Masked Language Modeling for Proteins via Linearly Scalable Long-Context Transformers

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Abstract
Transformer models have achieved state-of-the-art results across a diverse range of domains. However, concern over the cost of training the attention mechanism to learn complex dependencies between distant inputs continues to grow. In response, solutions that exploit the structure and sparsity of the learned attention matrix have blossomed. However, real-world applications that involve long sequences, such as biological sequence analysis, may fall short of meeting these assumptions, precluding exploration of these models. To address this challenge, we present a new Transformer architecture, Performer, based on Fast Attention Via Orthogonal Random features (FAVOR). Our mechanism scales linearly rather than quadratically in the number of tokens in the sequence, is characterized by sub-quadratic space complexity and does not incorporate any sparsity pattern priors. Furthermore, it provides strong theoretical guarantees: unbiased estimation of the attention matrix and uniform convergence. It is also backwards-compatible with pre-trained regular Transformers. We demonstrate its effectiveness on the challenging task of protein sequence modeling and provide detailed theoretical analysis.

1 Introduction and related work
Transformers [44,17] are powerful neural network architectures that have become SOTA in several areas of machine learning including Natural Language Processing (NLP) (e.g. speech recognition [32]), Neural Machine Translation (NMT) [6], document generation/summarization, time series prediction, generative modeling (e.g. image generation [56]), music generation [26], and analysis of biological sequences [39,33,30]. Transformers rely on a trainable attention mechanism that specifies complex dependencies between the elements of each input sequence (e.g. amino acids within a protein). Unfortunately, a standard Transformer scales quadratically with the number of tokens $L$ in the input sequence, which is prohibitively expensive for large $L$. Several solutions have been proposed to address this issue [1,23,5,7]. Most approaches restrict the attention mechanism to attend to local neighborhoods [56] or incorporate structural priors on attention such as sparsity [7], pooling-based compression [37] clustering/binning/convolution techniques (e.g. [41] which applies $k$-means clustering to learn dynamic sparse attention regions, or [28], where locality sensitive hashing is used to group together tokens of similar embeddings), sliding windows [1], or truncated targeting [4]. Thus these approaches do not aim to approximate regular attention, but rather propose simpler and more tractable attention mechanisms, often by incorporating additional constraints (e.g. identical query and key sets as in [28]), or by trading regular attention with sparse attention using more layers [7]. Furthermore, many of these works require special customized GPU operations (e.g. either writing C++ CUDA kernels [2] or using TVMs [1]). Other techniques which aim to improve the

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We show that regular attention can be considered a special case of a much larger class of kernel-driven methods with a wide variety of uses in computer vision [22], reinforcement learning [52], and even combinatorial optimization [46]. We demonstrate its effectiveness on the challenging task of protein modeling.

Orthogonal Random features works employing simpler statistical models that predict protein quaternary structure, protein-protein interactions, and protein interaction networks from evolutionary sequence data [47, 25, 35, 2, 13].

All proofs are given in full in the Appendix.

## 2 Generalized Attention via FAVOR mechanism

Below we describe in detail our FAVOR mechanism which is the backbone of our Performer architecture. We also present a general class of kernel-based attentions, called Generalized Attention (GA) (which includes regular attention as a special case), where FAVOR can be applied.
2.1 Preliminaries - standard attention mechanism

Let \( L \) be the size of an input sequence of tokens. Then regular dot-product attention \([44]\) is a mapping which accepts matrices \( Q, K, V \in \mathbb{R}^{L \times d} \) as input where \( d \) is the hidden dimension (dimension of the latent representation). Matrices \( Q, K, V \) are intermediate representations of the input and their rows can be interpreted as queries, keys and values of the continuous dictionary data structure respectively. Bidirectional (or non-directional \([18]\) dot-product attention has the following form:

\[
\text{Att}_{\rightarrow}(Q, K, V) = D^{-1}AV, \quad A = \exp(QK^\top / \sqrt{d}), \quad D = \text{diag}(A1_L),
\]

where \( \exp(\cdot) \) is applied elementwise, \( 1_L \) is the all-ones vector of length \( L \), and \( \text{diag}(\cdot) \) is a diagonal matrix with the input vector as the diagonal. The runtime complexity of computing \([1]\) is \( O(L^2d) \) because the attention matrix \( A \in \mathbb{R}^{L \times L} \) has to be computed and stored explicitly. Hence, in principle, dot-product attention of type \([1]\) is incompatible with end-to-end processing of long sequences.

