SFT: Sampling-based Foundational Transformer

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Abstract

The extraordinary success of transformers as a sequence processing model is hindered by two things: the quadratic complexity of self-attention modules and the difficulty of transformer training. In this paper, we introduce two mechanisms aiming to alleviate these two mentioned problems: a novel neural-guided down-sampling for self-attention and a new attention non-linearity with linear-scaled and convex characteristics. Those two procedures not only speed up the self-attention computation but also greatly ease the pain of meticulous hyper-parameter tuning. Moreover, our relative positional encoding procedure applies to many types of data structures as well as special restraints, such as rotational invariance (i.e. for 3D point clouds). It is important to emphasize that our model is a foundation model that can work with multiple types of data structures including point clouds, graphs, and long-range sequences. As a foundation model, we achieved competitive results on many data structures against specialized ones in standard benchmarks, while being faster and more efficient in inference than other state-of-the-art baselines. We release our source code in supplementary materials.

1 Introduction

Transformers (Vaswani et al., 2017) have been successfully applied to a wide variety of tasks on many data structures, namely sequence (Vaswani et al., 2017; Radford et al., 2019; Devlin et al., 2019), point cloud (Lee et al., 2019; Zhao et al., 2021; Yang et al., 2019), and graph (Yun et al., 2019; Rampášek et al., 2022; Shirzad et al., 2023; Ngo et al., 2023). Its successes can be characterized by the self-attention module. The self-attention module can model long-range dependencies without suffering from vanishing gradients like its predecessor - recurrent neural networks (RNN). It also can transform the whole sequence simultaneously like convolutional neural networks (CNN). This allows the model to scale up to a very big size, enabling large language modeling.

The problem is that self-attention has quadratic complexity, which forbids it from running on very long sequences. To reduce the computational complexity, a considerable body of literature has delved into sparsity patterns (Beltagy et al., 2020; Ainslie et al., 2020; Zaheer et al., 2020; Shirzad et al., 2023) and low-rank projection (Wang et al., 2020). Low-rank projection (Wang et al., 2020) although seems to be very promising, has inherent limitations on the performance at the larger end of scale. On the other hand, sparse transformers have proven themselves practical in large language modeling with hard-coded sparse patterns (Child et al., 2019).

In this work, we focus on sparse global attention along with some tweaks to trivialize the training process. We are interested in sparse global attention because its simplicity allows both a subquadratic asymptotic complexity and a **lower practical runtime**. We notice that most sparse attention mechanisms either utilize a fixed sparse pattern (Beltagy et al., 2020; Child et al., 2019) or rely on random sparse patterns (Shirzad et al., 2023) or a combination of these (Zaheer et al., 2020). Our initial idea is to use a differentiable sampling method to learn a subsampling pattern. Based on Gumbel-softmax reparameterization, we design sampling with and without replacement through neural importance score computation. This way, the sparse global self-attention can learn to attend to important tokens and is usable on non-sequential data structures like point clouds and graphs.

The attention nonlinearity we design is derived from the maxout network(Goodfellow et al., 2013). We combine it with a ReLU-based probability function instead of the Softmax function previously seen in transformers. The combination ultimately makes each of our transformer cells pseudoconvex on its parameters and is linear-scaled. This greatly alleviates the hyperparameter tuning pain of transformers. We further show that our maxout attention nonlinearity combined with the ReLU-based probability function allows better relative information aggregation. To demonstrate the effectiveness of relative information aggregation via positional encoding, we apply it to rotational invariant point cloud tasks, with coordinate information masked out of the input sequence. In this setting, only transformed Euclidean distance is introduced to the attention matrix. This technique (the ReLU-based probability function and the convex attention non-linearity) can be applied to any other self-attention-based model to increase the model expressivity.

In this paper, we conduct extensive experiments on point cloud, graph, and sequence datasets. For point clouds, we benchmarked the model via classification (Wu et al., 2015) and semantic segmentation (Chang et al., 2015; Armeni et al., 2016) tasks, in both conventional paradigms as well as rotational insensitive ones. For graphs, we evaluate our method using two Peptide datasets (Singh et al., 2015) and one Computer Vision dataset (Everingham et al., 2010). For sequences, we used the long-range arena benchmark (Tay et al., 2021) featuring four classification tasks and one retrieval task on these datasets: ListOps (Nangia & Bowman, 2018), IMDb review (Maas et al., 2011), ACL Anthology Network (Radev et al., 2009), Grayscaled CIFAR-10 (Krizhevsky & Hinton, 2009), and Pathfinder (Linsley et al., 2018). We achieve competitive results on these benchmarks as a foundation model working on both point clouds and sequences compared to the specialized ones, featuring faster empirical runtime.

In short, our contributions can be summarized as follows:

- Efficient linear complexity sparse self-attention in terms of the number of tokens,
- Differentiable and parallelizable sampling without replacement method that is optimization-friendly,
- Pseudoconvex transformer layer that does not suffer from gradient vanishing and exploding with theoretical backings,
- Zero-additional computing cost rotation-invariant addon for point cloud transformers,
- Outperformance over many well-known methods on standard benchmarks.

We provide the detailed theoretical analysis in the Appendix Section A.

2 Related works

Efficient Transformers. The scalability of transformers is hindered by the quadratic complexity of self-attention modules. Hence, numerous works have delved into sparsity (Beltagy et al., 2020; Ainslie et al., 2020; Zaheer et al., 2020; Shirzad et al., 2023), low-rank projection (Wang et al., 2020), hashing-based method (Kitaev et al., 2020), and kernel-based methods (Choromanski et al., 2021; Katharopoulos et al., 2020) to sacrifice the expressivity of transformers for a sub-quadratic construction. Our review of contemporary efficient transformers is influenced by this survey by (Tay et al., 2022). Linformer (Wang et al., 2020) is based on the low-rank assumption of self-attention matrices, realized via projection matrices. As one of the earliest works in efficient transformers, it has flaws in both scalability and fixed sequence length. Subsequent work like Linear Transformer (Katharopoulos et al., 2020) redesigns the similarity kernel previously as a softmax of dot-product score (or any other kernels) to one made of a linear probability cage. The modification frees them from the recomputation of the multiplication of key-value matrices, making attention computational cost $O(N)$, where N refers to the number of tokens. Methods like (Beltagy et al., 2020) utilize three choices of fixed-sparsity-patterns: sliding window, dilated sliding window, and global+sliding window. Similarly, (Zaheer et al., 2020) uses a combination of different sparse patterns at one time: random attention, window attention, and global attention. On graphs, (Shirzad et al., 2023) also combines different sparsity patterns but with a constraint on the random-generated one: it has to be an expander graph. The hard-coded sparsity effectively linearized the complexity of transformers and is empirically fast. However, intuitively, no pattern

or finite set of patterns fits all problems; therefore, there is also a line of work dedicated to a differentiable sparsity. (Roy et al., 2021) drew a relationship from MIPS problem (Maximum Inner Product Search) and the Nearest-Neighbor Search algorithm, when both the query and key vectors are unit vectors. With their online k-means algorithm, their method attends each query vector to every key vector belonging to the same cluster, thus, bringing the complexity down to $O(n^{1.5})$, with n is the number of tokens. Empirically, however, their method is not fast as it needs a k-means construction and extensive specialized implementation for sparse operators. We see that the literature currently lacks a fast learnable sparsity and this is what we provide, based on sampling method. (Lee et al., 2019), is most similar to our global attention scheme, as it is also based on sampling. Their method uses a multi-head attention stacked on one another to perform sampling. Except, our method learns a sparsity pattern for global attention, which has been proven to be more robust.

Point Clouds. Deep Learning has been applied in Point-Cloud-related problems, including 3-D Shape Classification, 3-D Point Cloud Segmentation, and others. Our literature review on Point Cloud methods is inspired from (Guo et al., 2021; Zhang et al., 2023; Gerken et al., 2023) and other contemporary literature, covering a wide range of geometric deep learning. Data structure-wise, point cloud works can be classified into three types: point/mesh, voxel, and multi-view; applied by different deep learning methods. Multi-view based methods like (Su et al., 2015; Yu et al., 2018) process point cloud via a sequence of rendered 2-D images of objects from different views, enjoying the early breakthroughs of deep learning-based computer vision (He et al., 2016). The voxel-based method (Maturana & Scherer, 2015; Qi et al., 2016) operates on a 3-D grid representing the object, which also uses convolutional neural networks. The voxel-based method is computing-intensive: the number of voxels grows cubically to the grid resolution. Therefore, numerous methods like (Riegler et al., 2017) are dedicated to the sparsification of the voxel grid. OctNet (Riegler et al., 2017) sparsify the voxel grid using an octree to allocate more memory and computation resources to denser areas of the voxel grid. In contrast, point/mesh-based methods like the works by (Charles et al., 2017; Qi et al., 2017; Zhao et al., 2021) use unprocessed inputs (3-D coordinates with/without surface normal vectors). These works often share several components: local permutation invariant point operators, global feature aggregation, and point downsampling operators. Methods-wise, point cloud works can be classified into types: local-aggregation-based methods and global-aggregation-based methods. Local aggregators in point cloud literature usually feature convolutional layers or point-to-point global aggregators with self-attention. Convolutional-powered local aggregators can take many forms depending on the data structure: 2-D convolutional layers (Su et al., 2015; Yu et al., 2018) for multi-view, 3-D convolutional layers (Maturana & Scherer, 2015; Qi et al., 2016) for voxel grid, graph convolutional layers (Shi & Rajkumar, 2020) for point graph (usually constructed using kNN or distance ball), and kNN-powered local feature aggregator (or point convolution operators) (Qi et al., 2017; Xu et al., 2018). Point-Conv (Wu et al., 2019) and Point-Transformer (Zhao et al., 2021) also feature point interpolation operators as an aggregation method. Global feature aggregation in point cloud literature is dominated by the likes of self-attention (Vaswani et al., 2017) popularized by the fact that the module has been so successful in modeling long-range dependencies in sequential processing. Point-Transformer (Zhao et al., 2021) is one of the works featuring long-range dependency modeling. It also takes account of each point's locality via nearest neighbor max pooling, which also allows the model to operate on higher-level features as they progress through deeper layers.

SO(3) Point Cloud. As point clouds exist in a 3-D Euclidean space, the rotation of objects should not change what those objects are. This is called the rotational invariance characteristics of some point cloud models and is an active area of research. Early research relies on data augmentation to achieve rotational invariance; however, it should be noted that covering all possible rotations is not achievable. Subsequent ones rely on modules satisfying one of the two characteristics: rotational invariant (Sun et al., 2019; Li et al., 2022; 2023) or rotational equivariant (Chen et al., 2021; Anderson et al., 2019; Deng et al., 2021; Kaba et al., 2023). Equivariant-based methods in point cloud, as a generalization to invariant-based ones, feature diverse mechanisms satisfying the equivariant constraint: $f(r(x, \alpha)) = r(f(x), \alpha)$, where f, r, and α is the equivariant mapping, the rotation function, and the rotation angle, respectively. As an early work, similar to the existing equivariant literature in other data structures like images, (Chen et al., 2021) develops a spherical point convolution operation. (Anderson et al., 2019; Thomas et al., 2018; Cohen et al., 2018) propose learning on Fourier domain by utilizing spherical tensors and Fast Fourier Transform on $SO(3)$ group. This allows them to retain perfect information of the whole point cloud on each layer, sequentially without a complicated multi-path model structure. (Deng et al., 2021) extends each neural node to have 3-D representation, with

different linear projection and non-linearity. Their method is elegant and simple enough to apply to any other point cloud framework. It sees performance degradation in (Charles et al., 2017) but retains full performance on (Su et al., 2015). In rotational-invariant literature, Euclidean distance is the most commonly used feature (Jing et al., 2021; Maron et al., 2019; Li et al., 2023). The reason: it is simple and it contains all geometric information of any point cloud (Satorras et al., 2021). (Li et al., 2023) further shows that GNN is incapable of distinguishing certain point cloud cases given distance matrix and proves that a k-tuple-distance is capable of capturing any k-order geometric features. In line with other rotational-invariant via GNN methods, we show that rotational invariance-via Euclidean features can be efficiently applied to transformers in the form of relational positional encodings, with significant architectural changes. In addition, we provide an empirical analysis of the ability of our transformer with relative positional encodings.

