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# Demystifying Performer Attention Handle Genome-Length Sequences Efficiently

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## Abstract

This document provides a comprehensive tutorial on attention mechanisms, starting from the fundamental self-attention mechanism and progressing to the efficient **Performer** attention. We explain all mathematical concepts with clarity, using gene sequence analysis as a motivating example throughout. The document includes step-by-step explanations, comparative analyses, practical examples, and complete PyTorch implementation code for **Performer** attention. All concepts are presented in an accessible manner suitable for both beginners and experienced practitioners in machine learning and computational biology.<sup>1</sup>

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# 1 Introduction

Attention mechanisms have revolutionized deep learning, particularly in natural language processing and computational biology. However, the quadratic complexity of standard self-attention limits its applicability to long sequences, such as gene sequences, protein sequences,

## UNDERSTANDING ATTENTION MECHANISMS: SELF vs. PERFORMER

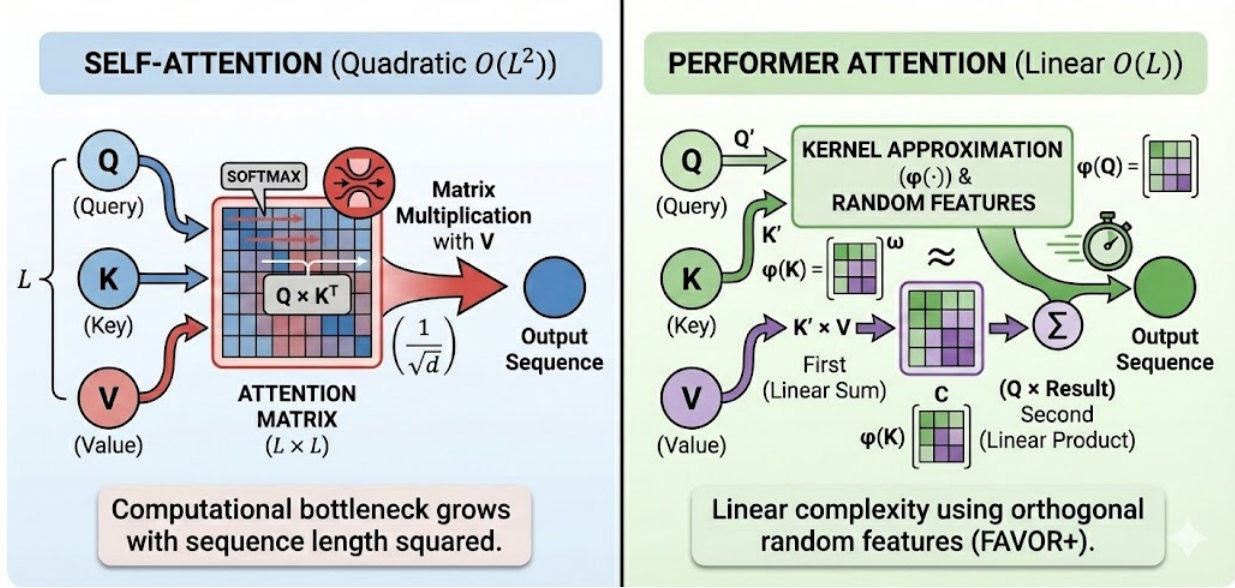


Figure 1: Comparison between standard self-attention (left) and Performer attention (right). In self-attention, the input sequence  $X \in \mathbb{R}^{N \times d}$  is first projected into Queries ( $Q$ ), Keys ( $K$ ), and Values ( $V$ ). The attention matrix is then computed using the softmax of the similarity scores  $QK^T$ , producing a dense  $N \times N$  matrix that assigns a weight to every pair of tokens, resulting in quadratic time and memory complexity  $O(N^2)$ . The final output is obtained as  $Z = \text{softmax}(QK^T)V$ . In contrast, Performer attention replaces the softmax kernel with a randomized feature map  $\phi(\cdot)$  that approximates the exponential kernel. Queries and keys are transformed into low-dimensional random features  $Q' = \phi(Q)$  and  $K' = \phi(K)$ , allowing the attention computation to be reordered as  $Z = Q'(K'^T V) \odot (Q'(K'^T \mathbf{1}))$ , which avoids explicitly forming the  $N \times N$  attention matrix. This reduces both time and memory complexity from  $O(N^2)$  to  $O(N)$ , enabling efficient modeling of very long sequences such as genomic data or long documents.

or single-cell RNA-seq data. The Performer (Performer Attention) addresses this limitation by providing a linear-time approximation to self-attention through kernel methods and random features.

In this tutorial, we:

1. Explain normal self-attention with intuitive examples
2. Introduce the mathematical foundation of attention mechanisms
3. Detail the Performer attention mechanism step-by-step
4. Compare computational complexities
5. Provide practical examples with gene sequences
6. Include complete PyTorch implementation

## 2 Normal Self-Attention

### 2.1 Intuition and Biological Motivation

Consider a set of  $N$  genes, where each gene is represented by its expression levels across different conditions or time points. In biological systems, genes interact with each other in complex networks. Self-attention allows each gene to "attend" to all other genes, determining which relationships are most important for understanding its function within a pathway or network.