Another important type of attention is unidirectional dot-product attention which has the form:

\[
\text{Att}_{\rightarrow}(Q, K, V) = \tilde{D}^{-1}\tilde{A}V, \quad \tilde{A} = \text{tril}(A), \quad \tilde{D} = \text{diag}(\tilde{A}1_L),
\]

where \( \text{tril}(\cdot) \) returns the lower-triangular part of the argument matrix including diagonal. As discussed in \([44]\), unidirectional attention is used for autoregressive generative modelling with Transformers when the output sequence \( o_1, \ldots, o_L \) is modelled as:

\[
p(o_1, \ldots, o_L) = p(o_1)p(o_2|o_1) \ldots p(o_L|o_1, \ldots, o_{L-1}).
\]

Therefore, the probability distribution over \( o_i \) can only depend on embeddings of tokens \( o_1, \ldots, o_{i-1} \). Unidirectional attention is used as self-attention in generative Transformers as well as the decoder part of Seq2Seq Transformers \([44]\), while bidirectional attention is used in encoder self-attention and encoder-decoder attention in Seq2Seq architectures.

A line of work relies on sparse approximation of the matrix \( A \) – either through restricting the sparsity pattern of \( A \) \([17]\) or learning it using Locality-Sensitive Hashing (LSH) techniques \([28]\). The latter results in \( O(Ld^2 \log L) \) runtime complexity. We will show that, without any structural assumptions, the matrix \( A \) can be approximated up to any precision in time \( O(Ld^2 \log(d)) \).

2.2 Generalized Attention (GA)

The idea of the attention mechanism is simple. New representations of tokens are obtained from previous ones by taking convex combinations of different value vectors with coefficients of the convex combinations interpreted as renormalized (i.e. all coefficients sum up to one) similarity measures between different tokens. High similarities imply strong attendance to the corresponding tokens. These similarity measures \( \text{sim} : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \) are simple ad-hoc “soft-max style” functions of a dot-product between query \( Q_i \) of token \( i \) and key \( K_j \) of token \( j \), namely:

\[
\text{sim}(o_i, o_j) = \exp\left(\frac{Q_i K_j^\top}{\sqrt{d}}\right),
\]

where: \( Q_i^\top, K_j^\top \in \mathbb{R}^d \). Note that \( \text{sim} \) is not a commutative operation here, and the \( \sqrt{d} \)-renormalizer is a technical modification to stabilize the range of \( \text{sim} \) and avoid very small/large values.

However, what if we use kernels instead of arbitrary similarity measures? Specifically, \( Q_i \) and \( K_j \) are entangled through a valid kernel function, by defining the attention matrix \( A \) as:

\[
A = A_{g,h}^K = [g(Q_i^\top)K(Q_j^\top, K_j^\top)h(K_j^\top)]_{i,j \in \{1, \ldots, L\}},
\]

where \( K : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R} \) is an arbitrary kernel function and \( g, h : \mathbb{R}^d \rightarrow \mathbb{R} \). We call this attention mechanism defined above Generalized Attention (GA) parameterized by \( K, g, h \).

Next we show that not only can FAVOR approximate regular attention governed by Eq. \([3]\) but it can be applied to GAs as long as the corresponding kernels can be effectively estimated via a random feature map mechanism \([38]\), which is the case for most kernels used in practice. We will in fact show that regular attention is a special case of GA for a specific choice of \( g, h \), and Gaussian kernel \( K \).

2.3 Towards FAVOR: approximating attention with random features (RFs)

Instead of computing and storing the attention matrix \( A \in \mathbb{R}^{L \times L} \) explicitly, we derive its unbiased stochastic approximation, which benefits from low-rank structure. We take our inspiration from a randomized scheme to train kernel Support Vector Machines with large training data \([38]\).
Let $Q_i$ and $K_i$ denote the $i$-th rows of matrices $Q$ and $K$ respectively. For regular attention, the $i, j$-th element of $A$ can be expressed as:

$$A_{i,j} = \exp(Q_i^T K_j^T) = \exp(\|Q_i\|^2 / 2\sqrt{d}) \cdot \exp(-\frac{\|Q_i - K_j\|^2}{\sigma^2} / 2\sqrt{d}) \cdot \exp(\|K_j\|^2 / 2\sqrt{d}).$$

