et al., 2019, Zaheer et al., 2020, Beltagy et al., 2020]. Beyond limiting the attention to fixed patterns, some approaches learn the patterns by determining token assignments to relevant groups [Kitaev et al., 2020, Roy et al., 2021]. Those models utilize local and global information in the attention score matrix to perform approximation, which coincides with the attempt to accelerate the computation in Gaussian processes [Snelson and Ghahramani, 2007].

The attention score matrix is known to exhibit a very fast rate of singular value decay [Bhojanapalli et al., 2020, Dong et al., 2021], similar to that of an empirical kernel matrix [Yang et al., 2017]. This near singular property motivates many low-rank attention approximation methods to skillfully leverage the computation techniques in kernel methods. Among them, Linformer [Wang et al.,

2020] compresses the size of key and value matrix with random projections based on the Johnson–Lindenstrauss transform, a common randomized sketching method in Gaussian processes [Yang et al., 2017]; Reformer [Kitaev et al., 2020] applies locality-sensitive hashing (LSH) [Har-Peled et al., 2012] to simplify the computation of the attention score matrix, which is widely used in kernel density estimation [Charikar and Siminelakis, 2017, Backurs et al., 2019]; Performer Choromanski et al. [2020] projects both query and key matrix through random Fourier features [Rahimi et al., 2007], heavily exploiting Bochner Theorem for stationary kernels.

The most related work to ours is Synthesizer [Tay et al., 2020a] and Nyströmformer [Xiong et al., 2021]. Synthesizer aims to modify the original self-attention by replacing the dot product before softmax with Synthetic Attention, which generates the alignment matrix independent of token-token dependencies; Nyströmformer applies the Nyström method [Williams and Seeger, 2001, Drineas et al., 2005], a powerful and effective method for large-scale kernel machines acceleration, to approximate the attention score matrix. However, Nyströmformer blindly applies the Nyström method to a non-PSD matrix, and thus fails to ultize the full potential of Nyström method. This issue is resolved in our proposed Skyformer by instead lifting the kernelized attention score matrix into a large PSD matrix which contains the target non-PSD matrix as its off-diagonal block. For more details on attention approximation methods, we refer readers to a survey paper on efficient transformers [Tay et al., 2020c].

3 Preliminaries and notations

3.1 Revisiting self-attention

For a given input sequence $\boldsymbol{X} \in \mathbb{R}^{n \times d_0}$ of length n and embedding dimension d_0, The dot-product attention for a single head in Transformer Vaswani et al. [2017] is defined as

$$\text{Attention}(\boldsymbol{Q}, \boldsymbol{K}, \boldsymbol{V}) = \text{softmax}\left(\frac{\boldsymbol{Q}\boldsymbol{K}^T}{\sqrt{p}}\right)\boldsymbol{V}$$

where $\boldsymbol{Q} = \boldsymbol{X}\boldsymbol{W}_Q$, $\boldsymbol{K} = \boldsymbol{X}\boldsymbol{W}_K$, and $\boldsymbol{V} = \boldsymbol{X}\boldsymbol{W}_V$, and $\boldsymbol{W}_Q$, $\boldsymbol{W}_K$ and $\boldsymbol{W}_V$ are the query, key, and value weight metrics that linearly project the input $\boldsymbol{X}$ of d_0 dimension to an output tensor of p dimensions.

To simplify the future analysis, the left softmax term can be rewritten into $\boldsymbol{D}^{-1}\boldsymbol{A}$, where $\boldsymbol{A} := \exp(\boldsymbol{Q}\boldsymbol{K}^T/\sqrt{p})$ is the un-normalized attention score matrix; $\boldsymbol{D}$ is a diagonal matrix whose diagonal is $\exp(\boldsymbol{Q}\boldsymbol{K}^T/\sqrt{p}) \cdot \mathbf{1}$ (by convention $\mathbf{1}$ is a size-n vector with all elements being 1). Following the notation in Performer [Choromanski et al., 2020], we define $\text{SM}(\boldsymbol{q}, \boldsymbol{k}) := \exp(\boldsymbol{q}^T\boldsymbol{k}/\sqrt{p})$ as the softmax kernel function, and represent $\boldsymbol{A}$ by the notation $\text{SM}(\boldsymbol{Q}, \boldsymbol{K})$, which means the element a_{ij} from the i-th row and j-th column in $\boldsymbol{A}$ is equal to $\text{SM}(\boldsymbol{q}_i, \boldsymbol{k}_j)$. Throughout this paper $\boldsymbol{q}_i$ (resp. $\boldsymbol{k}_j$) means the i-th (resp. j-th) row in $\boldsymbol{Q}$ (resp. $\boldsymbol{K}$).