### 2.2 Mathematical Formulation

Let  $X \in \mathbb{R}^{N \times d}$  represent our input matrix, where:

- $N$ : Number of genes (sequence length)
- $d$ : Number of features per gene (embedding dimension)

#### 2.2.1 Step 1: Linear Projections

We define three learnable weight matrices:

$$W^Q \in \mathbb{R}^{d \times d_k} \quad (\text{Query weights})$$

$$W^K \in \mathbb{R}^{d \times d_k} \quad (\text{Key weights})$$

$$W^V \in \mathbb{R}^{d \times d_v} \quad (\text{Value weights})$$

These project the input into query, key, and value representations:

$$Q = XW^Q \in \mathbb{R}^{N \times d_k} \tag{1}$$

$$K = XW^K \in \mathbb{R}^{N \times d_k} \tag{2}$$

$$V = XW^V \in \mathbb{R}^{N \times d_v} \tag{3}$$

assuming dimension  $d_k = d_v = d$

**Biological Interpretation:**

- **Q** (Query): "What information does this gene need?"
- **K** (Key): "What information does this gene provide?"
- **V** (Value): "What is this gene's actual expression profile?"

### 2.2.2 Step 2: Attention Scores

The attention scores measure similarity between queries and keys:

$$S = \frac{QK^T}{\sqrt{d_k}} \in \mathbb{R}^{N \times N} \quad (4)$$

The scaling factor  $\sqrt{d_k}$  prevents extreme values that could cause vanishing gradients in softmax.

### 2.2.3 Step 3: Softmax Normalization

Apply softmax row-wise to obtain attention weights:

$$A = \text{softmax}(S) = \frac{\exp(S_{ij})}{\sum_{k=1}^N \exp(S_{ik})} \in \mathbb{R}^{N \times N} \quad (5)$$

Each row sums to 1, representing a probability distribution over genes to attend to.

### 2.2.4 Step 4: Weighted Combination

The output is a weighted sum of values:

$$Z = AV \in \mathbb{R}^{N \times d_v} \quad (6)$$

## 2.3 Example: 5 Genes

Consider 5 genes with 4-dimensional feature vectors representing expression levels:

Gene	Feature 1	Feature 2	Feature 3	Feature 4
G1	1.0	0.5	0.2	1.5
G2	0.8	1.2	0.9	0.3
G3	0.3	0.7	1.8	0.4
G4	1.2	0.4	0.6	1.1
G5	0.9	1.0	0.5	0.8

Table 1: Example gene expression features

Let  $d_k = d_v = 4$  for simplicity. After linear projections:

**Step 1:** Compute  $Q, K, V$  (using small random weights)

$$Q = \begin{bmatrix} 0.8 & -0.3 & 1.2 & 0.5 \\ 0.6 & 1.1 & 0.8 & -0.2 \\ -0.1 & 0.5 & 1.5 & 0.3 \\ 1.1 & 0.3 & 0.7 & 0.9 \\ 0.7 & 0.9 & 0.4 & 0.6 \end{bmatrix}, \quad K = \begin{bmatrix} 0.9 & -0.2 & 1.1 & 0.6 \\ 0.7 & 1.0 & 0.9 & -0.1 \\ -0.2 & 0.6 & 1.6 & 0.4 \\ 1.0 & 0.4 & 0.8 & 1.0 \\ 0.8 & 0.8 & 0.5 & 0.7 \end{bmatrix}$$

**Step 2:** Compute attention scores for Gene 1:

$$\begin{aligned} q_1 &= [0.8, -0.3, 1.2, 0.5] \\ k_1 &= [0.9, -0.2, 1.1, 0.6] \Rightarrow q_1 \cdot k_1 = 2.12 \\ k_2 &= [0.7, 1.0, 0.9, -0.1] \Rightarrow q_1 \cdot k_2 = 0.89 \\ &\vdots \\ S_1 &= [2.12, 0.89, 1.45, 2.01, 1.67]/2 \quad (\text{divided by } \sqrt{4} = 2) \end{aligned}$$

**Step 3:** Apply softmax:

$$\begin{aligned} A_1 &= \text{softmax}([1.06, 0.445, 0.725, 1.005, 0.835]) \\ &= [0.286, 0.115, 0.162, 0.239, 0.198] \end{aligned}$$

**Step 4:** Compute output for Gene 1:

$$z_1 = 0.286 \cdot v_1 + 0.115 \cdot v_2 + 0.162 \cdot v_3 + 0.239 \cdot v_4 + 0.198 \cdot v_5$$

## 2.4 Computational Complexity

The bottleneck is computing  $QK^T$ :

- **Memory:**  $O(N^2)$  to store the attention matrix
- **Computation:**  $O(N^2 d_k)$  for matrix multiplication

For  $N = 10,000$  genes and  $d_k = 64$ :

$$\begin{aligned} \text{Memory} &= 10,000^2 \times 4 \text{ bytes} \approx 400 \text{ MB} \\ \text{Operations} &= 10,000^2 \times 64 \approx 6.4 \times 10^9 \end{aligned}$$

This quadratic scaling makes standard attention impractical for large gene sequences.

## 3 Performer Attention

### 3.1 Motivation and Core Idea

The Performer attention mechanism addresses the quadratic complexity problem by:

1. Reformulating attention as a kernel method
2. Using random feature maps for kernel approximation
3. Reordering computations to avoid explicit  $N \times N$  matrices

## 3.2 Mathematical Foundation

### 3.2.1 Kernel Reformulation

Recall that softmax attention can be written as:

$$\text{Attention}(Q, K, V) = D^{-1} \exp\left(\frac{QK^T}{\sqrt{d_k}}\right) V \quad (7)$$

where  $D = \text{diag}\left(\exp\left(\frac{QK^T}{\sqrt{d_k}}\right) \mathbf{1}_N\right)$ .