In other words, for $r = 2\sqrt{d}$, the attention matrix $A$ can be decomposed as:

$$A = D_QBD_K,$$

where $D \in \mathbb{R}^{L \times L}, q, j : B_{i,j} = \exp(-\|Q_i - K_j\|^2 / r)$.

$$D_T = \text{diag} \left( \exp(\|T_1\|^2 / r), \ldots, \exp(\|T_L\|^2 / r) \right),$$

for $T = Q, K$. Both $D_Q$ and $D_K$ can be computed in $O(Ld)$ time. Note that the $i, j$-th element of matrix $B$ is the value of the Gaussian kernel with $\sigma = \frac{d}{r}$:

$$B_{i,j} = K_{gauss}(Q_i^T, K_j^T) = \exp(-\frac{\|Q_i - K_j\|^2}{2\sigma^2}).$$

For GA, our analysis is similar. This time $D_Q, D_K$ have nonzero entries of the form $g(Q_i^T)$ and $h(K_j^T)$ (for regular attention we have: $g(x) = h(x) = \exp(\frac{\|x\|^2}{\sigma^2})$ respectively and furthermore the Gaussian kernel is replaced by a general kernel $K$, namely: $B_{i,j} = K(Q_i^T, K_j^T)$, as in Equation 3.

In the reminder of this section we will derive an unbiased stochastic approximation of matrix $B$ based on low-rank decomposition of $B$ with the use of random feature maps [38].

For a given kernel $K : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}$, the random feature $[RF]$ map $\phi_K : \mathbb{R}^d \to \mathbb{R}^M$ corresponding to $K$ is a probabilistic embedding satisfying

$$K(x, y) = \mathbb{E}[(\phi(x))^T \phi(y)],$$

where the expectation is with respect to the randomness of $\phi$, and $M$ denotes the number of random features (if $\mathbb{E}[(\phi(x))^T \phi(y)]$ only approximates $K(x, y)$ then we refer to the mechanism as an approximate random feature map). Efficient-to-compute random feature maps exist for virtually all classes of kernels used in machine learning, e.g., shift-invariant kernels [38], the pointwise nonlinear Gaussian kernel related to neural networks [24], and more, though the techniques used to derive these random mappings vary from class to class [12]. Even more interestingly, for most of these kernels, corresponding random feature maps have a similar structure, namely:

$$\phi(x) \overset{\text{def}}{=} \frac{c}{\sqrt{M}}(f(\omega_1^T x + b_1), \ldots, f(\omega_M^T x + b_M))^T = \frac{c}{\sqrt{M}} f(Wx + b)^T, $$

for some $f : \mathbb{R} \to \mathbb{R}$, $\omega_1, \ldots, \omega_M \overset{iid}{\sim} \Omega, b_1, \ldots, b_M \overset{iid}{\sim} \mathcal{B}$, distributions: $\Omega \in \mathcal{P}(\mathbb{R}^d), \mathcal{B} \in \mathcal{P}(\mathbb{R})$ and constant $c > 0$. Here $W \in \mathbb{R}^{M \times d}$ has rows $W_i = \omega_i^T$ and $b \overset{\text{def}}{=} (b_1, \ldots, b_M)^T$.

In particular, for the Gaussian kernel, we have $c = \sqrt{2}$ and:

$$\phi(x) \overset{\text{def}}{=} \sqrt{\frac{2}{M}}(\cos(\omega_1^T x + b_1), \ldots, \cos(\omega_M^T x + b_M))^T, $$

where $\omega_1, \ldots, \omega_M \overset{iid}{\sim} \mathcal{N}(0, \sigma^2 I_d)$ and $b_1, \ldots, b_M \overset{iid}{\sim} \text{Unif}(0, 2\pi)$. This particular form of $\phi$ is a consequence of the celebrated Bochner’s Theorem [38]. We now define $\tilde{Q}$ and $\tilde{K} \in \mathbb{R}^{L \times M}$ as:

$$\tilde{Q} = \frac{c}{\sqrt{M}} f(WQ^T + b)^T, \quad \tilde{K} = \frac{c}{\sqrt{M}} f(WK^T + b)^T. $$