We close this subsection with a short lemma to show $\text{SM}(\cdot, \cdot)$ is a positive semidefinite (PSD) kernel function [Wainwright, 2019, Definition 12.6] by relating it to Gaussian kernels.

Lemma 1. *$SM(\cdot, \cdot)$ is a PSD kernel function. Equivalently, for all integers $n \geq 1$ and elements $\{\boldsymbol{q}_i\}_{i=1}^n \subseteq \mathbb{R}^p$, the n-by-n matrix $\boldsymbol{C} = SM(\boldsymbol{Q}, \boldsymbol{Q})$ is PSD.*

Proof. We first state an important equation to connect the softmax kernel and Gaussian kernels as follows:

$$\text{SM}(\boldsymbol{q}_i, \boldsymbol{q}_j) = \exp\left(\frac{\boldsymbol{q}_i^T\boldsymbol{q}_j}{\sqrt{p}}\right) = \exp\left(\frac{\|\boldsymbol{q}_i\|^2}{2\sqrt{p}}\right)\exp\left(-\frac{\|\boldsymbol{q}_i - \boldsymbol{q}_j\|^2}{2\sqrt{p}}\right)\exp\left(\frac{\|\boldsymbol{q}_j\|^2}{2\sqrt{p}}\right).$$

The middle part $\exp\left(\frac{\|\boldsymbol{q}_i - \boldsymbol{q}_j\|^2}{2\sqrt{p}}\right)$ is exactly a Gaussian kernel with bandwidth $p^{\frac{1}{4}}$.

Through this equation, we can rewrite $\boldsymbol{C}$ as

$$\boldsymbol{C} = \boldsymbol{D}_Q^{1/2} \cdot \kappa\left(\frac{\boldsymbol{Q}}{p^{1/4}}, \frac{\boldsymbol{Q}}{p^{1/4}}\right) \cdot \boldsymbol{D}_Q^{1/2}, \tag{1}$$

where $\boldsymbol{D}_Q$ is a diagonal matrix with elements $(\boldsymbol{D}_Q)_{ii} = \frac{\|\boldsymbol{q}_i\|^2}{\sqrt{p}}, \forall i \in [n]$, and $\kappa(\boldsymbol{q}_i, \boldsymbol{q}_j) := \exp\left(-\|\boldsymbol{q}_i - \boldsymbol{q}_j\|^2/2\right)$ is the standard Gaussian kernel function.

We prove the lemma by using the fact that κ is a PSD kernel and $\kappa\left(\frac{\boldsymbol{Q}}{p^{1/4}}, \frac{\boldsymbol{Q}}{p^{1/4}}\right)$ is a PSD matrix. $\diamondsuit$

3.2 Nyström method

Due to the intrinsic low-rankness of an empirical kernel matrix $\boldsymbol{B}$, the so-called Nyström method that replaces $\boldsymbol{B}$ with its low-rank approximation $\tilde{\boldsymbol{B}}$, has been applied to accelerate kernel methods [Gittens and Mahoney, 2016, Kumar et al., 2009, Williams and Seeger, 2001]. Specially, the Nyström approximation of $\boldsymbol{B}$ is the matrix $\tilde{\boldsymbol{B}} = \boldsymbol{B}\boldsymbol{S}(\boldsymbol{S}^T\boldsymbol{B}\boldsymbol{S})^\dagger\boldsymbol{S}^T\boldsymbol{B}$, where $(\cdot)^\dagger$ denotes the Moore-Penrose pseudoinverse of a matrix, and $\boldsymbol{S} \in \mathbb{R}^{n\times d}$ is a zero-one sub-sampling matrix whose columns are a subset of the columns in $\boldsymbol{I}$, indicating which d observations have been selected. The formal definition of the uniform sub-sampling matrix is given as follows:

Definition 1 (Uniform sub-sampling matrix)**.** *For a random matrix $\boldsymbol{S} \in \mathbb{R}^{n\times d}$, if $\boldsymbol{S}$ has i.i.d. columns and the j-th column $\boldsymbol{S}^{(j)}$ can randomly be $\sqrt{\frac{1}{d}}\boldsymbol{e}_i$ with probability $\frac{1}{n}$, where $\boldsymbol{e}_i$ is the i-th column of the n-by-n identity matrix $\boldsymbol{I}_n$, then $\boldsymbol{S}$ is called a uniform sub-sampling.*

We close this subsection with a remark that it is not appropriate to directly extend the Nyström method from kernel method to self-attention due to a key requirement that $\boldsymbol{B}$ should be PSD with consideration of approximation performance improvement. We will show in the next section how to address this challenge and properly adapt Nyström method to non-PSD matrices.