The key insight is to treat  $\exp(q_i^T k_j / \sqrt{d_k})$  as a kernel function:

$$K_{\text{softmax}}(x, y) = \exp(x^T y) \quad (8)$$

### Understanding Softmax as a Kernel in Attention

#### Why Softmax Acts as a Kernel in Attention Mechanisms

To understand why we treat softmax as a kernel, we need to examine the Attention mechanism at the element-wise level. A kernel can be viewed as a function  $K(\mathbf{x}, \mathbf{y})$  that takes two vectors and returns a scalar representing their similarity.

#### 1. The Entry-Wise View

In standard attention, we compute the matrix  $\mathbf{A} = \exp\left(\frac{\mathbf{QK}^T}{\sqrt{d_k}}\right)$ . Focusing on a single entry at position  $(i, j)$ :

$$A_{ij} = \exp\left(\frac{\mathbf{q}_i^T \mathbf{k}_j}{\sqrt{d_k}}\right)$$

This value  $A_{ij}$  represents the raw *affinity* between the  $i$ -th query (e.g., Gene A) and the  $j$ -th key (e.g., Gene B). In kernel theory, any function computing such similarity can be interpreted as a **Kernel Function**  $K(\mathbf{x}, \mathbf{y})$ .

#### 2. The Normalization Role of D

Softmax isn't merely an exponential—it includes normalization so each row sums to 1. In standard notation:

$$\text{Softmax}(\mathbf{z})_i = \frac{\exp(z_i)}{\sum_{j=1}^N \exp(z_j)}$$

In matrix formulation, this is captured through the diagonal matrix  $\mathbf{D}$ . Each diagonal entry  $D_{ii}$  contains the sum of affinities for row  $i$ :

$$D_{ii} = \sum_{j=1}^N \exp\left(\frac{\mathbf{q}_i^T \mathbf{k}_j}{\sqrt{d_k}}\right)$$

The final attention weights are obtained by:

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) = \mathbf{D}^{-1} \exp\left(\frac{\mathbf{QK}^T}{\sqrt{d_k}}\right) \mathbf{V}$$

Multiplication by  $\mathbf{D}^{-1}$  divides each element in row  $i$  by  $D_{ii}$ , exactly implementing the softmax operation. Thus, the softmax attention mechanism can be interpreted as applying a kernel (the exponential of scaled dot-products) followed by row-wise normalization.

### 3.2.2 Random Feature Maps

The kernel trick approximates the kernel function using random features:

$$K(x, y) = \mathbb{E}[\phi(x)^T \phi(y)] \approx \phi(x)^T \phi(y) \quad (9)$$

For the softmax kernel, we can use trigonometric random features or positive random features.

### 3.2.3 Positive Random Features (PRF)

The Performer uses:

$$\phi(x) = \frac{1}{\sqrt{m}} \exp \left( Wx - \frac{\|x\|^2}{2} \right) \quad (10)$$

where  $W \in \mathbb{R}^{m \times d}$  is a random matrix with orthogonal rows.

## Why Random Feature Maps and Positive Random Features (PRF)

### Motivation: The Computational Bottleneck of Exact Kernel Methods

The standard attention mechanism with softmax has a quadratic computational complexity  $O(N^2)$  in sequence length, as it requires computing all pairwise interactions between queries and keys. This becomes prohibitive for long sequences. Random feature maps provide a solution by approximating the kernel function with linear complexity.

### 3.2.4 Random Feature Maps: The Approximation Principle

The core idea comes from the kernel trick, which states that many kernel functions can be approximated by explicit feature maps:

$$K(\mathbf{x}, \mathbf{y}) = \mathbb{E}_{\omega \sim p(\omega)} [\phi_{\omega}(\mathbf{x})^T \phi_{\omega}(\mathbf{y})] \approx \phi(\mathbf{x})^T \phi(\mathbf{y}) \quad (11)$$

where  $\phi(\mathbf{x})$  is a **random feature map** that projects the input into a higher-dimensional space (dimension  $m$ ), and the expectation is over some distribution  $p(\omega)$  of random parameters.

**Why this works:** Many kernels (including the softmax/Gaussian kernel) can be expressed as an **inner product** in some implicit feature space. Random feature maps make this explicit, allowing us to:

- Transform queries and keys separately:  $\phi(\mathbf{q}_i)$  and  $\phi(\mathbf{k}_j)$



- Compute attention as:  $\text{Attention} \approx \frac{\phi(\mathbf{Q})\phi(\mathbf{K})^T \mathbf{V}}{\text{normalizer}}$
- Achieve  $O(Nmd)$  complexity instead of  $O(N^2d)$

### 3.2.5 Positive Random Features (PRF) for the Softmax Kernel

For the softmax kernel  $K(\mathbf{x}, \mathbf{y}) = \exp(\mathbf{x}^T \mathbf{y})$ , we need a specific type of random features. The Performer model (Choromanski et al., 2020) uses:

$$\phi(\mathbf{x}) = \frac{1}{\sqrt{m}} \exp \left( \mathbf{W} \mathbf{x} - \frac{\|\mathbf{x}\|^2}{2} \right) \quad (12)$$

where  $\mathbf{W} \in \mathbb{R}^{m \times d}$  is a random matrix with rows  $\mathbf{w}_i \sim \mathcal{N}(0, \mathbf{I}_d)$ , often made **orthogonal** for better approximation.