Graphs. Graphs are used to represent relational data with a variety of use cases, e.g., small atomic structures (Wu et al., 2018; Townshend et al., 2022) for drug discovery, knowledge graphs (Hogan et al., 2021; Ko et al., 2021; Choudhary et al., 2021) for reliable information retrieval, etc. Modern graph pattern recognition relies on deep learning with the emerge of Messing Passing Neural Network (MPNN) (Gilmer et al., 2017). It is a learning paradigm where the computation of each node feature relies solely on its locality. Graph Convolutional Network (GCN) (Scarselli et al., 2009; Kipf & Welling, 2017) is the earliest work of this kind, where each node aggregates the feature of adjacency nodes using a permutation invariant operator. (Hy et al., 2018; 2019) extends the GCN model to higher-order while respecting the permutation symmetry by proposing the use of covariant tensor operators. Graph Attention Network (GAT) (Veličković et al., 2018) improves GCN by introducing a mechanism to select important nodes. These two are the classical graph neural networks and they suffer from overfocusing on locality; which prevents them from drawing meaningful long-range relationships (Dwivedi et al., 2022b; Ngo et al., 2023; Trang et al., 2024). Researchers have designed two mechanisms to tackle this with MPNN: virtual nodes (Pham et al., 2017) and k-hop neighborhood (Nikolentzos et al., 2020). Virtual nodes are designed to be nodes that connect to all nodes. This design provides information shortcuts for any two distant nodes, allowing global information to be propagated throughout all graph nodes. This concept is later explored and proved to be equivalent to low-rank-approximation-based transformer networks (Cai et al., 2023). K-hop MPNN aggregates information not only from the adjacency nodes but also the set of nodes that can be reached from the central node by following a path with a maximum of k edges. This increases the local receptive field of each graph node, which alleviates the mentioned problem, similar to the large convolutional kernel trend in computer vision (Ding et al., 2022). Transformer(Vaswani et al., 2017) operating on the complete graph domain (Bronstein et al., 2021), overcomes the mentioned problem purely through architectural design. While transformers are useful in extremely-large-scale learning tasks like language modeling, their performance is no good compared to traditional graph transformers in graph datasets, which often have few graphs with large numbers of nodes. Therefore, a considerable body of literature is devoted to making better handcrafted encodings as graph inductive bias (Ying et al., 2021; Dwivedi et al., 2022a; Rampášek et al., 2022). Graphormer (Ying et al., 2021) is one of the first graph transformer. It introduces several types of encodings: centrality encoding (how important the nodes are) and spatial encoding (how important the locality of each node is), which resembles how humans infer useful information from graphs. GraphGPS (Rampášek et al., 2022) designs a general pipeline for graph modeling by combining many prominent techniques into one: positional encoding (local PE, global PE, and relative PE), structural encoding, and multiple graph block types (MPNN layers (Brossard et al., 2021; Bresson & Laurent, 2018), attention layers (Vaswani et al., 2017; Choromanski et al., 2021; Zaheer et al., 2020)). Furthermore, (Ngo et al., 2023) proposes a multiscale version of graph transformer that learns to construct a hierarchy of coarsening graphs and a new form of positional encoding via graph wavelet transform. Our work focuses more on the scalability of the quadratic complexity graph transformer and the representative power of our relational information aggregation. This problem has been recently addressed by (Shirzad et al., 2023) where the attention mechanism is sparsified by virtual node and expander graphs. Learnable sparsity for sub-quadratic attention is relatively new technique, recently explored by (Trang et al., 2024). While the idea seems new and intriguing, it suffers from low convergence rate from stacked Gumbel-Softmax sampling layers to smoothen the discrete hierarchy. Here, we designed a more optimization-friendly differentiable sampler that can be stacked onto each other and a much simpler sparsity pattern (sampling versus hierarchy).

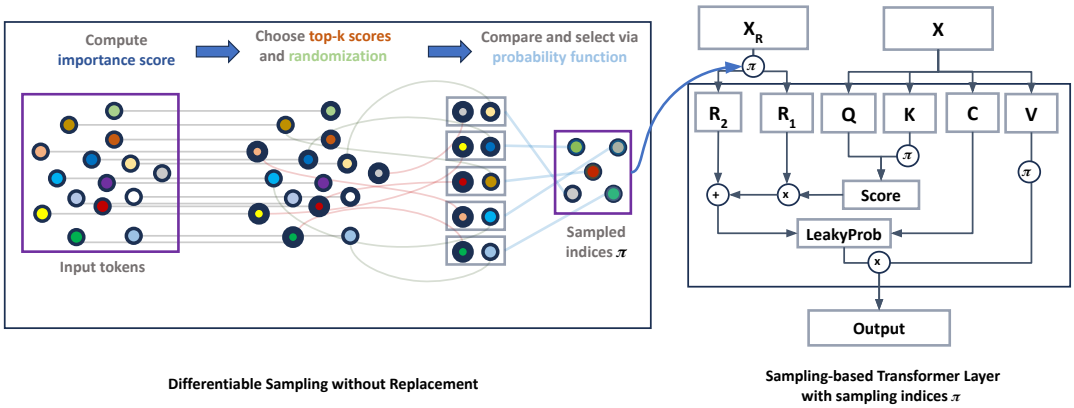

Figure 1: Overview of our proposed model sampling-based network. The sampled indices π are selected via top-k importance score (left), which then slices the matrices in our CASA network (right).

3 Background

The self-attention mechanism is a core component of transformer models to capture long-range dependencies. Let $\mathbf{X} = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n\} \in \mathbb{R}^{n \times d}$ represent a sequence of n d-dimensional vectors, $\mathbf{Q}$, $\mathbf{K}$, and $\mathbf{V}$ vectors representing query, key, and value vectors are created using three learnable linear transformation: $\text{Linear}(\mathbf{X}) : \mathbb{R}^d \to \mathbb{R}^d$. Then, using the $\mathbf{Q}$, $\mathbf{K}$, and $\mathbf{V}$ vectors, it creates another sequence by aggregating tokens satisfying certain criteria, expressed as follows:

$$\text{Attn}(\mathbf{X}) = f\left(g(\mathbf{Q}, \mathbf{K})\right)\mathbf{V}, \tag{1}$$

where f and g are attention non-linearity and attention score functions, respectively. The earliest transformer (Vaswani et al., 2017) uses softmax and scaled dot product functions as f and g. Replacements of f or g compared to the vanilla transformer (Katharopoulos et al., 2020; Wortsman et al., 2023; So et al., 2021; Shen et al., 2023) are created to address the problem of quadratic complexity, over-centralized attention, and ease of training or just motivated purely from empirical results. In our work, we introduce changes to both f and g to take care of the mentioned problems and further improve the theoretical expressivity of transformers, regarding relative positional encodings.

4 Method

4.1 Overview

Our method is a composition of neural-based sampling without replacement method, modifications to the self-attention mechanism with rigorous theoretical justifications, and supporting layers. Similar to Linformer (Wang et al., 2020) applying low-rank approximation to key and value vectors, we delve into the sampling procedure for key and value vectors, elaborated in Section 4.2. Next, we describe our easy-to-optimize attention score construction described in Section. The score is then combined with relative positional encodings via leaky probability formulation. These two processes are discussed in detail in Section 4.3. Finally, the layer ends with a feed-forward network, transforming the vector representation of the tokens. The method is summarized in Algorithm 1.

4.2 Differentiable Sampling Without Replacement

We formally define the operator that samples k of n real m-dimensional vectors as a function $\text{Sam}(\mathbf{X}) : \mathbb{R}^{nm} \to \mathbb{R}^{km}$. The sampling operator is a linear operator: $\text{S}(\mathbf{X}) = \mathbf{P}\mathbf{X}$. Here, $\mathbf{P}$ and $\mathbf{X}$ represent the selection

Algorithm 1 Sampling-based Transformer Layer

Input: Input token matrix $\mathbf{X}$, relative PE features $\mathbf{X_r}$
Output: Updated token matrix $\mathbf{X}$

1: **Transform token matrix to query, key, and value vectors**
2: $\mathbf{Q} \leftarrow \mathbf{X} * W_Q + B_Q$
3: $\mathbf{K} \leftarrow \mathbf{X} * W_K + B_K$
4: $\mathbf{V} \leftarrow \mathbf{X} * W_V + B_V$
5: **Compute importance score**
6: $\mathbf{S} \leftarrow \mathbf{X} * W_S + B_S + \text{Gumbel}(0, 1)$
7: $\pi \sim \text{Sample}(\mathbf{S})$
8: $\tilde{\mathbf{K}} \leftarrow \mathbf{K}[\pi]$
9: $\tilde{\mathbf{V}} \leftarrow \mathbf{V}[\pi]$
10: $\tilde{\mathbf{X}}_\mathbf{r} \leftarrow \mathbf{X_r}[\pi]$
11: **Compute attention score**
12: $\mathbf{C} \leftarrow \text{Softplus}(\tilde{\mathbf{V}} * W_C + B_C)$
13: $\mathbf{R_1} \leftarrow \text{F}_1(\tilde{\mathbf{X}}_\mathbf{r} * W_{R_1} + B_{R_1})$
14: $\mathbf{R_2} \leftarrow \text{F}_2(\tilde{\mathbf{X}}_\mathbf{r} * W_{R_2} + B_{R_2})$
15: $\mathbf{A} \leftarrow \text{Prob}(\text{Score}(\mathbf{Q}, \tilde{\mathbf{K}}, \mathbf{R_1}, \mathbf{R_2}), \mathbf{C})$
16: $\mathbf{X} \leftarrow \mathbf{X} + \mathbf{A} * \tilde{\mathbf{V}}$
17: $\mathbf{X} \leftarrow \text{LayerNorm}(\mathbf{X})$
18: **Feed-Forward Network**
19: $\mathbf{X} \leftarrow \mathbf{X} + \text{FFN}(\mathbf{X})$
20: $\mathbf{X} \leftarrow \text{LayerNorm}(\mathbf{X})$
21: **Return X**

matrix and the input token matrix. $\mathbf{P}$ is a row-wise concatenation of one-hot vectors defined as follows:

$$P = \begin{bmatrix} \text{onehot}(x_0) \\ \text{onehot}(x_1) \\ \vdots \\ \text{onehot}(x_{k-1}) \end{bmatrix}. \tag{2}$$

We sample the vectors based on importance scores: the vectors' importance scores represent the likeliness of being picked. The importance scores are computed via a learnable linear transformation: $\text{Linear}(x) : \mathbb{R}^m \to \mathbb{R}$. We use Gumbel distribution to include randomness to the importance scores, similar to (Jang et al., 2017). The Gumbel-Distribution PDF and importance score computation is given as follows:

$$\text{Gumbel}(0, 1)(x) = e^{-(x+e^{-x})},$$
$$\text{ImportanceScore}(x) = \text{Linear}(x) = x * W_S + B_S.$$

Gumbel-Softmax provides a differentiable choosing function via continuous relaxation of Gumbel-Distribution. The sampling procedure via Gumbel-Softmax is given as follows:

$$s(x, z, g) = \sum_i \left[\frac{\exp\left(\frac{z_i + g_i}{\tau}\right) * x_i}{\sum_j \exp\left(\frac{z_j + g_j}{\tau}\right)} \right], \tag{3}$$

where s, x, z, and g are the sampling function, the value vectors, the score vectors, and Gumbel random variables, respectively.

The problem is that Gumbel-Softmax gives off very small gradients due to its exponential nature. This is fine for its intended usage: to be put at the last layer or in a few specialized modules, but not a vital component in repeating sequential model cells. Hence, we linearize the probability formula. The formula of the Softplus

function and its sampling derivative is given as follows:

$$\text{Softplus}(x) = \log(1 + \exp(x)), \tag{4}$$

$$s(x, z, g) = \sum_i \left[\frac{\text{Softplus}\left(z_i + g_i\right) * x_i}{\sum_j \text{Softplus}\left(z_j + g_j\right)} \right]. \tag{5}$$

From here, we can derive the trivial sampling with replacement procedure by repeatedly applying Equation equation 3 or Equation equation 5, as follows:

$$\mathcal{S} = \text{ImportanceScore}(\mathbf{X}), \tag{6}$$

$$\text{Sam}(\mathbf{X}, k) = \text{Concat}_i^k \left(s(\mathbf{X}, \mathcal{S}, g_i) \right). \tag{7}$$

The drawback of sampling with replacement is repeating sampled vectors, which severely damages the model expressivity. We provide an analysis on how severe it damages the expressivity via drawing a relationship between the expected number of unique sampled vectors and the number of vectors as follows:

$$\mathbb{E}(N_k) = \sum_{i=0}^{k-1} (-1)^i \binom{k}{i+1} \frac{1}{N^i}. \tag{8}$$

Equation equation 8 shows that the expected number of unique sampled vectors is never equal to the number of vectors, no matter how many vectors we sample. Equivalently, the expressivity of a sampling-with-replacement-based self-attention is never equal to full self-attention, even when the computational cost is magnitudes higher.