3.3 Approximation evaluation

Beyond the time and space complexity, attention acceleration methods have been mostly evaluated with empirical experiment results, such as the perplexity of pretrained language models and the fine-tuned performance on downstream natural language understanding tasks. Specifically, Long Range Arena benchmark [Tay et al., 2020b] has been proposed to systematically evaluate the performance of efficient transformers with ten NLP tasks in long-context scenarios. However, such empirical results are indirect for theoretical analysis. Therefore, we introduce a common criterion used in matrix approximation, spectral norm, to ease the future discussion on performance.

Definition 2 (Spectral norm guarantee for matrix approximation (MA))**.** *Given a matrix $\boldsymbol{M} \in \mathbb{R}^{n_1\times n_2}$, two constants $\varepsilon > 0, \delta < \frac{1}{2}$, we say that its approximation matrix $\widetilde{\boldsymbol{M}} \in \mathbb{R}^{n_1\times n_2}$ satisfies (ε, δ)-MA property for $\boldsymbol{M}$, if*

$$\mathbb{P}\left\{\|\boldsymbol{M} - \widetilde{\boldsymbol{M}}\| > \varepsilon\|\boldsymbol{M}\|\right\} < \delta. \tag{2}$$

In previous works, the direct analysis of the approximation error to the entire output $\boldsymbol{D}^{-1}\boldsymbol{A}\boldsymbol{V}$ in the (ε, δ)-MA manner is usually spared due to the difficulty caused by the complex softmax structure. In this paper, with the new kernelized attention, we are allowed to perform the analysis through the existing theoretical results in kernel methods. Consequently, in Section 4.5 we are able to give a relatively precise error analysis on the approximation of Skyformer to the entire kernelized attention, which eases the future comparison with other methods approximating kernelized attention.

4 Method

4.1 Kernelized Attention

Kernelized Attention replaces the softmax structure in vanilla self-attention with a Gaussian kernel, and the new attention model is stated as:

$$\text{Kernelized-Attention}(\boldsymbol{Q}, \boldsymbol{K}, \boldsymbol{V}) = \boldsymbol{C}\boldsymbol{V} := \kappa\left(\frac{\boldsymbol{Q}}{p^{1/4}}, \frac{\boldsymbol{K}}{p^{1/4}}\right)\boldsymbol{V}, \tag{3}$$

where we define the n-by-n matrix $\boldsymbol{C}$ as the kernelized attention score matrix $\kappa(\boldsymbol{Q}/p^{1/4}, \boldsymbol{K}/p^{1/4})$.

The justification of using the kernelized attention model is as follows. A significant advantage of softmax attention is that tokens are allowed to attend to a limited number of other important tokens in the sequence. We observe that Gaussian kernel function can play a similar role. The expression of a Gaussian kernel is $\kappa(\boldsymbol{q}_i, \boldsymbol{k}_j) := \exp\left(-\|\boldsymbol{q}_i - \boldsymbol{k}_j\|^2/2\right)$. Via this expression, for token i in the query, Gaussian kernel assigns a large attention score to the token j when $\boldsymbol{k}_j$ is close to $\boldsymbol{q}_i$. The distance-based weight assignment is indeed considered as a major reason why kernel method is powerful. The form of Kernelized Attention also leads to an automatic normalization. Based on Equation (1), the new attention model can be rewritten in terms of the un-normalized attention score matrix $\boldsymbol{A}$ as

$$\text{Kernelized-Attention}(\boldsymbol{Q}, \boldsymbol{K}, \boldsymbol{V}) = \boldsymbol{D}_Q^{-1/2} \cdot \boldsymbol{A} \cdot \boldsymbol{D}_K^{-1/2},$$

where $\boldsymbol{D}_Q$ (resp. $\boldsymbol{D}_K$) is a diagonal matrix with elements $(\boldsymbol{D}_Q)_{ii} = \frac{\|\boldsymbol{q}_i\|^2}{\sqrt{p}}$ (resp. $(\boldsymbol{D}_K)_{ii} = \frac{\|\boldsymbol{k}_i\|^2}{\sqrt{p}}$), $\forall i \in [n]$. We remark the kernelized attention model can thus be formally taken as a variant of the original self-attention, which instead normalizes the matrix $\boldsymbol{A}$ in a form of $\boldsymbol{D}^{-1}\boldsymbol{A}$. Moreover, empirical evaluation in Section 5 supports our claim that the new attention model can attain a comparable performance to the original attention model.