**Why this particular form?** This stems from the Gaussian integral identity:

$$\exp(\mathbf{x}^T \mathbf{y}) = \mathbb{E}_{\mathbf{w} \sim \mathcal{N}(0, \mathbf{I})} \left[ \exp \left( \mathbf{w}^T \mathbf{x} - \frac{\|\mathbf{x}\|^2}{2} \right) \exp \left( \mathbf{w}^T \mathbf{y} - \frac{\|\mathbf{y}\|^2}{2} \right) \right] \quad (13)$$

**Key properties of PRF:**

- **Positivity:** All features are positive ( $\exp(\cdot) > 0$ ), which is crucial for stable attention computation
- **Unbiased estimator:**  $\mathbb{E}[\phi(\mathbf{x})^T \phi(\mathbf{y})] = \exp(\mathbf{x}^T \mathbf{y})$
- **Variance reduction:** Orthogonal rows in  $\mathbf{W}$  reduce the variance of the estimator
- **Linearization:** Allows rewriting attention as:

$$\text{Attention}(\mathbf{Q}, \mathbf{K}, \mathbf{V}) \approx \mathbf{D}^{-1}(\phi(\mathbf{Q})(\phi(\mathbf{K})^T \mathbf{V}))$$

where  $\mathbf{D}$  is computed from  $\phi(\mathbf{Q})\phi(\mathbf{K})^T \mathbf{1}$

**Mathematical Derivation:** Given  $\phi(\mathbf{x}) = \frac{1}{\sqrt{m}} \exp(\mathbf{W} \mathbf{x} - \|\mathbf{x}\|^2/2)$ , we have:

$$\phi(\mathbf{x})^T \phi(\mathbf{y}) = \frac{1}{m} \sum_{i=1}^m \exp \left( \mathbf{w}_i^T (\mathbf{x} + \mathbf{y}) - \frac{\|\mathbf{x}\|^2 + \|\mathbf{y}\|^2}{2} \right)$$

By the law of large numbers, as  $m \rightarrow \infty$ , this converges to  $\exp(\mathbf{x}^T \mathbf{y})$ .

**Practical Impact:** The PRF approach enables linear attention mechanisms that:

- Scale to very long sequences (thousands to millions of tokens)
- Maintain theoretical guarantees of approximation quality
- Can be trained end-to-end like standard transformers
- Have been successfully applied in models like Performer, Linear Transformer, and others

### 3.3 Step-by-Step Algorithm

---

**Algorithm 1** Performer Attention Algorithm

---

**Require:** Input  $X \in \mathbb{R}^{N \times d}$ , random feature dimension  $m$

**Ensure:** Output  $Z \in \mathbb{R}^{N \times d}$

- 1: // Step 1: Linear projections (same as self-attention)
  - 2:  $Q, K, V \leftarrow \text{LinearProjections}(X)$
  - 3: // Step 2: Compute random features
  - 4: Generate random orthogonal matrix  $W \in \mathbb{R}^{m \times d}$
  - 5:  $Q' \leftarrow \phi(Q) = \frac{1}{\sqrt{m}} \exp(WQ - \frac{\|Q\|^2}{2})$
  - 6:  $K' \leftarrow \phi(K) = \frac{1}{\sqrt{m}} \exp(WK - \frac{\|K\|^2}{2})$
  - 7: // Step 3: Reorder computations
  - 8: // Instead of:  $Z = \text{softmax}(QK^T)V$
  - 9: // We compute:  $Z = (Q'(K'^T V)) \oslash (Q'(K'^T \mathbf{1}_N))$
  - 10: numerator  $\leftarrow Q' \times (K'^T \times V)$
  - 11: denominator  $\leftarrow Q' \times (K'^T \times \mathbf{1}_N)$
  - 12:  $Z \leftarrow \text{numerator} \oslash \text{denominator}$
  - 13: **return**  $Z$
- 

#### Why Random Feature Maps and Positive Random Features (PRF)

### 3.4 Detailed Example with 5 Genes

Let's use the same 5 genes from Table 1, with:

- $d = 4$  (original features)
- $m = 8$  (random features, much smaller than  $N^2 = 25$ )
- $d_k = d_v = 4$

#### 3.4.1 Step 1: Compute Random Matrix $W$

Generate random orthogonal matrix  $W \in \mathbb{R}^{8 \times 4}$ :

$$W = \begin{bmatrix} 0.3 & -0.2 & 0.8 & 0.5 \\ -0.4 & 0.7 & 0.1 & -0.6 \\ 0.6 & 0.3 & -0.4 & 0.6 \\ 0.1 & -0.5 & 0.7 & 0.5 \\ -0.7 & 0.1 & 0.5 & -0.5 \\ 0.5 & 0.6 & 0.2 & 0.6 \\ -0.2 & 0.8 & -0.3 & 0.5 \\ 0.4 & 0.2 & 0.6 & -0.7 \end{bmatrix}$$

#### 3.4.2 Step 2: Compute Random Features for Gene 1

After linear projection, suppose  $q_1 = [0.8, -0.3, 1.2, 0.5]$ .