Here, we construct a data-driven differentiable sampling without replacement that is parallelizable, in contrast to existing sequential ones. Our method sorts the vectors by importance scores, selects k vectors with the highest scores in set $\mathcal{S}_1$ and k random vectors in set $\mathcal{S}_2$, satisfying this constraint: $\mathcal{S}_1 \cap \mathcal{S}_2 = \emptyset$, concatenates set $\mathcal{S}_1$ and set $\mathcal{S}_2$ into set of k binary bins $\mathcal{S}$, and finally selecting k vectors using Equation equation 5. While the sorting procedure is not differentiable, the whole procedure ensures the important tokens receive higher scores than the unimportant ones iteratively through a Softplus probability bin and gradient descent process. The algorithm is described in Algorithm 2.

4.3 Attention Matrix Construction

To recall, any generic self-attention is expressed as follows:

$$\begin{aligned}
\mathbf{Q} &= \text{Linear}_{\mathbf{Q}}(\mathbf{X}) = \mathbf{X} * W_Q + B_Q, \\
\mathbf{K} &= \text{Linear}_{\mathbf{K}}(\mathbf{X}) = \mathbf{X} * W_K + B_K, \\
\mathbf{V} &= \text{Linear}_{\mathbf{V}}(\mathbf{X}) = \mathbf{X} * W_V + B_V, \\
\text{Attn}(\mathbf{X}) &= f\left(g(\mathbf{Q}, \mathbf{K})\right) \mathbf{V}.
\end{aligned}$$

In vanilla transformer (Vaswani et al., 2017), function f and g are softmax and scaled-dot product, respectively, expressed as follows:

$$f(\mathbf{X})[i] = \frac{\exp(\mathbf{X_i})}{\sum_j \exp(\mathbf{X_j}) + \epsilon}, \tag{9}$$

$$g(\mathbf{X}, \mathbf{Y})[i, j] = \mathbf{1}^{\mathrm{T}} (\mathbf{X_i} \odot \mathbf{Y_j}), \tag{10}$$

$$\text{Attn}(\mathbf{X}) = \text{Softmax}\left(\frac{\mathbf{Q}\mathbf{K}^{\mathrm{T}}}{\sqrt{d}} \right) \mathbf{V}, \tag{11}$$

Algorithm 2 Differentiable Sampling Without Replacement

Input: Input set $\mathbf{X}$, number of sampled vectors k
Output: Sampled set $\tilde{\mathbf{X}}$

1: **Compute importance score**
2: $\mathbf{S} \leftarrow \mathbf{X} * W_S + B_S + \text{Gumbel}(0, 1)$
3: $\mathbf{X_S} \leftarrow \text{Concat}(\mathbf{X}, \mathbf{S})$
4: **Sort by importance score**
5: $\pi \leftarrow \text{Argsort}(\mathbf{S})$
6: $\mathbf{X_S} \leftarrow \mathbf{X_S}[\pi]$
7: **Generate set $\mathcal{S}_1$ and set $\mathcal{S}_2$**
8: $\mathcal{S}_1 \leftarrow \mathbf{X_S}[: k]$
9: $\mathbf{X_S} \leftarrow \mathbf{X_S}[k :]$
10: $\mathbf{X_S} \leftarrow \text{Shuffle}(\mathbf{X_S})$
11: $\mathcal{S}_2 \leftarrow \mathbf{X_S}[: k]$
12: **Sample via Binary Selection**
13: $\mathcal{S}_1[\mathbf{S}] \leftarrow \text{Softplus}(\mathcal{S}_1[\mathbf{S}])$
14: $\mathcal{S}_2[\mathbf{S}] \leftarrow \text{Softplus}(\mathcal{S}_2[\mathbf{S}])$
15: $\tilde{\mathbf{X}} \leftarrow \dfrac{\mathcal{S}_1[\mathbf{S}] * \mathcal{S}_1[\mathbf{X}]}{\mathcal{S}_1[\mathbf{S}] + \mathcal{S}_2[\mathbf{S}]} + \dfrac{\mathcal{S}_2[\mathbf{S}] * \mathcal{S}_2[\mathbf{X}]}{\mathcal{S}_1[\mathbf{S}] + \mathcal{S}_2[\mathbf{S}]}$
16: **Return $\tilde{\mathbf{X}}$**

with Equation equation 9 and Equation equation 10 constructs Equation equation 11 using Equation equation 1. Subsequent attention construction may only specify the attention nonlinearity function f and the attention score function g.

It is well-known that transformer is hard to optimize (Liu et al., 2020). We propose a conjecture that the ease of network training is strongly related to the componentwise convexity and the backpropagated gradient scale. This is based on a stark difference between transformers and other network architectures: convolutional neural networks and multi-layer perceptrons are all componentwise pseudoconvex but self-attention modules are not. We define a sequential model as componentwise pseudoconvex if and only if the model is a stack of pseudoconvex components to those components' weights.

We discovered the pairwise Maxout attention nonlinearity (derived from the Maxout activation (Goodfellow et al., 2013)) is convex. When combined with the attention module (including the feed-forward network), the whole transformer layer is pseudoconvex, with informal proof in Section 4.4 and formal one in the Appendix A.2. For computational efficiency, both $\text{Linear}_\mathbf{Q}$ and $\text{Linear}_\mathbf{K}$ project n-dimensional vectors into h-dimensional-vectors, where n and h are number of input dimensions and number of attention heads, respectively. The following equations express leaky factor, ReLU-probability function, and the pairwise Maxout attention nonlinearity, respectively:

$$
\begin{aligned}
&\mathbf{C} = \text{Linear}_\mathbf{C}(\mathbf{X}) = \mathbf{X} * W_C + B_C, \\
&f(\mathbf{X})[i] = \frac{\text{ReLU}(\mathbf{X_i})}{\sum_j \text{ReLU}(\mathbf{X_j}) + \sum \text{Softplus}(\mathbf{C}) + \epsilon}, \\
&g(\mathbf{X}, \mathbf{Y})[i, j] = \mathbf{1}^{\mathrm{T}} \max(\mathbf{X_i}, \mathbf{Y_j}).
\end{aligned}
$$

While the leaky factor is initially introduced for numerical stability, it allows better relative information aggregation. In practice, we use a linear combination for relative positional encoding alongside the leaky probability function. The relative positional encoding matrix receives different linear transformations projecting n-dimensional-vectors into h-dimensional-vectors for each layer. With $\mathbf{X_R}$ being the relative positional encoding matrix, the following equations express how we incorporate relative positional encoding

into attention scores:

$$W_{\mathbf{X_R}} = \text{Linear}_{\text{W}_{\mathbf{X_R}}}(\mathbf{X_R}),$$
$$B_{\mathbf{X_R}} = \text{Linear}_{\text{B}_{\mathbf{X_R}}}(\mathbf{X_R}),$$
$$g(\mathbf{X}, \mathbf{Y})[i, j] = \mathbf{1}^\top \max(\mathbf{X_i}, \mathbf{Y_j}) \odot \text{Softplus}(W_{\mathbf{X_R}}) + B_{\mathbf{X_R}}.$$

Leakiness injects rank. For any non-leaky probability function, the self-attention fails to distinguish any two tokens of a rank-1 uniform input, commonly known as the over-smoothing phenomenon (Noci et al., 2022; Dong et al., 2023). This case proves relative-positional-encoding-based (or RPE-based) Transformers' approximation power is far from being universal (Luo et al., 2022) as opposed to absolute-positional-encoding-based (APE-based) Transformer (Yun et al., 2020). This barrier limits Transformers' performances in relative positional data structures such as graphs and point clouds. In contrast, with the addition of the positive leaky component $\mathbf{C}$, we empirically show that the rank progression of token representation through our RPE-based Transformer gradually gain some rank. We will name this phenomenon **rank injection**. To visualize rank injection, in Figure 2, we use 30 samples of random weights to measure the rank progression of token representation with one random normal relational matrix over the layers.

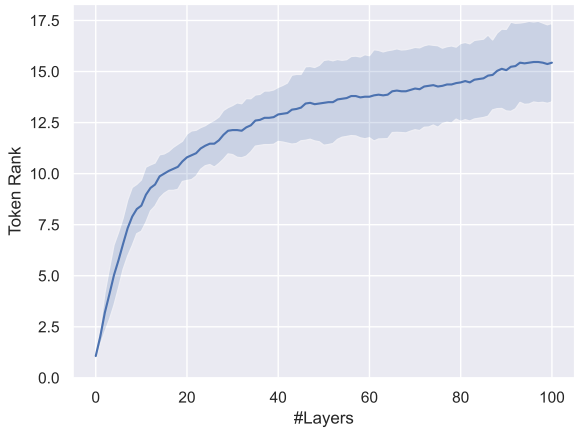

Figure 2: Rank progression of token representation with 256 tokens and embedding size 512 through 100 randomly initialized single head transformer layers with leaky probability function and pairwise maxout attention nonlinearity.

The reason to use a multiplicative relative positional encoding alongside the conventional relative attention bias is simple: we want the model to be able to zero-ize attention for very unrelated tokens efficiently. As this relative attention formulation can be very scale-sensitive, we introduce a learnable bounding activation trick to deal with out-of-distribution relative attention factors, expressed as the following equation:

$$\text{AttentionLimit}(\mathbf{A}, W_L) = \min(\mathbf{A}, \text{Softplus}(W_L)), \tag{12}$$

where $\mathbf{A}$ and W_L are the relative attention matrix and scalar bounding weight, respectively. This function is applied to $W_{\mathbf{X_R}}$ and $B_{\mathbf{X_R}}$. This can be useful for point cloud learning tasks given the distance between points can be very large. The technique is similar to the index clipping technique found in (Wu et al., 2021).

4.4 Theoretical Analysis Summary

In order to theoretically justify the effectiveness of our proposed model, we will analyze its convexity power. Even though rigorously, it is not possible for probability distribution functions to exhibits actual convexity (Tsurumi, 1966), a weaker yet significant function class that also draw heavy attention in optimization theory (Liu et al., 2012) (Qin et al., 2016) are **pseudoconvex functions**, defined as follows:

Definition 4.1. Let ∇ denote the gradient operator and $\mathcal{S} \subset \mathbb{R}^n$ is a convex open set, a function $f : \mathcal{S} \to \mathbb{R}$ is said to be pseudoconvex in $\mathcal{S}$ if for any $x_1, x_2 \in \mathcal{S}$ such that $\langle \nabla f(x_1), x_2 - x_1 \rangle \geq 0$, then $f(x_1) \geq f(x_2)$.

Pseudoconvex functions hold a very important lemma, which states that **every stationary point is also a global minimizer**. To visualize this concept, we sketched two functions with convex and pseudoconvex properties respectively in Figure 3. In application to deep learning, pseudoconvexity not only tackle tricky challenges in optimzations such as saddle points and local minimas but also improve the overall performance of artificial neural networks.