4.2 Skyformer: a modified Nyström method

Before jumping into details of Skyformer, we first propose a method to apply Nyström method to approximate an asymmetric (and thus non-PSD) empirical kernel matrix $\boldsymbol{B}$ constructed with any PSD kernel $\phi(\cdot, \cdot)$. Specifically, with two different n-by-p design matrices $\boldsymbol{Q}$ and $\boldsymbol{K}$, its element b_{ij} from the i-th row and j-th column in $\boldsymbol{B}$ is equal to $\phi(\boldsymbol{q}_i, \boldsymbol{k}_j)$, where $\boldsymbol{q}_i$ (resp. $\boldsymbol{k}_j$) is the i-th (resp. j-th) row in $\boldsymbol{Q}$ (resp. $\boldsymbol{K}$). We remark this type of empirical kernel matrices involves the un-normalized attention score matrix $\boldsymbol{A} := \mathrm{SM}(\boldsymbol{Q}, \boldsymbol{K})$, and the empirical Gaussian kernel matrix $\boldsymbol{C} := \kappa(\boldsymbol{Q}/p^{1/4}, \boldsymbol{K}/p^{1/4})$. Therefore this method leads to a low-rank approximation to the output of either self-attention $\boldsymbol{D}^{-1}\boldsymbol{A}\boldsymbol{V}$ or Kernelized Attention $\boldsymbol{C}\boldsymbol{V}$. ($\boldsymbol{D}$ in self-attention can be obtained by computing $\boldsymbol{A} \cdot \mathbf{1}$, and thus a low-rank approximation to $\boldsymbol{A}$ also implies an approximation to $\boldsymbol{D}$.)

Figure 1 shows our proposed method. Computational details are stated as follows. To tackle the challenge of approximating a non-PSD matrix $\boldsymbol{B}$, our first step is to complete the matrix into a PSD matrix $\bar{\boldsymbol{B}}$:

$$\bar{\boldsymbol{B}} := \phi\left(\begin{pmatrix}\boldsymbol{Q}\\ \boldsymbol{K}\end{pmatrix}, \begin{pmatrix}\boldsymbol{Q}\\ \boldsymbol{K}\end{pmatrix}\right). \tag{4}$$

Then we approximate $\bar{\boldsymbol{B}}$ with $\tilde{\bar{\boldsymbol{B}}}$ through

$$\tilde{\bar{\boldsymbol{B}}} = \bar{\boldsymbol{B}}\boldsymbol{S}(\boldsymbol{S}^T\bar{\boldsymbol{B}}\mathbf{S})^{\dagger}\mathbf{S}^T\bar{\boldsymbol{B}}, \tag{5}$$

where $\boldsymbol{S}$ is a $2n$-by-d uniform sub-sampling matrix as defined in Definition 1. The final approximation will be given as

$$\tilde{\boldsymbol{B}} := (\boldsymbol{I}, \mathbf{0})\tilde{\bar{\boldsymbol{B}}}(\mathbf{0}, \boldsymbol{I})^T. \tag{6}$$

The original matrix $\boldsymbol{B}$ can be well-approximated by $\tilde{\boldsymbol{B}}$ due to the following inequality

$$\|\boldsymbol{B} - \tilde{\boldsymbol{B}}\| = \|(\boldsymbol{I}, \mathbf{0})(\bar{\boldsymbol{B}} - \tilde{\bar{\boldsymbol{B}}})(\mathbf{0}, \boldsymbol{I})^T\| \leq \|\bar{\boldsymbol{B}} - \tilde{\bar{\boldsymbol{B}}}\|,$$

and thus we show our task of approximating the non-PSD matrix $\boldsymbol{B}$ boils down to well approximating the PSD matrix $\bar{\boldsymbol{B}}$.

Remark. The reason why $\boldsymbol{B}$ can be well approximated by a low-rank $\tilde{B}$ is that as an empirical kernel matrix the eigenvalues in $\bar{\boldsymbol{B}}$ usually decay fast, and thus there are many small eigenvalues in the long tail. In this case, theoretically a low-rank matrix (e.g. truncated singular value decomposition (SVD) of $\bar{\boldsymbol{B}}$) has enough potential to well approximate the original matrix $\bar{\boldsymbol{B}}$ (and $\boldsymbol{B}$ accordingly) in terms of spectral norm.

With the derivation above, we officially introduce our proposed Skyformer. As an approximation to Kernelized Attention, Skyformer simply applies the modified Nyström method to the kernelized attention score matrix $\boldsymbol{C}$. The next two subsections will continue our discussion on it, and respectively state the theoretical analysis of its approximation error and some details of its implementation in practice.