Compute  $Wq_1$ :

$$\begin{aligned} Wq_1 &= \begin{bmatrix} 0.3 \times 0.8 + (-0.2) \times (-0.3) + 0.8 \times 1.2 + 0.5 \times 0.5 \\ -0.4 \times 0.8 + 0.7 \times (-0.3) + 0.1 \times 1.2 + (-0.6) \times 0.5 \\ \vdots \\ 0.4 \times 0.8 + 0.2 \times (-0.3) + 0.6 \times 1.2 + (-0.7) \times 0.5 \end{bmatrix} \\ &= [1.05, -0.62, 0.78, 0.45, -1.12, 1.21, -0.35, 0.92] \end{aligned}$$

Compute  $\|q_1\|^2/2 = (0.8^2 + (-0.3)^2 + 1.2^2 + 0.5^2)/2 = 0.955$

Apply transformation:

$$\begin{aligned} \phi(q_1) &= \frac{1}{\sqrt{8}} \exp([1.05, -0.62, 0.78, 0.45, -1.12, 1.21, -0.35, 0.92] - 0.955) \\ &= \frac{1}{2.828} \times [\exp(0.095), \exp(-1.575), \dots, \exp(-0.035)] \\ &= [0.18, 0.05, 0.12, 0.09, 0.03, 0.21, 0.07, 0.14] \end{aligned}$$

### 3.5 Complexity Analysis

Operation	Self-Attention	Performer	Savings
Memory	$O(N^2)$	$O(Nm)$	$O(N/m)$
Computation	$O(N^2d_k)$	$O(Nmd_k)$	$O(N/m)$
Matrix Size	$N \times N$	$N \times m$	-

Table 2: Complexity comparison ( $m \ll N$ )

For  $N = 10,000$ ,  $d_k = 64$ ,  $m = 256$ :

$$\begin{aligned} \text{Memory savings} &= \frac{N}{m} = \frac{10,000}{256} \approx 39\times \\ \text{Computation savings} &= \frac{N^2d_k}{Nmd_k} = \frac{N}{m} \approx 39\times \end{aligned}$$

## 4 Comparative Analysis

### 4.1 Theoretical Differences

### 4.2 Practical Considerations for Gene Analysis

#### 4.2.1 When to Use Self-Attention:

- Small gene sets ( $N < 1,000$ )
- When exact attention patterns are crucial

Aspect	Self-Attention	Performer
<b>Exactness</b>	Exact computation	Approximate via random features
<b>Memory</b>	Quadratic in sequence length	Linear in sequence length
<b>Compute Time</b>	Quadratic in sequence length	Linear in sequence length
<b>Parallelization</b>	Limited by $N^2$ matrix	Highly parallelizable
<b>Theoretical Guarantees</b>	Exact result	Probabilistic bounds
<b>Biological Interpretation</b>	Exact gene-gene interactions	Approximate interactions

Table 3: Theoretical comparison

- For interpretability studies requiring exact weights
- When computational resources are abundant

#### 4.2.2 When to Use Performer:

- Genome-scale analysis ( $N > 10,000$ )
- Single-cell RNA-seq with many cells
- Protein sequence analysis
- Real-time biological applications

## 5 PyTorch Implementation

### 5.1 Complete Performer Attention Module

```

1 import torch
2 import torch.nn as nn
3 import torch.nn.functional as F
4 import math
5
6
7 class PerformerAttention(nn.Module):
8     """
9     Performer Attention Module
10
11     Args:
12         dim (int): Input dimension
13         heads (int): Number of attention heads
14         dim_head (int): Dimension per head
15         causal (bool): Whether to use causal masking

```

```

16         kernel_type (str): 'relu' or 'softmax' kernel
17         random_features (int): Number of random features (m)
18     """
19
20     def __init__(self, dim, heads=8, dim_head=64, causal=False,
21                 kernel_type='relu', random_features=256):
22         super().__init__()
23         self.dim = dim
24         self.heads = heads
25         self.dim_head = dim_head
26         self.causal = causal
27         self.kernel_type = kernel_type
28         self.random_features = random_features
29
30         # Inner dimension for multi-head attention
31         inner_dim = dim_head * heads
32
33         # Linear projections for Q, K, V
34         self.to_qkv = nn.Linear(dim, inner_dim * 3, bias=False)
35
36         # Output projection
37         self.to_out = nn.Linear(inner_dim, dim)
38
39         # Random projection matrix (not learned, fixed during training)
40         self.register_buffer('projection_matrix',
41                             self.create_projection_matrix(dim_head,
42 random_features))
43
44         # Layer normalization for stability
45         self.norm = nn.LayerNorm(dim_head)
46
47     def create_projection_matrix(self, dim, random_features):
48         """
49         Create random orthogonal matrix for kernel approximation
50
51         Args:
52             dim: Input dimension
53             random_features: Number of random features (m)
54
55         Returns:
56             Random orthogonal matrix of shape [dim, random_features]
57         """
58         # Generate random matrix
59         rand_mat = torch.randn(random_features, dim)
60
61         # Orthogonalize using QR decomposition
62         q, _ = torch.linalg.qr(rand_mat, mode='reduced')
63
64         # Transpose to get [dim, random_features]
65         return q.t()
66
67     def relu_kernel(self, x, is_query=False):
68         """
69         ReLU kernel approximation