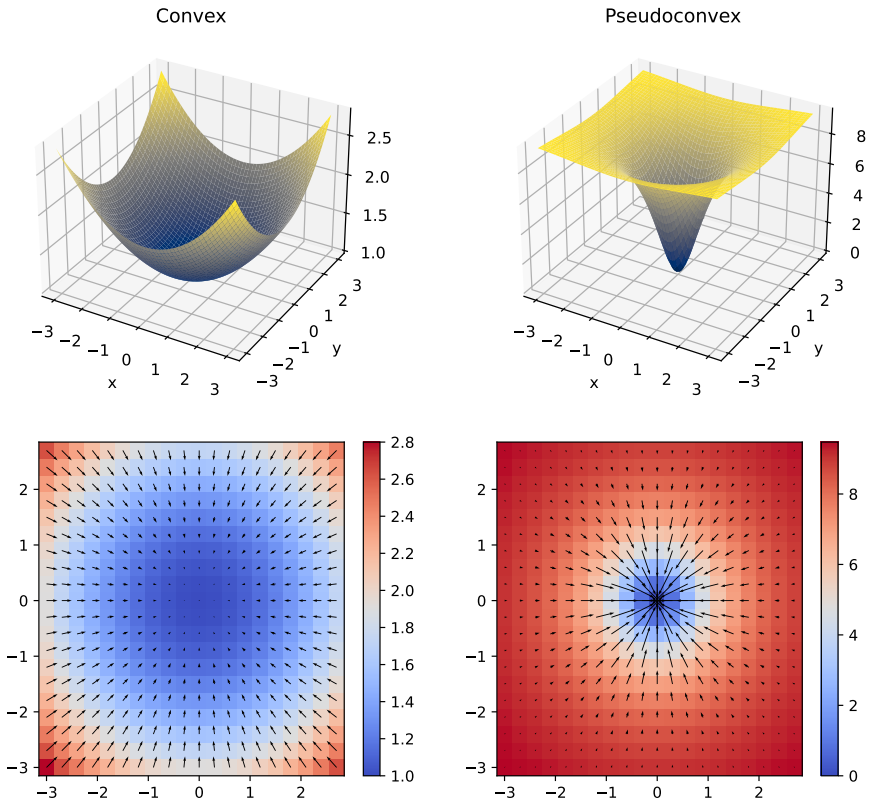

Figure 3: Comparison between a convex function $z = \frac{x^2+y^2+10}{10}$ (top-left) and a pseudoconvex function $z = \frac{10(x^2+y^2)}{x^2+y^2+1}$ (top-right) and their corresponding heatmaps with gradient vector fields (bottoms). The pseudoconvex function greatly resemble its convex counterpart regarding the search for the local minima.

In summary of our theoretical analysis, we will first show the convex inefficiency of two well-known attention settings, namely the vanilla attention (Vaswani et al., 2017) and ReLU-based attention with dot product (Shen et al., 2023) by handpicking some representative counterexamples. The details of the statements and corresponding proofs are provided at Appendix Section A.1.

Next, we will rigorously show that **CASA is pseudoconvex with both linear and GeLU activation in FFN layer**. Informally, we present the result as follows.

Theorem 4.2. ***(informal)*** *The CASA layer defined in Algorithm 1 with linear or GeLU FFN activation and no sampling is componentwise pseudoconvex with respect to certain combinations of weights.*

We provide the full theorem and proof in Appendix Section A.2.

In compensation to the non-decreasing gradient behaviour of pseudoconvex functions comparing to convex counterparts, we also derived an adaptive lower bound and global upper bound of the expectation of the Frobenius norm of the gradients of CASA, which is often referred as gradient norms for short, and analyze their complexity with respect to the number of tokens. The boundedness of the gradient norms should somewhat represent their magnitude and address the robustness of CASA against challenges such as gradient

vanishing and exploding while also show CASAs' resilience against phenomenas such as sharp minimas and flat minimas.

Theorem 4.3. ***(informal)*** *Let* $\mathbf{Sa} = \mathbf{Sa}(W_Q, W_K, W_V)$ *be the CASA attention layer output in Algorithm 1, then* $\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_V}\right\|_F^2$ *and* $\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_Q}\right\|_F^2$ *has complexity* $\Theta(n)$ *and* $\Theta(1)$ *respectively, where* n *is the number of tokens.*

Since the full proof for Theorem 4.3 is quite convoluted, we would like to sketch the proof as follows:

- Adaptive lower bound:
  - **Step 1:** Derive a fractional function form $f(\mathbf{W})/g(\mathbf{W})$ where $\mathbf{W}$ represents the set of parameters,
  - **Step 2:** Convexify the fractional form via the convex envelope derived by (Tawarmalani & Sahinidis, 2002),
  - **Step 3:** Evaluate the lower bound using the Jensen inequality,
  - **Step 4:** Make any simplification if necessary.
- Global upper bound: employ the norm product inquality and the Jensen inequality for concave functions.

The full statement and proof is at the Appendix Section A.3.

4.5 Complexity Analysis

Consider the input token $\mathbf{X} \in \mathbb{R}^{n \times d}$, query and key weights $W_Q, W_K \in \mathbb{R}^{d \times d_a}$.

The computational cost for each step is as follows:

- Linear transformations for $\mathbf{Q}, \mathbf{K}$ and $\mathbf{V}$: $O(nd^2)$,
- Importance score of the queries and keys: $O(nd)$,
- Selecting top-k importance score: $O(n \log n)$ with sorting method or $O(n)$ with quickselect algorithm,
- Attention from between n queries and top-k most important keys: $O(nkd_a)$,
- FFN network: $O(nd^2)$.

Given these complexities and considering the long-ranged data structures which can implies $n \gg d$, the asymptotic computational complexity of one single CASA layer is $O(n)$. The asymptotic space complexity of one single CASA layer is also $O(n)$.

5 Experiments

5.1 Objectives

The core of any foundation model is its efficacy in modeling diverse data modalities. And, the fundamental difference between data modalities is the different types of relationships between tokens. Therefore, we conduct extensive experiments to measure the ability of our attention mechanism to model dense low-rank (point clouds) and sparse high-rank relationships (graphs and sequences). As we propose our pseudoconvex mechanism, we also conduct a comparative experiment to measure the real runtime of our transformer formulation against the vanilla transformer.

In short, we answer three following questions:

- How effectively can leakiness encode relational information into the tokens' representation?
- How effectively can our sampling-based global attention model long-range interaction?
- How significant does our pseudoconvex formulation aid model convergence rate?

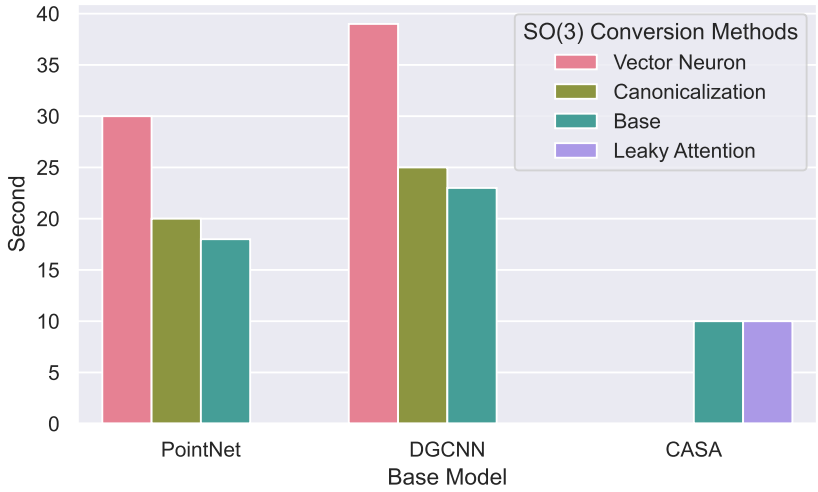

Figure 4: Inference time (in seconds) of the networks for ModelNet40 classification test split in 1 A100 GPU and 8 CPUs with a batch size of 32. The Vector Neuron (Deng et al., 2021) and Canonicalization (Kaba et al., 2023) framework is applied in PointNet (Charles et al., 2017) and DGCNN (Wang et al., 2019). The leaky attention function is applied to our CASA model. The results of others are taken from (Kaba et al., 2023).

5.2 Relational Learning

5.2.1 Dense Low-Rank Relational Learning

To measure the ability of our model in modeling dense low-rank relationship, we test our model on two point cloud tasks involving two datasets: Object Classification on ModelNet40 Wu et al. (2015), Part Segmentation on ShapeNetPart Chang et al. (2015); with/without rotational invariant constraint. The motivation we choose point cloud to experiment Dense Low-Rank Relational Learning is simple: rank of Euclidean Distance Matrix of p-dimensional points is at most $p + 2$ (Gower, 1985) and point cloud coordinates can be reconstructed from their Euclidean Distance Matrix through Multidimensional Scaling algorithm.

Our experiments on rotational invariant constraint specifically remove all of point cloud coordinates in input tokens, which forces our model to use only relational information to discriminate. By making our model rely solely on relational information, the experiment validates the generalizability of information obtained through rank injection phenomena. We further compare it against other dedicated rotational invariant models in Table 1 and it shows comparable performance to these dedicated rotational invariant methods, while can be inferenced **hundreds of percents** faster (computational time measured in Figure 4). Note that, our relative positional encoding scheme **can be dropped into any point cloud transformer**, making it rotational invariant with neglectable additional cost (because all of the point cloud transformers already feature relative positional encoding).

We also conduct experiments on point cloud datasets without rotational invariant constraints to measure how effective our method as a whole is in modeling non-sequential data in Table 2. It shows competitive results against other point cloud models. This is because our model does not include any data-modality-specific inductive bias (like the usage of kNN for locality heuristic) and is susceptible to overfitting in scenarios where data is not abundant.

5.2.2 Sparse High-Rank Relational Learning

To measure the ability of our model in modeling sparse high-rank relationship, we test our model on two data modalities: sequence and graph. For sequential tasks, we choose Long-Range-Arena Benchmark (Tay et al., 2021), a standard to measure the effectiveness of efficient transformer schemes in sequential modeling. For graph tasks, we choose three datasets: Peptides-func (Singh et al., 2015), Peptides-struct (Singh et al.,

Table 1: Experimental results to measure the effectiveness of leaky probability function in terms of transferring relative information to tokens' representation. The table shows shape classification results on ModelNet40 dataset (Wu et al., 2015) and part segmentation results on ShapeNetPart dataset (Chang et al., 2015) under rotational invariant constraint with popular baselines in rotational invariance/equivariant literature. z/z, z/SO(3), SO(3)/SO(3) signifies the model trained with 3D coordinates (no rotational invariant constraint), the model trained with rotational invariant features/trained using rotational equivariant transformation, and trained with random rotation data augmentation, respectively.

Method	**ModelNet40**		**ShapeNetPart**	
	z/z$^{\uparrow}$	**z/SO(3)**$^{\uparrow}$	**z/SO(3)**$^{\uparrow}$	**SO(3)/SO(3)**$^{\uparrow}$
SFCNN (Rao et al., 2019)	91.4	84.8	-	-
TFN (Thomas et al., 2018)	88.5	85.3	76.8	76.2
RI-Conv (Zhang et al., 2019)	86.5	86.4	75.3	75.3
SPHNet (Poulenard et al., 2019)	87.7	86.6	-	-
ClusterNet (Chen et al., 2019)	87.1	87.1	-	-
GC-Conv (Zhang et al., 2020)	89.0	89.1	77.2	77.3
RI-Framework (Li et al., 2022)	89.4	89.4	79.2	79.4
VN-PointNet (Deng et al., 2021)	77.5	77.5	72.4	72.8
VN-DGCNN (Deng et al., 2021)	89.5	89.5	81.4	81.4
CN(NL)-PointNet (Kaba et al., 2023)	79.9	79.6	73.5	73.6
CN(NL)-DGCNN (Kaba et al., 2023)	88.7	88.8	78.4	78.5
CASA (Ours)	91.1	87.2	78.3	-

Table 2: Experimental results to measure the effectiveness of our sparse attention on non-sequential data structure, particularly spatial data structure. The table shows shape classification results on ModelNet40 dataset (Wu et al., 2015) and part segmentation results on ShapeNetPart dataset (Chang et al., 2015) along with popular baselines in the point cloud analysis literature.

Method	**ModelNet40**		**ShapeNetPart**	
	mAcc$^{\uparrow}$	**OA**$^{\uparrow}$	**c. IoU**$^{\uparrow}$	**i. IoU**$^{\uparrow}$
PointNet (Charles et al., 2017)	86.2	89.2	80.4	83.7
Set Transformer (Lee et al., 2019)	-	90.4	-	-
PointNet++ (Qi et al., 2017)	-	91.9	81.9	85.1
SpecGCN (Wang et al., 2018)	-	92.1	-	-
PointCNN (Li et al., 2018)	88.1	92.2	84.6	86.1
DGCNN (Wang et al., 2019)	90.2	92.2	82.3	85.1
PointWeb (Zhao et al., 2019)	89.4	92.3	-	-
SpiderCNN (Xu et al., 2018)	-	92.4	81.7	85.3
PointConv (Wu et al., 2019)	-	92.5	82.8	85.7
Point2Sequence (Liu et al., 2019)	90.4	92.6	-	85.2
KPConv (Thomas et al., 2019)	-	92.9	85.1	86.4
InterpCNN (Mao et al., 2019)	-	93.0	84.0	86.3
Point Transformer (Zhao et al., 2021)	90.6	93.7	83.7	86.6
Sequoia (Trang et al., 2024)	88.4	92.0	80.6	83.8
CASA (Ours)	88.2	91.1	81.3	84.5

2015), and PascalVOC-sp (Everingham et al., 2010) in Long-Range-Graph-Benchmark (Dwivedi et al., 2022b), which is the equivalent of Long-Range-Arena-Benchmark for graph transformers.