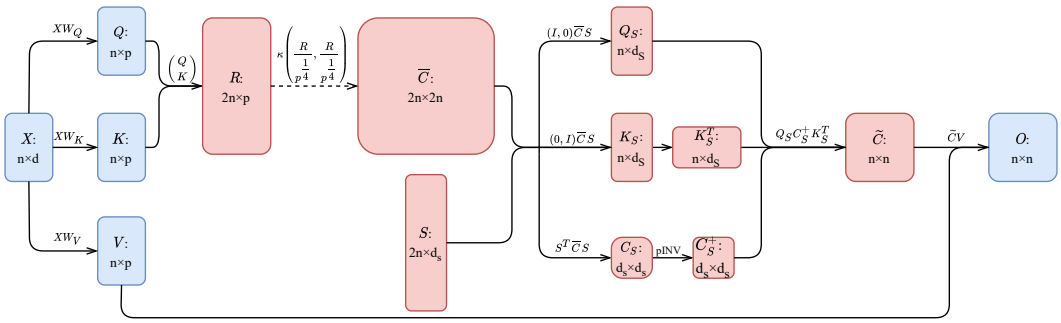

Figure 1: An overview of the proposed attention approximation method. This method approximates the original softmax matrix with a low dimensional randomized sketch of the complete symmetric matrix. Each box represents a matrix with the box size representing matrix size. The red boxes are matrices introduced by the proposed method besides the vanilla self-attention matrices in blue boxes. The dash line means that during computation, instead of the full $\bar{\boldsymbol{C}}$ we only compute the selected columns of $\bar{\boldsymbol{A}}$ with a sampling matrix $\boldsymbol{S}$.

4.3 Error analysis of Skyformer

As mentioned, an implicit advantage of using Kernelized Attention is that we can leverage the existing conclusions for kernel methods to analyze the theoretical properties of the model. In this subsection we aim to provide some theoretical analysis of its approximation error.

We state a high probability bound on the size d of the sub-sampling matrix used in Skyformer to attain (ε, δ)-MA property for the kernelized attention score matrix $\boldsymbol{C}$ by the following theorem. We refer the readers to the proof in Appendix D to take a closer look at our claim that the matrix to be approximated should be PSD is a key to the theoretical guarantee of Nyström method.

Theorem 2 (Adapted from Lemma 9 and Theorem 3 [Musco and Musco, 2017])**.** *Consider the query, key, and value matrix $\boldsymbol{Q}, \boldsymbol{K}, \boldsymbol{V} \in \mathbb{R}^{n\times p}$ and two positive constants $\varepsilon < 1, \delta < \frac{1}{2}$. Let $\lambda := \varepsilon\|\boldsymbol{C}\| < \|\bar{\boldsymbol{C}}\|$, where $\bar{\boldsymbol{C}}$ is constructed as substituting the Gaussian kernel with bandwidth $p^{1/4}$ for the arbitrary kernel function ϕ in Equation (4). To ease the analysis, we specifically define the i-th diagonal element of $\bar{\boldsymbol{C}}(\bar{\boldsymbol{C}} + \lambda \boldsymbol{I}_{2n})^{-1}$ as leverage score $\ell_i, \forall i = 1, \ldots, 2n$, and define their sum $\mathrm{Tr}\left(\bar{\boldsymbol{C}}(\bar{\boldsymbol{C}} + \lambda \boldsymbol{I})^{-1}\right)$ as the statistical dimension d_{stat}. Suppose $\boldsymbol{S}$ is a uniform sub-sampling matrix, and assume there exists a constant $\beta \in (0, 1]$ such that $\beta \leq \frac{d_{stat}}{2n\ell_i}, \forall i = 1, \ldots, 2n$. For the approximation matrix $\tilde{\bar{\boldsymbol{C}}}$ constructed with $\bar{\boldsymbol{C}}, \boldsymbol{S}$ as in Equation (5), there exists a constant C such that if*

$$d \geq C\frac{d_{stat}}{\beta}\log\frac{n}{\delta}$$

then $\tilde{\bar{\boldsymbol{C}}} \preccurlyeq \bar{\boldsymbol{C}} \preccurlyeq \tilde{\bar{\boldsymbol{C}}} + \lambda \boldsymbol{I}$ with probability $1 - \delta$. Here $\preccurlyeq$ denotes the Loewner ordering: $\boldsymbol{B} \preccurlyeq \boldsymbol{A}$ means $\boldsymbol{A} - \boldsymbol{B}$ is positive semidefinite. Furthermore, for our approximation $\tilde{\boldsymbol{C}}$ in Equation (6) to the kernelized attention score $\boldsymbol{C}$, we have

$$\|\tilde{\boldsymbol{C}} - \boldsymbol{C}\| \leq \lambda = \varepsilon\|\boldsymbol{C}\|.$$

This theorem implies the time and space complexity of our proposed approximation depends on the statistical dimension d_{stat}. If we directly use the conclusion from Gaussian kernels, d_{stat} should be $\tilde{\mathcal{O}}(1)$ (complexity modulo poly-log term) [Yang et al., 2017] due to the exponential eigenvalue decay rate of Gaussian kernels, which is comparable to the complexity of most other efficient transformers. However, different than the case in the classical kernel methods, the distribution of the query and key matrix $\boldsymbol{Q}$ and $\boldsymbol{K}$ varies during the training procedure, which may invalidate the conclusion about d_{stat}. Therefore we leave the exact non-asymptotic analysis of the computational complexity for future work.