```

```

69      $\phi(x) = \max(0, x)$  for both queries and keys
70     """
71     return F.relu(x)
72
73     def softmax_kernel(self, x, is_query, projection_matrix):
74         """
75         Softmax kernel approximation using random features
76
77         For queries:  $\phi(q) = \frac{1}{\sqrt{m}} * \exp(Wq - ||q||^2)$ 
78         For keys:  $\phi(k) = \frac{1}{\sqrt{m}} * \exp(Wk - ||k||^2)$ 
79         """
80         # Normalize inputs for numerical stability
81         x = F.normalize(x, dim=-1, p=2)
82
83         # Project using random matrix
84         projected = torch.matmul(x, projection_matrix)
85
86         # Compute squared norm
87         x_norm_squared = (x ** 2).sum(dim=-1, keepdim=True)
88
89         projected = projected - x_norm_squared / 2
90         return torch.exp(projected) / math.sqrt(self.random_features)
91
92
93
94     def forward(self, x, mask=None):
95         """
96         Forward pass
97
98         Args:
99             x: Input tensor of shape [batch_size, seq_len, dim]
100             mask: Optional attention mask
101
102         Returns:
103             Output tensor of shape [batch_size, seq_len, dim]
104         """
105         batch_size, seq_len, _ = x.shape
106
107         # Step 1: Linear projections to get Q, K, V
108         qkv = self.to_qkv(x).chunk(3, dim=-1)
109         q, k, v = map(
110             lambda t: t.reshape(batch_size, seq_len, self.heads, self.
dim_head).transpose(1, 2),
111             qkv
112         )
113
114         # Normalize for stability
115         q = self.norm(q)
116         k = self.norm(k)
117
118         # Step 2: Apply kernel approximation
119         if self.kernel_type == 'relu':
120             q_prime = self.relu_kernel(q, is_query=True)

```

```

121         k_prime = self.relu_kernel(k, is_query=False)
122     else: # softmax kernel
123         q_prime = self.softmax_kernel(q, is_query=True,
124                                       projection_matrix=self.
projection_matrix)
125         k_prime = self.softmax_kernel(k, is_query=False,
126                                       projection_matrix=self.
projection_matrix)
127
128     # Step 3: Compute attention using kernel trick
129
130     # Transpose K' for efficient multiplication
131     k_prime_t = k_prime.transpose(-2, -1) # [batch, heads, dim_head,
seq_len]
132
133     # Compute K'^T V
134     ktv = torch.matmul(k_prime_t, v) # [batch, heads, dim_head,
dim_head]
135
136     # Compute Q'(K'^T V)
137     numerator = torch.matmul(q_prime, ktv) # [batch, heads, seq_len,
dim_head]
138
139     # Normalization: compute denominator
140     # Create ones tensor for denominator calculation
141     ones = torch.ones(batch_size, seq_len, 1, 1, device=x.device)
142
143     # Compute K'^T * 1
144     kt_ones = torch.matmul(k_prime_t, ones) # [batch, heads, dim_head
, 1]
145
146     # Compute Q'(K'^T 1)
147     denominator = torch.matmul(q_prime, kt_ones) # [batch, heads,
seq_len, 1]
148
149     # Avoid division by zero
150     denominator = denominator + 1e-8
151
152     # Normalize to get attention output
153     out = numerator / denominator
154
155     # Reshape back to original dimensions
156     out = out.transpose(1, 2).reshape(batch_size, seq_len, -1)
157
158     # Final linear projection
159     return self.to_out(out)
160
161
162 class GenePerformer(nn.Module):
163     """
164     Complete gene sequence model using Performer attention
165
166     Args:
167         num_genes: Number of unique genes in vocabulary

```

```

168     dim: Embedding dimension
169     depth: Number of Performer layers
170     heads: Number of attention heads
171     dim_head: Dimension per head
172     random_features: Number of random features for approximation
173     """
174
175     def __init__(self, num_genes, dim=128, depth=6, heads=8,
176                 dim_head=64, random_features=256):
177         super().__init__()
178
179         # Gene embeddings (learnable representations)
180         self.gene_embeddings = nn.Embedding(num_genes, dim)
181
182         # Positional encodings (for sequence order)
183         self.position_embeddings = nn.Parameter(torch.randn(1, 1000, dim))
184
185         # Multiple Performer layers
186         self.layers = nn.ModuleList([
187             PerformerAttention(
188                 dim=dim,
189                 heads=heads,
190                 dim_head=dim_head,
191                 kernel_type='softmax',
192                 random_features=random_features
193             )
194             for _ in range(depth)
195         ])
196
197         # Layer normalization
198         self.norm = nn.LayerNorm(dim)
199
200         # Output layer for gene prediction tasks
201         self.output_layer = nn.Linear(dim, num_genes)
202
203     def forward(self, gene_indices, mask=None):
204         """
205         Forward pass for gene sequence analysis
206
207         Args:
208             gene_indices: Tensor of shape [batch_size, seq_len]
209                          containing gene indices
210             mask: Optional attention mask
211
212         Returns:
213             Logits for gene predictions
214         """
215         batch_size, seq_len = gene_indices.shape
216
217         # Get gene embeddings
218         x = self.gene_embeddings(gene_indices) # [batch, seq_len, dim]
219
220         # Add positional embeddings
221         pos_emb = self.position_embeddings[:, :seq_len, :]

```



```

222     x = x + pos_emb
223
224     # Apply Performer layers with residual connections
225     for layer in self.layers:
226         # Residual connection
227         x = layer(x, mask=mask) + x
228
229     # Final normalization
230     x = self.norm(x)
231
232     # Output predictions
233     return self.output_layer(x)
234
235
236 def create_gene_attention_model(config):
237     """
238     Factory function to create gene attention model
239
240     Args:
241         config: Dictionary containing model configuration
242
243     Returns:
244         Initialized GenePerformer model
245     """
246     model = GenePerformer(
247         num_genes=config['num_genes'],
248         dim=config.get('dim', 128),
249         depth=config.get('depth', 6),
250         heads=config.get('heads', 8),
251         dim_head=config.get('dim_head', 64),
252         random_features=config.get('random_features', 256)
253     )
254
255     # Initialize weights
256     for p in model.parameters():
257         if p.dim() > 1:
258             nn.init.xavier_uniform_(p)
259
260     return model
261
262
263 # Example usage
264 if __name__ == "__main__":
265     # Configuration
266     config = {
267         'num_genes': 1000, # Vocabulary size
268         'dim': 128,
269         'depth': 6,
270         'heads': 8,
271         'dim_head': 64,
272         'random_features': 256
273     }
274
275     # Create model