The reason we chose these two data modalities to represent sparse high-rank relational learning is intuitive: both the causal relationship of sequences and graph adjacency matrix is very sparse yet high rank. The competitive experimental results of our model in Long-Range-Arena-Benchmark and Long-Range-Graph-Benchmark are shown in Table 4 and Table 3, respectively.

In sequential tasks, our model has competitive results against many other efficient transformers and the full attention transformer. However, it should be note that we did not reach the performance level of models designed specifically for sequential tasks like MEGA (Ma et al., 2023) and S4 (Gu et al., 2022). The EMA inductive bias or locality bias of SSM cannot be applied into other data structures like point clouds and graphs.

In graphs tasks, our model has relatively good results in peptides dataset compared to other efficient transformers, full attention transformer, and superior results to all classical message passing neural networks. However, since our transformer construction for graph is simple and does not rely on local information aggregation like GraphGPS Rampášek et al. (2022), it does not perform well on PascalVOC-sp dataset. This show a limitation on how our method's relational information aggregation.

Table 3: (Long Range Graph Benchmark) Performance on Peptide and Computer-Vision Graph datasets. The performance of our model on peptide-func, peptide-struct, and the computer vision-based PascalVOC datasets is measured using Average Precision (AP), Mean Absolute Error (MAE), and F1-score metrics, respectively.

Method	**Pept-func** $\uparrow$	**Pept-struct** $\downarrow$	**PasVOC-sp** $\uparrow$
GCN (Kipf & Welling, 2017)	0.5930	0.3496	0.1268
GCNII (Chen et al., 2020)	0.5543	0.3471	0.1698
GINE (Brossard et al., 2021)	0.5498	0.3547	0.1265
GatedGCN (Bresson & Laurent, 2018)	0.5864	0.3420	0.1265
GatedGCN (RWPE) (Bresson & Laurent, 2018)	0.6069	0.3357	0.1265
Transformer (LapPE) (Vaswani et al., 2017)	0.6326	0.2529	0.2694
Transformer (RWPE) (Vaswani et al., 2017)	0.6502	0.2620	0.2718
SAN (LapPE) (Kreuzer et al., 2021)	0.6384	0.2683	0.3230
SAN (RWPE) (Kreuzer et al., 2021)	0.6562	0.2545	0.3216
GPS (Rampášek et al., 2023)	0.6535	0.2500	0.3748
GPS-Sequoia-RWPE (Trang et al., 2024)	0.6755	0.2453	0.3379
CASA (Ours)	0.6674	0.2661	0.1961
CASA-RWPE (Ours)	0.6902	0.2655	0.2181

Table 4: (Long Range Arena) Accuracy on the full suite of long range arena (LRA) tasks. The performance of our model on peptide-func, peptide-struct, and the two computer vision-based datasets is measured using Average Precision (AP), Mean Absolute Error (MAE), and F1-score metrics, respectively.

Method	**ListOps**	**Text**	**Retrieval**	**Image**	**Pathfinder**
BigBird (Zaheer et al., 2020)	36.05	64.02	59.29	40.83	74.87
Reformer (Kitaev et al., 2020)	37.27	56.10	53.40	38.07	68.50
Performer (Choromanski et al., 2021)	18.01	65.40	53.82	42.77	77.05
Linformer (Wang et al., 2020)	35.70	53.94	52.27	38.56	76.34
Luna-256 (Ma et al., 2021)	37.98	65.78	79.56	47.86	78.55
Transformer (Vaswani et al., 2017)	36.37	64.27	57.46	42.44	71.40
Sequoia (Trang et al., 2024)	37.70	75.10	67.04	49.88	87.30
S4 (Gu et al., 2022)	88.65	76.02	87.09	86.09	86.05
MEGA (Ma et al., 2023)	63.14	90.43	91.25	90.44	96.01
CASA-Relative (Ours)	39.95	64.54	71.33	47.65	78.39

Table 5: Performance Gap between Relational and Absolute Positional Information Aggregation

	ModelNet40↑	ShapeNetPart↑	Peptides-func↑	Peptides-struct↓	PascalVOC-sp↑
Relational	87.2	78.3	0.67	0.2661	0.20
Absolute	91.1	81.3	0.69	0.2655	0.22
Performance Gap	3.9	3.0	0.02	-0.001	0.02

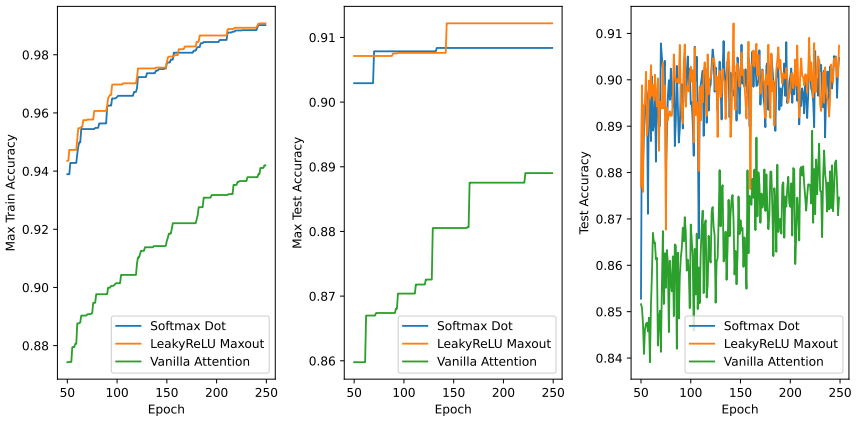

Figure 5: Comparison between learning curves of CASA with Leaky Relu-based + Maxout (orange), with softmax + dot product (blue) and vanilla transformer without relative information (green) on ModelNet40 throught 256 epochs. The actual test accuracy curve is shown (right) while the max accuracy through all epochs are also visualized during training (left) and testing (middle).

5.2.3 Performance Gap between Relational and Absolute Positional Information Aggregation

Additionally, we compare two variants of our models (with/without absolute position) on both Dense-Low-Rank and Sparse-High-Rank experiments. Despite promising results, we notice a significant performance gap on all of the experimented datasets: ModelNet40, ShapeNetPart, Peptides-func, Peptides-struct, PascalVOC-sp; shown in Table 5.

We suspect this is related to how we construct relational information since we only use one linear layer to transform relational information, which is an open question to future research. We have experimented with multi-layer-perceptron to transform relational information, but it proved to be too slow in practice.

5.3 Learning Curve Analysis

We also make the pseudoconvex formulation of CASA justifiable via an ablation experiment. In Figure 5. , the learning curve of different models are shown, including CASA with leaky ReLU + maxout and vanilla transformer with no relative encoding. Our results show that leaky ReLU-based CASA converges faster in the training phase than the other two counterparts thanks to its unique pseudoconvexity.

5.4 Sampling Rate-Performance Tradeoff

It is also much-needed for efficient models to examine the efficiency-performance tradeoff. In this case, the sampling rate represents CASAs' efficiency. In Figure 6, we show the result of CASA performance with five different sampling rates. Our results suggest that the increment between 25% and 50% is not significant and thus show that CASA can converge relative well even with low sampling rate.

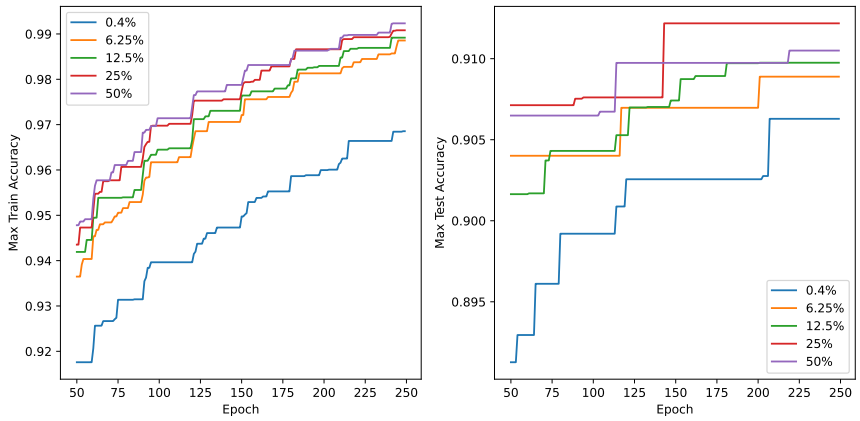

Figure 6: The influence of sampling rate onto the performance of CASA at five different sampling rates. The accuracy during training (left) and testing (right) are taken by max through 256 epochs.

Table 6: Model runtime measured in seconds (10 runs averaged).

	CASA (Ours)					**Transformer**
#Sampling	32	64	128	256	512	1024
%Sampling	3.13%	6.25%	12.5%	25.0%	50.0%	100%
Runtime$^{\downarrow}$	0.30s	0.32s	0.34s	0.46s	0.64s	0.64s

5.5 Runtime Analysis

To precisely measure the runtime of models, we run with one CPU thread. CASA layers with various numbers of sampled points are compared against the vanilla transformer (using the built-in implementation in PyTorch to measure). The input is a batch of 4 1024-length sequences. The result is shown in Table 6, which shows that our model is more efficient than the vanilla transformer when the sampling percentage is less than 50%.

6 Conclusion

In this paper, we made three contributions: a data-driven differentiable sampling without replacement method, self-attention formulation with pseudoconvexity and bounded gradient norm, and leaky probability function for relative positional encoding. Two of our three contributions aim at lowering the complexity of training transformers while the last one significantly improves the expressivity of transformer regarding relative positional encoding. We have empirically demonstrated the usefulness of the three modules and show at least one application: zero-additional computing cost to achieve rotational invariant - a desired property for multiple point cloud problems (e.g., molecular modeling). By easing the hyperparameter tuning pain, it may pave the way for very deep transformer networks to be trained at small facilities. In short, we make transformers more powerful and easier to train.

Limitations. We have yet to incorporate dedicated point cloud modules into our model as well as use the leaky positional encoding for prominent state-of-the-art point cloud transformers. Our model with leaky positional encoding overfits the dataset and has to heavily rely on weight decay to simplify the model on rotational invariant experimental settings. This shows that our model learns to generate not-so-useful features at the start and fixes itself through regularization when the training loss is close to zero. Future work would be to develop regularization to simplify the transformer model for generalization, to fully discretize the sampling operator at convergence.

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A Theoretical Analysis

A.1 Nonconvexity of Other Attention Settings

As mentioned in Section 4.4, the definition of pseudoconvex functions is defined below.

Definition A.1. Let ∇ denote the gradient operator and $\mathcal{S} \subset \mathbb{R}^n$ is a convex open set, a function $f : \mathcal{S} \to \mathbb{R}$ is considered pseudoconvex if for any $x_1, x_2 \in \mathcal{S}$ such that $\langle \nabla f(x_1), x_2 - x_1 \rangle \geq 0$ then $f(x_1) \geq f(x_2)$.

In this section, we will show the nonpseudoconvexity of two well-known Transformer variations: the vanilla Transformer (Vaswani et al., 2017) and ReLU-based attention with dot-product (Shen et al., 2023). Specifically, we will point out some simplified counterexamples with well-defined inputs to achieve this goal. Note that these counterexample can easily be generalized into arbitrary settings, but we handpicked them rather for simplicity.

Theorem A.2. *Let* $\mathbf{S}(W_Q, W_K) = \mathrm{SM}(\mathbf{X}W_Q W_K^\top \mathbf{X}^\top)\mathbf{X}\overline{W_V} + \mathbf{X}$ *be the vanilla attention layer where* SM *is the softmax function with respect to query and key, then there exists a setting in which* $\mathbf{S}$ *is not pseudoconvex with respect to all pairs of weight entries.*

Proof. Let $\mathbf{X} \in \mathbb{R}^{3\times 3}$, $W_Q, W_K \in \mathbb{R}^3$ and $\overline{W_V} \in \mathbb{R}^{3\times 3}$. We consider a counterexample by letting $\mathbf{X} = \overline{W_V} = \mathbf{I}_3$. Calculating the output we have

$$\mathbf{S}(W_Q, W_K)[i, j] = \frac{e^{w_{Qi} w_{Kj}}}{\sum_{k=1}^{3} e^{w_{Qi} w_{Kk}}} \qquad \forall i, j \in \{1, 2, 3\}.$$

where w_{Qi} and w_{Kj} is the ith and j^{th} entry of the vectors W_Q and W_K respectively.