Note that we have: $\tilde{Q}_i = \phi(Q_i^T)^T$ and $\tilde{K}_i = \phi(K_i^T)^T$, where $\tilde{Q}_i$ and $\tilde{K}_i$ stand for the $i$th row of $\tilde{Q}$ and $\tilde{K}$ respectively. Then according to Equation 6, we have: $B \approx \mathbb{E}[\tilde{Q}\tilde{K}]$. Thus with $Q', K'$ given as: $Q' = D_Q\tilde{Q}, K' = D_K\tilde{K}$, we obtain:

$$A \approx \mathbb{E}[Q'(K')^T].$$

We conclude that the attention matrix $A$ can be approximated without bias as: $\hat{A} = Q'(K')^T$. We will leverage this unbiased approximate low-rank (if $M \ll L$) decomposition of $A$ in our algorithm, even though we will not explicitly compute $\hat{A}$.
We are ready to present the full FA VOR algorithm. In the bidirectional case, our approximate attention

where

we show in Secs. 3 and 4 that they do indeed lead to more accurate approximations and substantially

better downstream results. Below we briefly review the most efficient ORF mechanisms (based on

their strengths and costs) that we will use in Sec. 2.6 in the analysis of FA VOR.

2.5 FA VOR: Fast Attention via Orthogonal Random Features

For isotropic $\Omega$ (true for most practical applications, including regular attention), instead of sampling

$\omega_i$ independently, we can use orthogonal random features (ORF) [51][12][11]: these maintain (exactly

or approximately) the marginal distributions of samples $\omega_i$ while enforcing that different samples are

orthogonal. If we need $M > d$, ORFs still can be used locally within each $d \times d$ block of $W$ [51].

ORFs were introduced to reduce the variance of Monte Carlo estimators [51][12][11][9][40][8][10] and

we show in Secs. 3 and 4 that they do indeed lead to more accurate approximations and substantially

better downstream results. Below we briefly review the most efficient ORF mechanisms (based on

their strengths and costs) that we will use in Sec. 2.6 in the analysis of FAVOR.

(1) Regular ORFs [R-ORFs]: Applies Gaussian orthogonal matrices [51]. Encodes matrix $W$ in

$O(Md)$ space. Provides algorithm for computing $Wx$ in $O(Md)$ time for any $x \in \mathbb{R}^d$. Gives

unbiased estimation. Requires one-time $O(Md^2)$ preprocessing (Gram-Schmidt orthogonalization).

(2) Hadamard/Givens ORFs [H/G-ORFs]: Applies random Hadamard [12]/Givens matrices [10].

Encodes matrix $W$ in $O(M)/O(M \log(d))$ space. Provides algorithm for computing $Wx$ in

$O(M \log(d))$ time for any $x \in \mathbb{R}^d$. Gives small bias (going to 0 with $d \to \infty$).

2.5 FAVOR: Fast Attention via Orthogonal Random Features

We are ready to present the full FAVOR algorithm. In the bidirectional case, our approximate attention

computed by FAVOR is given as:

$$\hat{\text{Att}}_{\leftrightarrow}(Q, K, V) = \hat{D}^{-1}\hat{A}V = \hat{D}^{-1}(Q'(\hat{K}')^T V),$$

(13)

where $\hat{D} = \text{diag}(Q'(\hat{K}')^T 1_L))$. The placement of brackets determines the order in which computations are conducted. Note that we never explicitly compute $\hat{A}$ and consequently, avoid $\Theta(L^2)$ time complexity and storing the $L \times L$ approximate attention matrix (see: Sec. 2.6 for rigorous analysis).

2.5.1 Prefix-sums for unidirectional FAVOR

For the unidirectional case, our analysis is similar but this time our goal is to compute

$\text{tril}(Q'(\hat{K}')^T)C$ without constructing and storing the $L \times L$-sized matrix $\text{tril}(Q'(\hat{K}')^T)$ explicitly, where $C = [V \ 1_L] \in \mathbb{R}^{L \times (d+1)}$. In order to do so, observe that $\forall 1 \leq i \leq L$:

$$[\text{tril}(Q'(\hat{K}')^T)C]_i = G^\text{PS}_{i,:} \times Q'_i, \quad G^\text{PS}_{i,:} = \sum_{j=1}^i G_{j,:}, \quad G_{j,:} = K'_j C^T_j \in \mathbb{R}^{M \times (d+1)},$$

(14)

where $G, G^\text{PS} \in \mathbb{R}^{L \times M \times (d+1)}$ are 3d-tensors. Each slice $G^\text{PS}_{i,:}$ is therefore a result of a prefix-sum (or cumulative-sum) operation applied to $G_{i,:}$. $G^\text{PS}_{i,:} = \sum_{j=1}^i G_{j,:}$. An efficient algorithm to compute the prefix-sum of $L$ elements takes $O(L)$ total steps and $O(\log L)$ time when computed in parallel [29][15]. See Algorithm 1 for the whole approach.