4.4 Implementation details

A potential limitation with the implementation of the proposed method lies in the tricky fact that the matrix inversion on GPU is much slower and numerically less stable than the same operation on CPU due to the different back-end libraries in the two platforms. We attempt to circumvent the problem by adapting the strategy in Nyströmformer [Xiong et al., 2021] to our setting. Specifically, we use the matrix-product-based iterative method [Razavi et al.] for finding approximate inverses, instead of some division-based methods (such as the conjugate gradient method) which induces some instability in model training.

To apply the iterative method and inverse matrix $\boldsymbol{M} = \boldsymbol{S}^T\bar{\boldsymbol{C}}\mathbf{S}$, we need to satisfy its assumption [Razavi et al., Theorem 2] that $\|\boldsymbol{I} - \boldsymbol{M}\| < 1$. In practice, we instead pass the matrix $\boldsymbol{D}_M^{-1/2}(\boldsymbol{M} + \gamma\boldsymbol{I})\boldsymbol{D}_M^{-1/2}$ as an input to the iterative method, where $\gamma > 0$ is a small constant and the diagonal matrix $\boldsymbol{D}_M$ is defined as $\mathrm{diag}(\boldsymbol{M} + \gamma\boldsymbol{I})\mathbf{1}$. We give the following lemma to justify our practical usage of the method. The proof is deferred to Appendix E.

Lemma 3. *Given a constant $\gamma > 0$, if matrices $\boldsymbol{M}$ is constructed as $\boldsymbol{S}^T\bar{\boldsymbol{C}}\boldsymbol{S}$, and $\boldsymbol{D}_M$ are defined as above, then all the singular values of $\boldsymbol{D}_M^{-1/2}(\boldsymbol{M} + \gamma\boldsymbol{I})\boldsymbol{D}_M^{-1/2}$ are within $(0, 1)$, which implies that $\|\boldsymbol{I} - \boldsymbol{D}_M^{-1/2}(\boldsymbol{M} + \gamma\boldsymbol{I})\boldsymbol{D}_M^{-1/2}\| < 1$.*

4.5 Empirical approximation evaluation

Spectral norm, the maximum singular value of a matrix, is a computation-light indicator of matrix approximation performance. In this work we compare the spectral norm of the difference between the outputs from attention functions and the output from vanilla self-attention with the same input.

We use the initialized and pretrained bert-base-cased models from Huggingface's implementation [Wolf et al., 2019] . The input vector X is embedded from the tokenized raw text in Wikitext-2 dataset [Merity et al., 2017]. The query, key and value weight matrices in initialized or pretrained models transform input X into Q, K, V of different distributions. We compare the results with different sequence lengths and different number of features used in attention approximation methods. We set the number of features in the range of 2^4 to 2^8. More features usually require more computation resources.

Figure 2 shows the performance of the modified Nyström method on approximation error with regards to the number of features. We conclude that for Skyformer the approximation is significantly better with the increased number of features, while for other methods the gain is not obvious. The good performance of the modified Nyström method also validates our previous claim that the Nyström method is currently one of the most powerful methods in large-scale kernel machines acceleration.

5 Experimental Results

Tasks and Datasets. We evaluate the proposed methods on four classification tasks on LRA benchmark [Tay et al., 2020b], which focuses on model quality under long-context scenarios: ListOps [Nangia and Bowman, 2018], Text Classification on IMDb review dataset [Maas et al., 2011], Document Retrieval on AAN dataset [Radev et al., 2013], and Pathfinder [Linsley et al., 2018]. The LRA benchmark covers diverse long-sequence tasks in sequence length, task difficulty and inspecting model abilities. For example, ListOps and Pathfinder evaluate the abilities to capture the long-range hierarchical dependency and spatial dependency, respectively, which places challenges for sparse attention pattern based methods. We report the classification accuracy on test set, training time, and peak memory usage during training for each task.

Baselines. Aside from the vanilla quadratic self-attention, we compare with Big Bird [Zaheer et al., 2020], Performer [Choromanski et al., 2020], Linformer [Wang et al., 2020], Nyströmformer [Xiong et al., 2021], Informer [Zhou et al., 2020], and Reformer [Kitaev et al., 2020]. Most methods are approximating the full attention for efficiency and thus are not expected to have better performance. As it is not realistic to exhaustively fine-tune all models and search for the best performance under limited computation resources, we instead only replace the self-attention module with the various attention methods and keep other experimental setting the same for fair comparisons.