From here, we will prove that $\mathbf{S}$ is not quasiconvex, thus not pseudoconvex, with respect to all pairs of scalar weight entries.

- $\mathbf{S}$ is not quasiconvex with respect to the pair (w_{Qs}, w_{Qr}) for any $s \neq r$ and $s, r \in \{1, 2, 3\}$.

  Since we are considering convexity within the entries of the query, it is reasonable to fix $W_K = \overline{W_K} = \begin{pmatrix} 1 & 1 & 1 \end{pmatrix}^\top$ and consider the first entry $\mathbf{S}$, which is simply

  $$\mathbf{s}(w_{Q1}, w_{Q2}, w_{Q3}) = \frac{e^{w_{Q1}}}{e^{w_{Q1}} + e^{w_{Q2}} + e^{w_{Q3}}}$$

  Without loss of generality let us fix $w_{Q1} = \overline{w_{Q1}} = 0$ and consider the convexity with respect to the pair (w_{Q2}, w_{Q3}). By taking the sublevel set defined by some level $\alpha \in (0, 1)$, one can easily observe that

  $$L_{\mathbf{s}}(\alpha) := \left\{ (w_{Q2}, w_{Q3}) \in \mathbb{R}^2 \quad \text{s.t} \quad e^{w_{Q2}} + e^{w_{Q3}} \geq \frac{1}{\alpha} - 1 \right\}$$

  is evidently not a convex set in two dimensional space. Therefore, $\mathbf{S}$ is not quasiconvex w.r.t (w_{Q2}, w_{Q3}).

- $\mathbf{S}$ is not quasiconvex with respect to the pair (w_{Qs}, w_{Kr}) for any $s, r \in \{1, 2, 3\}$.

  Without loss of generality, let $w_{Qs} = \overline{w_{Qs}} = w_{Ks} = \overline{w_{Ks}} = 0$ for $s \in \{2, 3\}$ and consider the function representing the $[2, 1]$ location entry of the $\mathbf{S}(W_Q, W_K)$ output

  $$\mathbf{s}(w_{Q1}, w_{K1}) = \frac{1}{e^{w_{Q1} w_{K1}} + 2}.$$

  Similarly, by taking the sublevel set defined by some level $\alpha \in (0, 1)$, it is obvious that this set is not a convex set. Hence, the proof is complete.

□

Not only vanilla attention fails to exhitbit the pseudoconvex property, but also attention settings with the presence of the dot product.

Theorem A.3. *Let* $\mathbf{R}(W_Q, W_K) = \mathrm{PR}(\mathbf{X}W_Q W_K^\top \mathbf{X}^\top)\mathbf{X}\overline{W_V} + \mathbf{X}$ *be the ReLU based attention with dot product where*

$$\mathrm{PR}(\mathbf{A})[i,j] = \frac{\mathrm{ReLU}(\mathbf{A}[i,j])}{\sum_{k=1}^{n} \mathrm{ReLU}(\mathbf{A}[i,k])},$$

then there exists a setting in which $\mathbf{R}(W_Q, W_K)$ *is not pseudoconvex w.r.t all pair of entry weight* (w_{Qs}, w_{Kr})*.*

The proof of this theorem is somewhat trivial and similar to the second counterexample in Theorem A.2. Therefore, we will skip the full proof.

A.2 Convexity of CASA

Even though a complete convex analysis is not possible due to the structure of the probability distribution function Prob, it is possible to prove the efficiency of this function during the training process via its pseudoconvexity, as all stationary points in a pseudoconvex are also global minimizers. The pseudoconvexity of the rational function class is verified by the following lemma.

Lemma A.4. *(Cambini & Martein, 2008) Let* $z(x, c) = \frac{f(x)}{g(x)}$ *be the ratio of two differentiable functions* f *and* g *defined on an open convex set* $\mathcal{S} \subset \mathbb{R}^n$*. If* f *is convex and* g *is positive and affine, then* z *is a pseudoconvex function.*

Since ReLU is indifferentiable, the pseudoconvexity of Prob should be analyzed in separated orthants $\mathcal{O}_\mathcal{I}$ where $I \subset [n]$ is defined via the non-negativity of the input entries. Lemma A.4 directly implies that

Theorem A.5. *The probability distribution function* $\mathrm{Prob} : \mathbb{R}^n \times \mathbb{R}^+ \to \mathbb{R}^n$ *defined as*

$$\mathrm{Prob}(\mathbf{x}, c)[i] = \frac{\mathrm{ReLU}(\mathbf{x}[i])}{\sum_k \mathrm{ReLU}(\mathbf{x}[k]) + c},$$

where $i \in [n]$ *is a pseudoconvex function in orthant* $\mathcal{O}_\mathcal{I}$ *for all* $\mathcal{I} \subset [n]$*.*

Proof. Without loss of generality, consider the Prob function in the orthant $\mathcal{O}_1 = \mathcal{O}_{[n]\setminus\{1\}}$, which means that for any $\mathbf{x} \in \mathcal{O}_1$

$$\mathrm{Prob}(\mathbf{x}, c)[i] = \begin{cases} 0 & \text{if } i = 1, \\ \dfrac{\mathbf{x}[i]}{\sum_k \mathbf{x}[k] + c} & \text{otherwise.} \end{cases}$$

From here, it is evident that the proof follows Lemma A.4 since $\mathbf{x}[k]$ is non-negative for all $k \neq 1$. Therefore, Prob is pseudoconvex in orthant $\mathcal{O}_1$ and, thus, in all orthants of $\mathbb{R}^n$. □

The probability distribution function Prob can only be pseudoconvex in each individual orthant $\mathcal{O}_\mathcal{I}$. However, due to the complete separation property, the stability during training is preserved. Consequently, we derive the pseudoconvexity power of CASA. But first, let us consider a modified version of CASA with linear activation in the FFN layer as follows:

Theorem A.6. *The CASA block in Algorithm 1 with FFN linear activation and no sampling has the following componentwise properties:*

- *Pseudoconvex with respect to* W_Q*,* B_Q*,* W_K *and* B_K*;*
- *Pseudoconvex with respect to* $W_{R_1}, B_{R_1}, W_{R_2}$ *and* B_{R_2}*;*
- *Pseudoconvex with respect to* W_C*,* B_C*.*

Proof. Let $\mathbf{M} = CASA(W_Q, B_Q, W_K, B_K, W_{R_1}, W_{R_2}, W_C)$ be the output of a CASA block in Algorithm 1.

- $\mathbf{M}$ is pseudoconvex with respect to W_Q, W_K, B_Q and B_K.

  Consider the orthant $\mathcal{O}_{\mathbf{Q+K}} \cap \mathcal{O}_{\mathbf{Q-K}}$ of $\mathbf{Q}$ and $\mathbf{K}$, where $\mathcal{O}_{\mathbf{Q-K}}$ and $\mathcal{O}_{\mathbf{Q+K}}$ are the orthants in which the score function $\text{Score}(\mathbf{Q}, \mathbf{K})$ is differentiable and affine. Thus, it follows rom Theorem A.5 that each entry of the output of the Prob function can be written in the form $f(W_Q, W_K, B_Q, B_K)/(g(W_Q, W_K, B_Q, B_K) + C)$ where f and g are affine and g is positive.

  As the remaining parts of CASA layer are linear transformations, they do not affect the affinity of f. Therefore, Lemma A.4 states the pseudoconvexity of the CASA block with respect to the inspected weights.

- $\mathbf{M}$ is pseudoconvex with respect to W_{R_1}, W_{R_2}, B_{R_1} and B_{R_2}.

  This proof is similiar to which of W_Q and W_K and therefore is neglected.

- $\mathbf{M}$ is pseudoconvex with respect to W_C and B_C. For the sake of simplity, Consider the ith entry of $\mathbf{C}$, denoted as $\mathbf{C}[i] = \mathbf{X}[i]W_C + b_C$ where $\mathbf{1}_d b_C = B_C$, let there exist W_{C1} and W_{C2} such that:

$$\nabla \mathbf{M}(W_{C1})(W_{C2} - W_{C1}) \geq 0. \tag{13}$$

  To prove the pseudoconvex dependency of $\mathbf{M}$ with respect to W_C and B_C, consider the dependencies of $\mathbf{P}(W_C)$ with respect to W_C, and the pseudoconvexity w.r.t b_C is analogous, where

$$\mathbf{P}(W_C) = CASA(\overline{W_Q}, \overline{B_Q}, \overline{W_K}, \overline{B_K}, \overline{W_{R_1}}, \overline{W_{R_2}}, W_C, \overline{b_C}),$$

  and the overlined weights are treated as constants. This function can be written in a simpler form regarding each of its entry

$$\mathbf{P}(W_C)[i, j] = \frac{C_1}{C_2 + \text{SP}(\mathbf{X}[i]W_C + b_C)} + C_3,$$

  where C_1, C_2, C_3 and C_4 are all constants, $C_2 > 0$ and SP denotes the softplus non-linearity. Returning to (13), we have:

$$-\frac{C_1}{(C_2 + \text{SP}(\mathbf{X}[i]W_{C1} + C_4))^2} \text{SG}(\mathbf{X}[i]W_{C1} + C_4)\mathbf{X}[i](W_{C2} - W_{C1}) \geq 0, \tag{14}$$

  given that SG denotes the sigmoid function $\text{SG}(x) = 1/(1 + \exp(-x))$. Assume that $C_1 > 0$ (similar for $C_1 < 0$), then it follows from equation 14 that:

$$\mathbf{X}[i](W_{C2} - W_{C1}) \leq 0.$$

  Thus for every W_{C2} and W_{C1} satisfying equation 13, we have:

$$\mathbf{P}(W_{C2}) \leq \mathbf{P}(W_{C1}).$$

  By definition, $\mathbf{M}$ is pseudoconvex with respect to W_C and b_C.

□

However, in our proposed model, the FFN activation is GeLU. In order to show the pseudoconvexity of the our original CASA block, we analyze this via its quasiconvexity with the following theorem:

Theorem A.7. *(Ivanov, 2001) A function $f : \mathbb{R}^m \to \mathbb{R}^n$ that is quasiconvex is also pseudoconvex if the set of stationary points coincides with the set of global minimizers.*

From here, the pseudoconvexity of our model is proved.

Theorem A.8. *The CASA block in Algorithm 1 with FFN GeLU activation and no sampling exhibits the same properties as in Theorem A.6.*

Proof. Let $\sigma(\cdot)$ be the shorthand notion of the GeLU non-linearity and $\mathbf{M}(\cdot)$ be the function of the linear activation FFN CASA block. Then, the function of our proposed CASA block is $\mathbf{G} := \sigma \circ \mathbf{M}$.

For the sake of simplicity, let $\mathbf{G}(\cdot)$ and $\mathbf{M}(\cdot)$ be a single-matrix-input and scalar-output function, which can represent any weight and entry respectively.

- Pseudoconvexity w.r.t the query, key, $\mathbf{R_1}$ and $\mathbf{R_2}$ scalers.

  Since the output of $\mathbf{M}(\cdot)$ is a fractional function with respect to these weights, as illustrated in the proof of Theorem A.6, it has no stationary points. Furthermore, due to the uniqueness of the global minimizer of σ, one can easily derive that $\mathbf{G}$, if quasiconvex, is also pseudoconvex by Theorem A.7.

  Now we will prove the quasiconvexity of $\mathbf{G}(\cdot)$. Given that σ is a quasiconvex scalar non-linearity, we consider the sublevel set of $\mathbf{G}$, defined as

$$\begin{aligned} L_{\mathbf{G}}(\alpha) &= \{\mathbf{W} \text{ s.t } \mathbf{G}(\mathbf{W}) \leq \alpha\} \\ &= \{\mathbf{W} \text{ s.t } u_1(\alpha) \leq \mathbf{M}(\mathbf{W}) \leq u_2(\alpha)\}\,. \end{aligned}$$

  where $u_1(\cdot)$ and $u_2(\cdot)$ represent the lower and upper scalar bound of σ with some level input.