**Algorithm 1: FAVOR (bidirectional or unidirectional).**

**Input:** $Q, K, V \in \mathbb{R}^{L \times d}$, isBidirectional - binary flag.

**Result:** $\hat{\text{Att}}_{\leftrightarrow}(Q, K, V) \in \mathbb{R}^{L \times L}$ if isBidirectional, $\hat{\text{Att}}_{\rightarrow}(Q, K, V) \in \mathbb{R}^{L \times L}$ otherwise.

Compute $D_Q, D_K$ as explained in Sec. 2.3.

Compute $Q, K$ according to [11] and take $Q' := D_Q Q, \quad K' := D_K K, \quad C := [V \ 1_L]$;

if isBidirectional then

Compute $G$ and its prefix-sum tensor $G^\text{PS}$ according to [14];

Compute $G^\text{PS} := \left[ G^\text{PS}_{1,:} Q'_1, \ldots, G^\text{PS}_{L,:} Q'_L \right]^T \in \mathbb{R}^{L \times (d+1)}$;

end

$\text{return diag}(buf_4)^{-1}buf_3$.

else

Compute $D$ and $G$ and take $D' := D_D D, \quad G' := D_D G$;

Compute $G^\text{PS} := \left[ G^\text{PS}_{1,:} Q'_1, \ldots, G^\text{PS}_{L,:} Q'_L \right]^T \in \mathbb{R}^{L \times (d+1)}$;

end

$\text{return diag}(buf_4)^{-1}buf_3$.


2.6 Time and space complexity analysis

We see that a variant of bidirectional FAVOR using regular RFs (based on iid samples) or R-ORFs has \(O(Md + Ld + ML)\) space complexity as opposed to \(\Theta(L^2 + Ld)\) space complexity of the baseline. Unidirectional FAVOR using fast prefix-sum precomputation in parallel [29, 15] has \(O(MLd)\) space complexity to store \(G^{PS}\) which can be reduced to \(O(Md + Ld + ML)\) by running a simple (though non-parallel in \(L\)) aggregation of \(G^{PS}\), without storing the whole tensor \(G^{PS}\) in memory. From Sec. [24] we know that if instead we use G-ORFs, then space complexity is reduced to \(O(M \log(d) + Ld + ML)\) and if the H-ORFs mechanism is used, then space is further reduced to \(O(M + Ld + ML) = O(Ld + ML)\). Thus for \(M, d \ll L\) all our variants provide substantial space complexity improvements since they do not need to store the attention matrix explicitly.

The time complexity of Algorithm 1 is \(O(LMd)\) (note that constructing \(Q\) and \(\hat{K}\) can be done in time \(O(LMd)\) via Eq. [1]) if samples from \(\Omega\) and \(B\) can be obtained in time \(O(d)\) and \(O(1)\) respectively (which is the case for all practical applications). Note that the time complexity of our method is much lower than \(O(L^2d)\) of the baseline for \(L \gg M\).

As explained in Sec. [24] the R-ORF mechanism incurs an extra one-time \(O(Md^2)\) cost (negligible compared to the \(O(LMd)\) term for \(L \gg d\)). H-ORFs or G-ORFs do not have this cost, and when FAVOR uses them, computing \(Q^*\) and \(K^*\) can be conducted in time \(O(L \log(Md))\) as opposed to \(O(LMd)\) (see: Sec. [24]). Thus even though H/G-ORFs do not change the asymptotic time complexity, they improve the constant factor from the leading term. This plays an important role for training very large models.

The number of random features \(M\) allows a trade-off between computational complexity and the level of approximation: bigger \(M\) results in higher computation costs, but also in a lower variance of the estimate of \(A\). In the next section we will show that in practice we can take \(M = \Theta(d \log(d))\).

Observe that the algorithm obtained is highly-parallelizable, and benefits from fast matrix multiplication and broadcasted operations on GPUs or TPUs.