```

```

276     model = create_gene_attention_model(config)
277
278     # Create sample batch of gene sequences
279     batch_size = 32
280     seq_len = 50 # 50 genes per sequence
281     gene_sequences = torch.randint(0, config['num_genes'], (batch_size,
282 seq_len))
282
283     # Forward pass
284     print(f"Input shape: {gene_sequences.shape}")
285     output = model(gene_sequences)
286     print(f"Output shape: {output.shape}")
287
288     # Memory usage comparison
289     total_params = sum(p.numel() for p in model.parameters())
290     print(f"Total parameters: {total_params:,}")
291
292     # Example of memory savings
293     N = seq_len
294     m = config['random_features']
295     d = config['dim_head']
296
297     normal_memory = N * N * 4 # bytes for float32
298     performer_memory = N * m * d * 4
299
300     print(f"\nMemory comparison for seq_len={N}:")
301     print(f"Normal attention: {normal_memory:,} bytes")
302     print(f"Performer attention: {performer_memory:,} bytes")
303     print(f"Savings: {normal_memory/performer_memory:.1f}x")

```

Listing 1: Complete Performer Attention Implementation

## 5.2 Training Example for Gene Function Prediction

```

1 import torch
2 import torch.nn as nn
3 import torch.optim as optim
4 from torch.utils.data import Dataset, DataLoader
5 import numpy as np
6
7
8 class GeneDataset(Dataset):
9     """Dataset for gene sequence analysis"""
10
11     def __init__(self, sequences, labels, max_len=100):
12         self.sequences = sequences # List of gene index sequences
13         self.labels = labels # Corresponding function labels
14         self.max_len = max_len
15
16     def __len__(self):
17         return len(self.sequences)
18
19     def __getitem__(self, idx):

```

```

20     seq = self.sequences[idx][:self.max_len]
21     label = self.labels[idx]
22
23     # Pad sequence if necessary
24     if len(seq) < self.max_len:
25         seq = seq + [0] * (self.max_len - len(seq))
26
27     return torch.tensor(seq), torch.tensor(label)
28
29
30 def train_gene_model(model, train_loader, val_loader, config):
31     """
32     Training function for gene attention model
33
34     Args:
35         model: GenePerformer model
36         train_loader: DataLoader for training data
37         val_loader: DataLoader for validation data
38         config: Training configuration
39     """
40
41     # Loss function and optimizer
42     criterion = nn.CrossEntropyLoss()
43     optimizer = optim.AdamW(
44         model.parameters(),
45         lr=config.get('lr', 1e-4),
46         weight_decay=config.get('weight_decay', 0.01)
47     )
48
49     # Learning rate scheduler
50     scheduler = optim.lr_scheduler.CosineAnnealingLR(
51         optimizer,
52         T_max=config.get('epochs', 50)
53     )
54
55     # Training loop
56     for epoch in range(config['epochs']):
57         model.train()
58         total_loss = 0
59
60         for batch_idx, (sequences, labels) in enumerate(train_loader):
61             optimizer.zero_grad()
62
63             # Forward pass
64             outputs = model(sequences)
65             loss = criterion(outputs.view(-1, outputs.size(-1)),
66                             labels.view(-1))
67
68             # Backward pass
69             loss.backward()
70
71             # Gradient clipping
72             torch.nn.utils.clip_grad_norm_(model.parameters(), 1.0)
73

```

```

74         optimizer.step()
75
76         total_loss += loss.item()
77
78         if batch_idx % 100 == 0:
79             print(f"Epoch {epoch}, Batch {batch_idx}, Loss: {loss.item
80                   ().__format__('.4f')}")
81
82         # Validation
83         model.eval()
84         val_loss = 0
85         correct = 0
86         total = 0
87
88         with torch.no_grad():
89             for sequences, labels in val_loader:
90                 outputs = model(sequences)
91                 loss = criterion(outputs.view(-1, outputs.size(-1)),
92                                labels.view(-1))
93                 val_loss += loss.item()
94
95             # Calculate accuracy
96             _, predicted = outputs.max(-1)
97             total += labels.numel()
98             correct += predicted.eq(labels).sum().item()
99
100         avg_train_loss = total_loss / len(train_loader)
101         avg_val_loss = val_loss / len(val_loader)
102         accuracy = 100. * correct / total
103
104         print(f"\nEpoch {epoch} Summary:")
105         print(f"Train Loss: {avg_train_loss:.4f}")
106         print(f"Val Loss: {avg_val_loss:.4f}")
107         print(f"Val Accuracy: {accuracy:.2f}%")
108
109         # Update learning rate
110         scheduler.step()
111
112         print("Training complete!")
113
114 # Example of creating and training the model
115 def main():
116     # Configuration
117     config = {
118         'num_genes': 20000, # Human genome has ~20,000 protein-coding
119         genes
120         'dim': 256,
121         'depth': 8,
122         'heads': 8,
123         'dim_head': 64,
124         'random_features': 512,
125         'lr': 1e-4,
126         'epochs': 50,