  However, as illustrated in Theorem A.6, $\mathbf{M}(\mathbf{W})$ is a fractional function with respect to $\mathbf{W}$ and so it is both pseudoconvex and pseudoconcave. Hence, $\mathbf{M}$ is also both quasiconvex and quasiconcave, which means that if we let

$$L^1_{\mathbf{M}}(\alpha_1) = \{\mathbf{W} \text{ s.t } \mathbf{M}(\mathbf{W}) \geq \alpha_1\} \text{ and } L^2_{\mathbf{M}}(\alpha_2) = \{\mathbf{W} \text{ s.t } \mathbf{M}(\mathbf{W}) \leq \alpha_2\}$$

  be the superlevel and sublevel set of $\mathbf{M}(\mathbf{W})$ respectively, then they are convex sets for all α_1 and α_2. Therefore,

$$L_{\mathbf{G}}(\alpha) = L^1_{\mathbf{M}}(u_1(\alpha)) \cap L^2_{\mathbf{M}}(u_2(\alpha))$$

  is also a convex set and the quasiconvexity of $\mathbf{G}(\mathbf{W})$ is derived.

- Pseudoconvexity w.r.t the leaky attention weights W_C and b_C.

  Consider the function $\mathbf{P}(W_C)$ defined in Theorem A.6, by following the same proof steps, one can prove that $-\mathbf{P}(W_C)$ is also pseudoconvex. As a result, $\mathbf{P}(W_C)$ is pseudoconcave.

  It is also evident that $\mathbf{P}(W_C)$ has no stationary points. Hence, by replicating the proof of the other weights, it is sufficient to show that the CASA block is also pseudoconvex with respect to W_C, and also to b_C.

□

A.3 Gradient Analysis of CASA

To theoretically analyze the effectiveness of CASA against gradient vanishing and exploding, we evaluate the local adaptive lower bound and a global upper bound for the gradient norm squared of the weights.

Theorem A.9. *Let* $\mathbf{Sa} = \mathbf{Sa}(W_Q, W_K, W_V) = \mathrm{Prob}(\mathrm{Score}(\mathbf{X}W_Q, \mathbf{X}W_K), \mathbf{C})\mathbf{X}W_V + \alpha\mathbf{X}$ *be the CASA self-attention layer output with the simplication of* $\mathbf{C}$ *being treated as a positive constant matrix. Assume that all weights are initialized via He initialization He et al. (2015) where each entry independently follows the normal distribution* $\mathcal{N}(0, \sigma^2)$ *and let* $W_D = W_Q - W_K$*, then for any positive matrices* $W^L_{QQ}, W^U_{QQ}, W^L_{KK}, W^U_{KK}, W^L_{DD}, W^U_{DD}$ *such that* $W^L_{QQ} < W^U_{QQ}$*,* $W^L_{KK} < W^U_{KK}$*,* $W^L_{DD} < W^U_{DD}$ *and* $W_Q W_Q^\top \in [W^L_{QQ}, W^U_{QQ}]$*,* $W_K W_K^\top \in [W^U_{KK}, W^U_{KK}]$ *and* $W_D W_D^\top \in [W^U_{DD}, W^U_{DD}]$ *there exist two positive scalar-valued positive function* f_1, f_2 *and positive constants* C_Q, C_V *such that:*

$$\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_V}\right\|_F^2 \in \left(f_V(W^L_{QQ}, W^U_{QQ}, W^L_{KK}, W^U_{KK}), C_V\right),$$

$$\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_Q}\right\|_F^2 \in \left(f_Q(W_{DD}^L, W_{DD}^U, W_{KK}^L, W_{KK}^U), C_Q\right).$$

and

$$f_V(W_{QQ}^L, W_{QQ}^U, W_{KK}^L, W_{KK}^U) = \Omega(n), \qquad C_V = O(n),$$

$$f_Q(W_{DD}^L, W_{DD}^U, W_{KK}^L, W_{KK}^U) = \Omega(1), \qquad C_Q = O(1).$$

Proof. First, let us note some remarks on matrix calculus and properties of the Kronecker product $\otimes$, shown at Magnus & Neudecker (1999) Singh et al. (2021). Given some matrices $\mathbf{A} \in \mathbb{R}^{s_1 \times s_2}, \mathbf{B} \in \mathbb{R}^{s_2 \times s_3}, \mathbf{C} \in \mathbb{R}^{s_3 \times s_4}, \mathbf{D} \in \mathbb{R}^{s_4 \times s_5}$ and a matrix variable $\mathbf{W} \in \mathbb{R}^{s_2 \times s_2}$, then:

$$\frac{\partial \mathbf{AWB}}{\partial \mathbf{W}} = \mathbf{A} \otimes \mathbf{B}^\top.$$

Additionally, we also mention some useful properties regarding the trace operator, denoted as $\mathrm{tr}(\cdot)$,

$$\begin{aligned} \mathrm{tr}(\mathbf{A} \otimes \mathbf{B}) &= \mathrm{tr}(\mathbf{A})\,\mathrm{tr}(\mathbf{B}), \\ (\mathbf{AC}) \otimes (\mathbf{BD}) &= (\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}). \end{aligned}$$

We would also like to recall to the Jensen inequality for the expectation of convex and concave function. Let $\mathbb{E}$ denotes the expectation operator, and X be a random variable. Then, for any scalar function $\phi : \mathbb{R} \to \mathbb{R}$,

- $\mathbb{E}(\phi(X)) \geq \phi(\mathbb{E}(X))$ if ϕ is convex,
- $\mathbb{E}(\phi(X)) \leq \phi(\mathbb{E}(X))$ if ϕ is concave.

Now we are ready for the proof, let us consider the gradient norm w.r.t W_V. For simplicity, we have the notations

$$\begin{aligned} \mathbf{T}_i &= \mathrm{Score}(\mathbf{X}[i]W_Q, \mathbf{X}W_K), \\ \mathbf{R}_i &= \mathrm{Prob}(\mathbf{T}_i). \end{aligned}$$

Note that

$$\begin{aligned} \left\|\frac{\partial \mathbf{Sa}}{\partial W_V}\right\|_F^2 &= \sum_{i=1}^n \left\|\frac{\partial \mathbf{Sa}[i]}{\partial W_V}\right\|_F^2 \\ &= \sum_{i=1}^n \|\mathbf{R}_i \mathbf{X} \otimes \mathbf{I}_d\|_F^2 \\ &= \sum_{i=1}^n \mathrm{tr}\left(((\mathbf{R}_i X) \otimes \mathbf{I}_d)\left((X^\top \mathbf{R}_i^\top) \otimes \mathbf{I}_d\right)\right) \\ &= \sum_{i=1}^n \mathrm{tr}\left((\mathbf{R}_i \mathbf{X}\mathbf{X}^\top \mathbf{R}_i^\top) \otimes \mathbf{I}_d\right) \\ &= \sum_{i=1}^n d\,\mathrm{tr}\left(\mathbf{R}_i \mathbf{X}\mathbf{X}^\top \mathbf{R}_i^\top\right) \\ &= \sum_{i=1}^n d\,\|\mathbf{R}_i \mathbf{X}\|_F^2 \\ &= \sum_{i=1}^n \sum_{j=1}^n d\,\|\mathbf{R}_i[j]\mathbf{X}[j]\|_F^2. \end{aligned}$$

However, we have:

$$\mathbf{R}_i[j] = \frac{\mathrm{ReLU}\left(\max(\mathbf{Q}[i], \mathbf{K}[j])\right)}{\sum_{k=1}^{n} \mathrm{ReLU}\left(\max(\mathbf{Q}[i], \mathbf{K}[k])\right) + \mathbf{C}[i]}.$$

In order to linearize the max operator, let $e_{ij} \in \{0, 1\}$ be the query-key indicator such that:

$$\max(\mathbf{Q}[i], \mathbf{K}[j]) = e_{ij}\mathbf{Q}[i] + (1 - e_{ij})\mathbf{K}[j].$$

Similiar to the e_{ij}, let $d_{ij} \in \{0, 1\}$ represents the ReLU non-linearity by having

$$\mathrm{ReLU}\left(\max(\mathbf{Q}[i], \mathbf{K}[j])\right) = d_{ij} \max(\mathbf{Q}[i], \mathbf{K}[j]) = d_{ij}\left(e_{ij}\mathbf{Q}[i] + (1 - e_{ij})\mathbf{K}[j]\right).$$

By this formulation, we have

$$\begin{aligned}
\left\| \frac{\partial \mathbf{Sa}}{\partial W_V} \right\|_F^2 &= d \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{d_{ij} e_{ij} \mathbf{Q}[i]\mathbf{Q}^\top[i] + d_{ij}(1 - e_{ij})\mathbf{K}[j]\mathbf{K}^\top[j]}{\left(\sum_{k=1}^{n} d_{ik} e_{ik} \mathbf{Q}[i] + d_{ik}(1 - e_{ik})\mathbf{K}[k] + \mathbf{C}[i]\right)^2} \left\| \mathbf{X}[j] \right\|_F^2 \\
&= d \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{d_{ij} e_{ij} \operatorname{tr}(\mathbf{X}^\top[i]\mathbf{X}[i] W_Q W_Q^\top) + d_{ij}(1 - e_{ij}) \operatorname{tr}(\mathbf{X}^\top[j]\mathbf{X}[j] W_K W_K^\top)}{\left(\sum_{k=1}^{n} d_{ik} e_{ik} \operatorname{tr}(\mathbf{X}[i] W_Q) + d_{ik}(1 - e_{ik}) \operatorname{tr}(\mathbf{X}[i] W_K) + \mathbf{C}[i]\right)^2} \left\| \mathbf{X}[j] \right\|_F^2 \\
&\geq \frac{d}{3n} \sum_{i=1}^{n} \sum_{j=1}^{n} \frac{d_{ij} e_{ij} \operatorname{tr}(\mathbf{X}^\top[i]\mathbf{X}[i] W_Q W_Q^\top) + d_{ij}(1 - e_{ij}) \operatorname{tr}(\mathbf{X}^\top[j]\mathbf{X}[j] W_K W_K^\top)}{\sum_{k=1}^{n} d_{ik} e_{ik} \operatorname{tr}(\mathbf{X}^\top[i]\mathbf{X}[i] W_Q W_Q^\top) + d_{ik}(1 - e_{ik}) \operatorname{tr}(\mathbf{X}^\top[k]\mathbf{X}[k] W_K W_K^\top) + \mathbf{C}[i]^2} \left\| \mathbf{X}[j] \right\|_F^2.
\end{aligned}$$

To express this more concisely, we have following shorthand notations:

$$\begin{aligned}
\mathbf{A}_{Qi} &= \frac{d}{3n} \sum_{j=1}^{n} d_{ij} e_{ij} \left\| \mathbf{X}[j] \right\|_F^2 \mathbf{X}^\top[i]\mathbf{X}[i], \\
\mathbf{A}_{Ki} &= \frac{d}{3n} \sum_{j=1}^{n} d_{ij}(1 - e_{ij}) \left\| \mathbf{X}[j] \right\|_F^2 \mathbf{X}^\top[j]\mathbf{X}[j], \\
\mathbf{B}_{Qi} &= \sum_{k=1}^{n} d_{ik} e_{ik} \mathbf{X}^\top[i]\mathbf{X}[i], \\
\mathbf{B}_{Ki} &= \sum_{k=1}^{n} d_{ik}(1 - e_{ik}) \mathbf{X}^\top[k]\mathbf{X}[k].
\end{aligned}$$

By doing this, we derive that:

$$\left\| \frac{\partial \mathbf{Sa}}{\partial W_V} \right\|_F^2 \geq \sum_{i=1}^{n} \frac{\operatorname{tr}(\mathbf{A}_{Qi} W_{QQ}) + \operatorname{tr}(\mathbf{A}_{Ki} W_{KK})}{\operatorname{tr}(\mathbf{B}_{Qi} W_{QQ}) + \operatorname{tr}(\mathbf{B}_{Ki} W_{KK}) + \mathbf{C}[i]^2},$$

where $W_{QQ} = W_Q W_Q^\top$ and $W_{KK} = W_K W_K^\top$.

We delve into the concept of convex envelope, which seeks the highest convex underestimator of a given function. Additionally, the local minina of the convex envelope is also the global minima of the primal function.