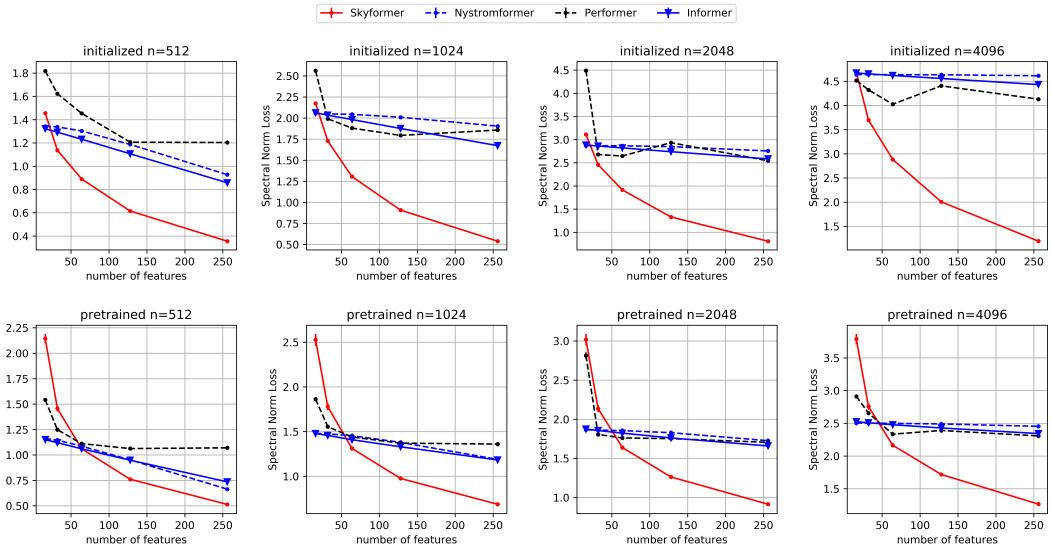

Figure 2: Spectral norm results with different sequence lengths under different W_Q, W_K, W_V settings, either from initialized or pretrained BERT models. Y axis: Lower spectral loss means better approximation. X axis: Higher d (number of features) means visiting more elements in the original matrix and bringing more computation costs.

Implementation Details. We conduct experiments on one Tesla V100 SXM2 16GB. We use the LRA evaluation benchmark reimplemented in PyTorch by Xiong et al. [2021]. We use a 2-layer transformer model with 64 embedding dimension, 128 hidden dimension, 2 attention heads and mean pooling for classification. Batch size is selected conditioned on the memory requirements of standard self-attention method, which leads to 16 for Text Classification, 32 for ListOps, 16 for Document Retrieval, and 128 for Pathfinder. Learning rate is set to $1e-4$ for Text Classification and ListOps, and $2e-4$ for Retrieval and Pathfinder. Each model on each task is trained for $50k$ steps, during which the best checkpoint with highest accuracy on development set will be saved for evaluation. For comparable computation complexity, we control the number of features to be 128 used in all methods (except Big Bird), under which setting the models will visit $128 \cdot n$ elements in the attention matrix. For numerical consistency, all experiment results are averaged across three runs with different random seeds.

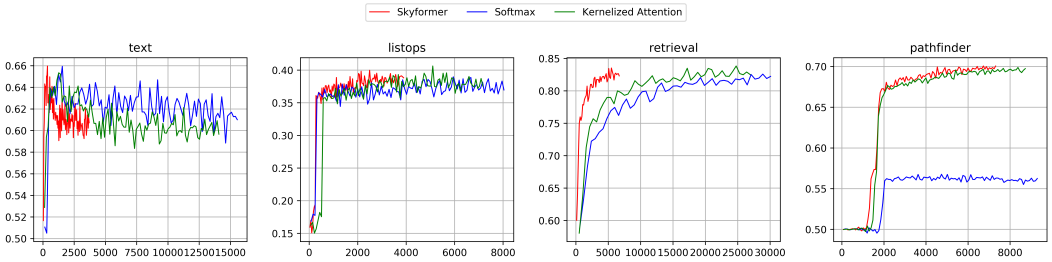

Figure 3: Validation accuracy changes with respect to training time for $50k$ steps.

Results. The training process of the standard softmax-based method is unstable as observed in Figure 3: it takes more steps to reach the stationary distribution of long-time limit, and it is more easily getting stuck in local minimum. Runs with different random seeds may bring much divergent performances, and thus leads to lower averaged scores. We have also tried directly approximating the self-attention method with the Nyström method and observed numerical instability during training.

Replacing the softmax structure with Gaussian kernel somehow alleviates this instability problem with boosted performance as shown in Table 1. However, the time and space requirement of Kernelized

Table 1: Classification accuracy (%) on LRA benchmark.