3 Theoretical convergence analysis

In contrast to other methods approximating the attention matrix \(A\), our algorithm provides provable strong uniform convergence theoretical guarantees for compact domains. We show that \(M_{opt}\), the optimal number of random features, does not depend on \(L\) but only on \(d\). In fact, we prove that if we take \(M_{opt} = \Theta(d \log(d))\), then with \(O(Ld^2 \log(d))\)-time, we can approximate \(A\) up to any precision, regardless of the number of tokens \(L\). In order to provide those guarantees for FAVOR, we leverage recent research on the theory of negative dependence for ORFs [31]. The following is true:

**Theorem 1** (Uniform convergence of FAVOR). Take the generalized attention mechanism defined by \(g, h : \mathbb{R}^d \rightarrow \mathbb{R}\) (see: Sec. [2.2]) and a radial basis function (RBF) kernel \([17]\) \(K\) with corresponding spectral distribution \(\Omega\) (e.g. Gaussian kernel for which \(\Omega = \mathcal{N}(0, L)\)). Assume that the rows of matrices \(Q\) and \(K\) are taken from a ball \(B(\mathcal{R})\) of radius \(\mathcal{R}\), centered at 0 (i.e. norms of queries and keys are upper-bounded by \(\mathcal{R}\)). Define \(l = Rd^{-\frac{1}{2}}\) and take \(g^* = \max_{x \in B(l)} |g(x)|, h^* = \max_{x \in B(l)} |h(x)|\). Then for any \(\epsilon > 0\), \(\delta = \frac{\epsilon}{\sqrt{\mathcal{R}}}\) and the number of random features \(M = \Omega(d \log(\frac{\delta \mathcal{R}}{\sqrt{\epsilon}}))\) for \(\sigma = \mathbb{E}_{\omega \sim \Omega} [\omega^T \omega]\) the following holds: \(\|\hat{A} - A\|_1 \leq \epsilon\) with any constant probability, where \(\hat{A}\) approximates generalized attention matrix via FAVOR with R-ORFs.

The result holds in particular for regular attention using Gaussian kernels (see: Sec. [2.2]) for which \(M_{opt} = \Omega(\frac{d \log(\frac{d \mathcal{R}}{\sqrt{\epsilon}}})\) since \(\sigma = d\).

4 Experiments

We implement our setup on top of pre-existing Transformer training code in Jax [21], and complement our theory with empirical evidence to demonstrate FAVOR’s practicality in the protein setting. Unless explicitly stated, a Performer replaces only the attention component with FAVOR, while all other components are exactly the same as for the regular Transformer. Furthermore, since we use the cross-entropy loss in our generative training experiments, we use standard the accuracy metric as defined from supervised learning.
4.1 Computation costs

We compared speed-wise the backward pass, as it is one of the main computational bottlenecks during training, for a Transformer and a Performer in two settings: when the architecture \((n_{\text{heads}}, n_{\text{layers}}, d_{\text{ff}}, d_f)\) is mostly composed of attention while other dimensions are small \((1, 6, 64, 64)\), as well as the regular default size \((8, 6, 2048, 512)\), where \(d_{\text{ff}}\) denotes the width of the MLP layers of the Transformer. We observed (Fig. 1) that in terms of \(L\), the Performer reaches nearly linear time complexity as opposed to the Transformer’s quadratic time complexity. Furthermore, the Performer’s memory consumption is sub-quadratic (as it does not store the explicit \(O\left(L^2\right)\) sized attention matrix), which allows both higher batch sizes and longer sequence lengths. The combination of both memory and backward pass efficiencies for large \(L\) has profound implications for training speed, as it allows respectively, large batch training and lower wall clock time per gradient step, contributing to total train time reduction. We present additional results, including the forward pass, in the Appendix A by varying layers and architecture sizes as well.

![Backward Pass (Small)](image1)
![Backward Pass (Regular)](image2)

Figure 1: Comparison of Transformer and Performer in terms of backward pass speed and maximum \(L\) allowed. Plots shown up to when a model produces an out of memory error on a V100 GPU with 16GB. Best in color.

4.2 Approximation error and compatibility with regular Transformer

We further examined the approximation error of the attention matrix implicitly defined in FAVOR in Fig. 2 (and in Fig. 8 in Appendix B), which thus directly affects the accuracy of FAVOR’s output. We demonstrate that orthogonal features generally produce lower error than unstructured features.

![Attention Matrix Approx. Error](image3)
![Attention Output Approx. Error](image4)

Figure 2: Approximation errors for both the attention matrix and output of the mechanism itself. We took \(L = 4096\), \(d = 16\), and varied the number of random features \(M\). Standard deviations shown across 10 samples.