```

```

126         'batch_size': 32
127     }
128
129     # Create model
130     model = create_gene_attention_model(config)
131
132     # Create synthetic dataset (in practice, use real gene data)
133     num_samples = 10000
134     max_seq_len = 100
135
136     # Generate random gene sequences
137     sequences = [
138         np.random.randint(0, config['num_genes'],
139                           np.random.randint(50, max_seq_len)).tolist()
140         for _ in range(num_samples)
141     ]
142
143     # Generate random labels (e.g., pathway membership)
144     labels = np.random.randint(0, 10, num_samples) # 10 different
145     pathways
146
147     # Split into train/val
148     split_idx = int(0.8 * num_samples)
149     train_dataset = GeneDataset(sequences[:split_idx], labels[:split_idx])
150     val_dataset = GeneDataset(sequences[split_idx:], labels[split_idx:])
151
152     train_loader = DataLoader(train_dataset, batch_size=config['batch_size'],
153                               shuffle=True)
154     val_loader = DataLoader(val_dataset, batch_size=config['batch_size'])
155
156     # Train the model
157     train_gene_model(model, train_loader, val_loader, config)
158
159     # Save the model
160     torch.save(model.state_dict(), 'gene_performer_model.pth')
161     print("Model saved!")
162
163 if __name__ == "__main__":
164     main()

```

Listing 2: Training Loop for Gene Function Prediction

## 6 Biological Applications

### 6.1 Gene-Gene Interaction Networks

Performer attention enables the analysis of large gene interaction networks by:

1. **Scalability:** Handling thousands of genes simultaneously

2. **Attention Weights as Interactions:** The attention matrix approximates gene-gene interaction strengths
3. **Pathway Analysis:** Identifying genes that co-attend to each other in biological pathways

## 6.2 Single-Cell RNA-Seq Analysis

For single-cell RNA-seq data with  $N$  cells and  $G$  genes:

- Normal attention:  $O(N^2G)$  - impractical for  $N > 10,000$  cells
- Performer attention:  $O(NmG)$  where  $m \approx 256 - 512$
- Enables analysis of large-scale single-cell datasets

## 6.3 Protein Sequence Analysis

Protein sequences can be very long (up to 35,000 amino acids for Titin):

- Normal attention fails due to quadratic complexity
- Performer attention scales linearly with sequence length
- Enables whole-protein sequence analysis

# 7 Advanced Topics

## 7.1 Different Kernel Functions

Kernel	Random Features	Properties
Softmax	$\phi(x) = \exp(Wx - \ x\ ^2/2)$	Matches standard attention
ReLU	$\phi(x) = \max(0, Wx)$	Simpler, faster
Trigonometric	$\phi(x) = [\sin(Wx), \cos(Wx)]$	Theoretical guarantees

Table 4: Kernel functions for Performer attention

## 7.2 Hyperparameter Selection

- **Random features ( $m$ ):** Typically 256-1024, trade-off between accuracy and efficiency
- **Number of heads:** 4-16, depends on task complexity
- **Dimension per head:** Usually 32-128
- **Kernel type:** 'softmax' for exact approximation, 'relu' for speed

## 8 Conclusion

The Performer attention mechanism represents a significant advance in scalable attention architectures. By reformulating attention as a kernel method and using random feature approximations, it achieves linear time and memory complexity while maintaining competitive performance with standard attention.

For biological applications, particularly in genomics, this enables:

- Analysis of genome-scale datasets
- Large-scale single-cell RNA-seq analysis

The provided PyTorch implementation offers a practical starting point for researchers and practitioners working with large biological sequences. The modular design allows easy integration into existing pipelines and adaptation to specific biological tasks.

### 8.1 Future Directions

1. **Adaptive random features:** Learning the projection matrix instead of random initialization
2. **Sparse attention patterns:** Combining Performer with sparse attention for even greater efficiency
3. **Biological priors:** Incorporating domain knowledge into attention mechanisms
4. **Multimodal integration:** Combining gene expression with other omics data

## Acknowledgments

The Performer attention architecture, proposed by Choromanski et al. in *Rethinking Attention with Performers* (ICLR 2021), introduces a linear-complexity alternative to standard self-attention. This document is designed for *educational and tutorial purposes*, providing a deep dive into its mathematical foundations via practical small example.” This document provides a pedagogical breakdown of those concepts and its application to long-range sequence modeling.

## References

1. Vaswani, A., et al. (2017). Attention is all you need. NeurIPS.
2. Choromanski, K., et al. (2021). Rethinking attention with performers. ICLR.

## A Appendix: Mathematical Derivations

### A.1 Softmax Kernel Derivation

The softmax kernel is defined as:

$$K_{\text{softmax}}(x, y) = \exp(x^T y) \quad (14)$$

We can rewrite this using the identity:

$$\exp(x^T y) = \exp\left(\frac{\|x\|^2 + \|y\|^2 - \|x - y\|^2}{2}\right) \quad (15)$$

$$= \exp\left(\frac{\|x\|^2}{2}\right) \exp\left(\frac{\|y\|^2}{2}\right) \exp\left(-\frac{\|x - y\|^2}{2}\right) \quad (16)$$

The Gaussian kernel  $\exp(-\|x - y\|^2/2)$  can be approximated using random Fourier features.

### A.2 Random Feature Maps for Gaussian Kernel

For the Gaussian kernel  $K(x, y) = \exp(-\|x - y\|^2/(2\sigma^2))$ , we have:

$$K(x, y) = \mathbb{E}_{w \sim \mathcal{N}(0, I)}[\cos(w^T(x - y))] \quad (17)$$

This leads to the random feature map:

$$\phi(x) = \frac{1}{\sqrt{m}}[\cos(w_1^T x), \sin(w_1^T x), \dots, \cos(w_m^T x), \sin(w_m^T x)] \quad (18)$$