Model	Text	ListOps	Retrieval	Pathfinder	AVG.
Self-Attention [Vaswani et al., 2017]	61.95	38.37	80.69	65.26	61.57
Kernelized Attention	60.22	38.78	81.77	**70.73**	62.87
Nystromformer [Xiong et al., 2021]	**64.83**	38.51	80.52	69.48	63.34
Linformer [Wang et al., 2020]	58.93	37.45	78.19	60.93	58.88
Informer [Zhou et al., 2020]	62.64	32.53	77.57	57.83	57.64
Performer [Choromanski et al., 2020]	64.19	38.02	80.04	66.30	62.14
Reformer [Kitaev et al., 2020]	62.93	37.68	78.99	66.49	61.52
BigBird [Zaheer et al., 2020]	63.86	**39.25**	80.28	68.72	63.03
Skyformer	64.70	38.69	**82.06**	**70.73**	**64.05**

Table 2: Running time (hour) and peak memory usage (GB). **TC**: Text Classification. **LO**: ListOps. **RE**: Retrieval. **PF**: Pathfinder.

Model	Time (h)				Memory (GB)			
	TC	LO	RE	PF	TC	LO	RE	PF
Self-Attention [Vaswani et al., 2017]	4.3	2.2	8.3	2.6	10.4	5.4	10.8	5.7
Kernelized Attention	3.9	2.0	7.5	2.4	5.7	5.9	10.5	6.4
Nystromformer [Xiong et al., 2021]	0.7	0.7	1.3	1.5	1.2	1.4	2.4	3.4
Linformer [Wang et al., 2020]	0.7	0.6	1.1	1.1	1.0	1.0	1.9	2.0
Informer [Zhou et al., 2020]	1.6	1.2	2.9	2.4	5.1	4.9	5.8	4.8
Performer [Choromanski et al., 2020]	0.8	0.7	1.4	1.4	1.1	1.1	2.2	2.2
Reformer [Kitaev et al., 2020]	0.9	0.9	1.7	1.7	1.6	1.6	3.0	3.2
BigBird [Zaheer et al., 2020]	2.0	1.9	3.8	3.4	2.8	2.7	5.0	5.0
Skyformer	1.0	1.3	1.9	2.0	1.6	1.7	3.2	4.1

Self-Attention is not significantly improved compared to the original version, which serves as the motivation to approximate Kernelized Self-Attention with Nyström method.

Though not necessarily the fastest, our proposed Skyformer can efficiently converge to the long-time limit with comparable general performance in classification accuracy (Table 1) and resource consumption (Table 2). The advantages over the standard self-attention is significant: consistently less training time and generally better performance. For example, Skyformer brings nearly 4 times speed-up on text classification and document retrieval while with 2.75% and 1.37% accuracy improvement over the standard self-attention.

6 Conclusions and future work

Motivated by the connection between kernel methods and self-attention, we introduce Kernelized Attention that replace the softmax structure in self-attention with a Gaussian kernel. We also propose Skyformer that adapts the Nyström method to Kernelized Attention to improve its efficiency. We expect the new model can enjoy more stable training while inheriting the strong performance from self-attention. Extensive experiments verify our intuitions and show that both Kernelized Attention and its Nyström approximation variant have comparable accuracy to the original Transformer on the LRA benchmark.

A direct development of this work is the incorporation of further computation tricks in kernel methods, such as the local and global approximation for gram matrix [Snelson and Ghahramani, 2007] and the importance sampling in Nyström methods [Musco and Musco, 2017]. Other related questions include the choice of the kernel other than the Gaussian kernel in our kernelized attention model. It is expected that for different tasks there will be specific kernels more proper than the commonly used Gaussian kernels. The results in this work also shed new light on the design of the attention mechanism, which may benefit board downstream NLP tasks.

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Checklist

1. For all authors...
   (a) Do the main claims made in the abstract and introduction accurately reflect the paper's contributions and scope? [Yes]
   (b) Did you describe the limitations of your work? [Yes] In section 4.4
   (c) Did you discuss any potential negative societal impacts of your work? [No]
   (d) Have you read the ethics review guidelines and ensured that your paper conforms to them? [Yes]
2. If you are including theoretical results...
   (a) Did you state the full set of assumptions of all theoretical results? [N/A]
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3. If you ran experiments...
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   (c) Did you report error bars (e.g., with respect to the random seed after running experiments multiple times)? [Yes] Error bar is plotted in Figure 2
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   (d) Did you discuss whether and how consent was obtained from people whose data you're using/curating? [Yes] In README of code.
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5. If you used crowdsourcing or conducted research with human subjects...
   (a) Did you include the full text of instructions given to participants and screenshots, if applicable? [N/A]
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