![Backward Compatibility](image5)

Figure 3: We transferred the original pretrained Transformer’s weights into the Performer, which produces an initial non-zero 0.07 accuracy (dotted orange line). However, once fine-tuned, the Performer quickly recovers accuracy in less than 1/6th the original number of gradient steps.

Notice that the accuracy can be further boosted by applying a resampling strategy that reconstructs samples periodically. We set this period as a hyperparameter of our overall algorithm.
Figure 4: Black dashed line corresponds to the baseline using regular attention. To emphasize the highest accuracy runs, we set y-axis to be log-scale. We tested four kernels defined by four different functions $f$ (see: Sec. 2.2): sigmoid, exponential, identity and cosine.

Figure 5: Generative training for Transformer (Small) and Performer.

The approximation error can propagate when applying the other components (MLPs, multiple heads, multiple layers, etc.) of a Transformer, which we demonstrate in Fig. 7 (Appendix). This implies we cannot immediately directly transfer the weights from a pretrained Transformer onto the Performer. However, this can be resolved by finetuning the Performer on the trained task. We demonstrate this technique for a pretrained BERT model [18] on the LM1B dataset [5] in Fig. 3.

4.3 Generalized Attention

We investigated Generalized Attention mechanisms (Sec. 2.2) on protein datasets [14] of up to length 512 for various kernel functions. Using hyperparameter sweeps across multiple variables in FAVOR, we compared several kernels and also renormalization on/off (Fig. 4, Renormalize corresponds to applying $D^{-1}$ operator in attention, as for the standard mechanism; though we noticed that disabling it does not necessarily hurt accuracy) to produce the best training configuration for the Performer. We found the sigmoid kernel with renormalization ON was the optimal configuration for the Performer.

4.4 Training on concatenated protein sequences

Finally, we demonstrate that the Performer can model multiple concatenated protein sequences as required to model and predict interactions among groups of proteins from sequence data. For this proof of principle study, we use protein sequences from the Jan. 2019 release of Trembl [14], and concatenated protein sequences to length $L = 8192$, long enough to model protein interaction networks without the large sequence alignments required by existing methods [13]. We train models on a Cloud TPU v3, containing 16GB RAM per chip. At this length, a baseline Transformer overloads memory even at a batch size of 1 per chip by a wide margin. Thus as a baseline we were forced to use a significantly smaller variant, reducing to $(n_{\text{heads}}, n_{\text{layers}}, d_{ff}, d) = (2, 1, 256, 128)$. Meanwhile, the Performer trains efficiently at a batch size of 16 per chip using the standard $(8, 6, 2048, 512)$ architecture. We see in Fig. 5 that the Transformer is quickly bounded at $\approx 17\%$, while the Performer is able to train continuously, increasing its performance as training progresses.

5 Conclusion

We presented Performer, a new type of Transformer, relying on our Fast Attention Via Orthogonal Random features (FAVOR) mechanism to significantly improve space and time complexity of regular Transformers. Our mechanism is to our knowledge the first unbiased estimation of the original algorithm with linear space and time complexity with respect to $L$. Further, FAVOR could be applied to other tasks of approximate attention, including hierarchical attention networks (HANS) [49], graph attention networks [45], image processing [22], and reinforcement learning/robotics [43].
6 Broader impact

We believe that the presented algorithm can be impactful in various ways:

**Biology and Medicine:** Our method has the potential to directly impact research on biological sequence analysis by enabling the Transformer to be applied to much longer sequences without constraints on the structure of the attention matrix. The initial application that we consider is the prediction of interactions between proteins on the proteome scale. Recently published approaches require large evolutionary sequence alignments, a bottleneck for applications to mammalian genomes [13]. The potentially broad translational impact of applying these approaches to biological sequences was one of the main motivations of this work. We believe that modern bioinformatics can immensely benefit from new machine learning techniques with Transformers being among the most promising. Scaling up these methods to train faster more accurate language models opens the door to the ability to design sets of molecules with pre-specified interaction properties. These approaches could be used to augment existing physics-based design strategies that are of critical importance for example in the development of new nanoparticle vaccines [34].

**Environment:** As we have shown, Performers with FAVOR are characterized by much lower compute costs and substantially lower space complexity which can be directly translated to CO₂ emission reduction [42] and lower energy consumption [50], as regular Transformers require very large computational resources.

**Research on Transformers:** We believe that our results can shape research on efficient Transformers architectures, guiding the field towards methods with strong mathematical foundations. Our research may also hopefully extend Transformers also beyond their standard scope (e.g. by considering the Generalized Attention mechanism and connections with kernels). Exploring scalable Transformer architectures that can handle $L$ of the order of magnitude few thousands and more, preserving accuracy of the baseline at the same time, is a gateway to new breakthroughs in bio-informatics, e.g. language modeling for proteins, as we explained in the paper. Our presented method can be potentially a first step.

**Backward Compatibility:** Our Performer can be used on the top of a regular pre-trained Transformer as opposed to other Transformer variants. Even if up-training is not required, FAVOR can be still used for fast inference with no loss of accuracy. We think about this backward compatibility as a very important additional feature of the presented techniques that might be particularly attractive for practitioners.

**Attention Beyond Transformers:** Finally, FAVOR can be applied to approximate exact attention also outside the scope of Transformers. This opens a large volume of new potential applications including: hierarchical attention networks (HANS) [49], graph attention networks [45], image processing [22], and reinforcement learning/robotics [43].

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APPENDIX: Masked Language Modeling for Proteins via Linearly Scalable Long-Context Transformers

A Extended computation costs

In this subsection, we empirically measure computational costs in terms wall clock time for both the forward and backward passes when we replace the attention mechanism on a regular Transformer-based architecture. Since some of the computational bottleneck in the Transformer may originate from the extra feed-forward layers, we thus focus on the attention part of our mechanism (which is primarily dependent on $L$) by varying both the number of layers and sequence length, while fixing the other components to be relatively minor - i.e., $n_{\text{heads}} = 1, d_{ff} = 64, d = 64$ with a batch size of 1.

![Figure 6: Using log-scale with time $T$ in seconds, we see that both the forward and backward passes scale in nearly linear time with respect to the length $L$, allowing for fast inference and training respectively. The linear regime begins to take place at approximately $2^{13} = 8192$ length size, where vanilla Transformers begin to overload GPU memory.](image)

B Extended approximation results

Although mentioned previously (Sec. 4.2) that the Performer with additional finetuning is backwards compatible with the Transformer, we demonstrate below error propagation due to non-attention components of the Transformer is one of the primary reasons that pretrained Transformer weights cannot be immediately used for inference on the corresponding Performer.

![Figure 7: Output approximation errors between a vanilla Transformer and a Performer (with orthogonal features) for varying numbers of layers.](image)

We further extend the hyperparameter sweep setting from Figure 4 in the main body of the paper, and see that across varying hyperparameters, training with orthogonal features is generally is the most accurate.
Figure 8: Orthogonality vs Unstructured usage when varying across various hyperparameters.

C Theoretical results

We provide here the proof of Theorem 1 from the main body.

Proof. We consider first the case of the default FAVOR setting with R-ORF mechanism turned on. We rely on Theorem 3 from [31]. Note that we can apply it in our case, since for RBF kernels the corresponding function $f$ is $\cos$ (thus in particular it is bounded). Also, it is not hard to observe (see for instance analysis in Claim 1 from [38]) that $L_f = 1$. Using Theorem 3 from [31], we conclude that:

$$\| \hat{B} - B \|_1 \leq \delta$$  \hspace{1cm} (15)

with any constant probability as long as $M = \Omega(\frac{d}{\sigma^2}) \log(\frac{\sigma \cdot \text{diam}(\mathcal{M})}{\delta})$, where $\sigma = \mathbb{E}[\omega^\top \omega]$ and $\mathcal{M}$ is the diameter of the smallest ball containing all vectors of the form $z = Q_i - K_j$. Since $\|Q_i\|_2, \|K_j\|_2 \leq R$, we conclude that $\|z\|_2 \leq \frac{2R}{d^{\frac{1}{4}}}$ and thus one can take $\text{diam}(\mathcal{M}) = \frac{4R}{d^{\frac{1}{4}}}$. We have:

$$\| \hat{A} - A \|_1 = \| D_Q (\hat{B} - B) D_K \|_1 \leq \| D_Q \|_1 \| \hat{B} - B \|_1 \| D_K \|_1 \leq \delta g^* h^*$$  \hspace{1cm} (16)

Taking $\delta = \frac{\epsilon}{\sigma^2 R^2}$ completes the proof. \qed