However, in this proof, we only focus on the convex properties. Specifically, consider the non-convex lower bound function

$$\mathbf{LB}_i(W_{QQ}, W_{KK}) = \frac{\operatorname{tr}(\mathbf{A}_{Qi} W_{QQ}) + \operatorname{tr}(\mathbf{A}_{Ki} W_{KK})}{\operatorname{tr}(\mathbf{B}_{Qi} W_{QQ}) + \operatorname{tr}(\mathbf{B}_{Ki} W_{KK}) + \mathbf{C}[i]^2}, \tag{15}$$

and based on the convex envelope of the bivariate rational function discovered at Tawarmalani & Sahinidis (2002), we can convexify the multivariate rational function $\mathbf{LB}_i$ by considering the convexity with respect to

each entry one at a time. For convenience, we let $\mathbf{Af}_i(W_{QQ}, W_{KK})$ be the affine function denominator of equation 15. As a result, we can derive a componentwise convex lower bound of $\mathbf{LB}_i$ called $\mathbf{CCLB}_i$, which can be expressed in the form

$$\mathbf{CCLB}_i(W_{QQ}, W_{KK}) = \frac{r_i}{\mathbf{Af}_i(W_{QQ}, W_{KK})} \prod_{s,k,p,q=1}^{d} \mathbf{Cci}_{Qsr}\left(\frac{\left(w_{Qsr} + \sqrt{w^L_{Qsr} w^U_{Qsr}}\right)^2}{\left(\sqrt{w^L_{Qsr}} + \sqrt{w^U_{Qsr}}\right)^2}\right) \mathbf{Cci}_{Kpq}\left(\frac{\left(w_{Kpq} + \sqrt{w^L_{Kpq} w^U_{Kpq}}\right)^2}{\left(\sqrt{w^L_{Kpq}} + \sqrt{w^U_{Kpq}}\right)^2}\right)$$

where:

- w_{Qsr}, w_{Kpq} is the $[s, r]$ and $[p, q]$ location entry of W_{QQ} and W_{KK} respectively,
- w^L_{Qsr} and w^U_{Qsr} are the lower and upper bound of w_{Qsr},
- w^L_{Kpq} and w^U_{Kpq} are the lower and upper bound of w_{Kpq},
- r_i is a constant and is independent of the bounds,
- $\mathbf{Cci}_{Qsr}(\cdot)$ is the identity function if w_{Qsr} is concave in the $\mathbf{LB}_i$ function, and 1 otherwise,
- $\mathbf{Cci}_{Kpq}(\cdot)$ is defined similar to $\mathbf{Cci}_{Qsr}(\cdot)$.

With this formulation, we take the expectation of the gradient norm square and use the Jensen inequality, which leads to:

$$\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_V}\right\|_F^2 \geq \sum_{i=1}^{n} \frac{r_i}{\mathbf{Af}_i(\sigma^2 \mathbf{I}_n, \sigma^2 \mathbf{I}_n)} \prod_{s,r,p,q=1}^{d} \mathbf{Cci}_{Qsr}\left(\frac{\left(\sigma^2\delta_{sr} + \sqrt{w^L_{Qsr} w^U_{Qsr}}\right)^2}{\left(\sqrt{w^L_{Qsr}} + \sqrt{w^U_{Qsr}}\right)^2}\right) \mathbf{Cci}_{Kpq}\left(\frac{\left(\sigma^2\delta_{pq} + \sqrt{w^L_{Kpq} w^U_{Kpq}}\right)^2}{\left(\sqrt{w^L_{Kpq}} + \sqrt{w^U_{Kpq}}\right)^2}\right) \tag{16}$$

$$\triangleq f_V(W^L_{QQ}, W^U_{QQ}, W^L_{KK}, W^U_{KK}) = \Omega(n), \tag{17}$$

where $\delta_{sr} = 1$ if $s = r$ and 0 otherwise.

Now let us consider the gradient norm with respect to the query:

$$\left\|\frac{\partial \mathbf{Sa}}{\partial W_Q}\right\|_F^2 = \sum_{i=1}^{n} \left\|\frac{\partial \mathbf{Sa}[i]}{\partial W_Q}\right\|_F^2.$$

Consider the gradient norm for each $i \in [n]$, by applying the chain rule we have:

$$\begin{aligned}\left\|\frac{\partial \mathbf{Sa}[i]}{\partial W_Q}\right\|_F^2 &= \left\|\frac{\partial \mathbf{Sa}[i]}{\partial \mathbf{R}_i}\frac{\partial \mathbf{R}_i}{\partial \mathbf{T}_i}\frac{\partial \mathbf{T}_i}{\partial \mathbf{Q}[i]}\frac{\partial \mathbf{Q}[i]}{\partial W_Q}\right\|_F^2 \\ &= \left\|W_V^\top \mathbf{X}^\top \frac{\partial \mathbf{R}_i}{\partial \mathbf{T}_i} \mathbf{e}_i \mathbf{X}[i]\right\|_F^2,\end{aligned}$$

where $\mathbf{e}_i = (e_{ij})_{j\in[n]}$ is the query-key binary gate vector. Continuing the formulation,

$$\begin{aligned}
\mathbb{E}\left\|\frac{\partial \mathbf{Sa}[i]}{\partial W_Q}\right\|_F^2 &= \mathbb{E}\left(\operatorname{tr}\left(W_V W_V^\top \mathbf{X}^\top \frac{\partial \mathbf{R}_i}{\partial \mathbf{T}_i}\mathbf{e}_i \mathbf{X}[i]\mathbf{X}^\top[i]\mathbf{e}_i^\top \frac{\partial \mathbf{R}_i^\top}{\partial \mathbf{T}_i^\top}\mathbf{X}\right)\right) \\
&= \sigma^2 \left\|\mathbf{X}[i]\right\|_F^2 \operatorname{tr}\left(\mathbf{X}\mathbf{X}^\top \mathbb{E}\left(\frac{\partial \mathbf{R}_i}{\partial \mathbf{T}_i}\mathbf{e}_i\mathbf{e}_i^\top \frac{\partial \mathbf{R}_i^\top}{\partial \mathbf{T}_i^\top}\right)\right) \\
&= \sigma^2 \left\|\mathbf{X}[i]\right\|_F^2 \mathbb{E}\left\|\mathbf{X}^\top \frac{\partial \mathbf{R}_i}{\partial \mathbf{T}_i}\mathbf{e}_i\right\|_F^2 \\
&= \sum_{k=1}^{d} \sigma^2 \left\|\mathbf{X}[i]\right\|_F^2 \mathbb{E}\left\|\mathbf{X}[:,k]^\top \frac{\partial \mathbf{R}_i}{\partial \mathbf{T}_i}\mathbf{e}_i\right\|_F^2 .
\end{aligned}$$

Let $W_D = W_Q - W_K$ and $\mathbf{Z}_i = \dfrac{\partial \mathbf{R}_i}{\partial \mathbf{T}_i}\mathbf{e}_i$, we have:

$$\mathbf{Z}_i[j] = \frac{d_{ij}e_{ij}\left(\sum_{\substack{k=1\\k\neq j}}^{n} d_{ik}\mathbf{T}_i[k] - d_{ik}\mathbf{T}_i[j]\right)}{\left(d_{ik}\mathbf{T}_i[k] + \mathbf{C}[i]\right)^2}.$$

And since $\mathbf{T}_i[k] = e_{ik}\mathbf{Q}[i] + (1-e_{ik})\mathbf{K}[k] = e_{ik}\mathbf{X}[i]W_D + \left((1-e_{ik})\mathbf{X}[k] + e_{ik}\mathbf{X}[i]\right)W_K$, we derive that:

$$\begin{aligned}
\left\|\mathbf{X}[:,k]^\top \mathbf{Z}_i\right\|_F^2 &= \frac{\sum_{j=1}^{n}\mathbf{X}[j,k]^2 d_{ij}e_{ij}\left(\sum_{\substack{k=1\\k\neq j}}^{n} d_{ik}\left(1-e_{ik}\right)\right)^2 \left(\mathbf{X}[i]W_D\right)^2}{\left(\sum_{k=1}^{n} d_{ik}e_{ik}\mathbf{X}[i]W_D + d_{ik}\left((1-e_{ik})\mathbf{X}[k] + e_{ik}\mathbf{X}[i]\right)W_K + \mathbf{C}[i]\right)^4} \\
&\geq \frac{1}{9n^2}\frac{\sum_{j=1}^{n}\mathbf{X}[j,k]^2 d_{ij}e_{ij}\left(\sum_{\substack{k=1\\k\neq j}}^{n} d_{ik}\left(1-e_{ik}\right)\right)^2 \left(\mathbf{X}[i]W_D\right)^2}{\left(\sum_{k=1}^{n} d_{ik}e_{ik}(\mathbf{X}[i]W_D)^2 + d_{ik}\left(\left((1-e_{ik})\mathbf{X}[k] + e_{ik}\mathbf{X}[i]\right)W_K\right)^2 + \mathbf{C}[i]^2\right)^2}.
\end{aligned}$$

Now let $W_{DD} = W_D W_D^\top$ and confine W_{DD} in a hypercube (W_{DD}^L, W_{DD}^U) similarly to W_{QQ} and W_{KK}, we have

$$(\mathbf{X}[i]W_D)^2 = \operatorname{tr}(\mathbf{X}[i]^\top\mathbf{X}[i]W_D W_D^\top) \leq \left\|\mathbf{X}[i]\right\|_F^2 \left\|W_{DD}\right\|_F \leq \left\|\mathbf{X}[i]\right\|_F^2 C\left(W_{DD}^L, W_{DD}^U\right),$$

where $C(\cdot,\cdot)$ is some scalar-valued positive function dependent only on the bounds of W_{DD}.

By applying similar evaluations for W_{KK} and following the techniques used for the analysis W_V gradient norm, such that it is sufficient to deduce that for some constant matrices A_{Di}, B_{Di} and B_{Ki} that are bound-independent, we have:

$$\left\|\mathbf{X}[:,k]^\top \mathbf{Z}_i\right\|_F^2 \geq C\left(W_{DD}^L, W_{DD}^U, W_{KK}^L, W_{KK}^U\right)\frac{\operatorname{tr}(A_{Di}W_{DD})}{\operatorname{tr}(B_{Di}W_{DD}) + \operatorname{tr}(B_{Ki}W_{KK}) + \mathbf{C}[i]^2}.$$

It is evident of the proof from this point as it is analogous to the previous part. Therefore, we deduce another adaptive lower bound for the gradient norm of W_Q as there exist a non-negative scalar function f_Q such that:

$$\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_Q}\right\|_F^2 \geq f_Q\left(W_{DD}^L, W_{DD}^U, W_{KK}^L, W_{KK}^U\right) = \Omega(1). \tag{18}$$

Regarding the upper bound, we will achieve this by acquiring a sufficiently large universal constant. Simply by the norm product inequality, we have:

$$\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_V}\right\|_F^2 \leq d \max_i \|\mathbf{X}[i]\|_F^2 \sum_{i=1}^n \|\mathbf{R}_i\|_F^2 \leq dn \max_i \|\mathbf{X}[i]\|_F^2 \triangleq C_V = O(n). \tag{19}$$

Combining Eq equation 17 and Eq equation 19, the complexity of $\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_V}\right\|_F^2$ is derived to be $\Theta(n)$.

Also,

$$\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_Q}\right\|_F^2 \leq \sum_{i=1}^n \sum_{k=1}^d \sigma^2 \|\mathbf{X}[i]\|_F^2 \mathbb{E}\left\|\mathbf{X}[:,k]^\top \mathbf{Z}_i\right\|_F^2.$$

Since $W_D = W_Q - W_K$, we get $\mathrm{Var}(W_D) = \mathrm{Var}(W_Q) + \mathrm{Var}(W_K) = 2\sigma^2 \mathbf{I}_n$. Alongside this, notice that the indicators d_{ij} where $i, j \in [n]$ can be treated as binary gates that filter out negative values, therefore:

$$\begin{aligned}
\mathbb{E}\left\|\mathbf{X}[:,k]^\top \mathbf{Z}_i\right\|_F^2 &\leq \mathbb{E}\frac{\sum_{j=1}^n \mathbf{X}[j,k]^2 d_{ij} e_{ij} \left(\sum_{\substack{k=1\\k\neq j}}^n d_{ik}\left(1-e_{ik}\right)\right)^2 \left(\mathbf{X}[i]W_D\right)^2}{\left(\sum_{k=1}^n d_{ik} e_{ik} \mathbf{X}[i] W_D + \mathbf{C}[i]\right)^4} \\
&\leq \mathbb{E}\frac{\sum_{j=1}^n \mathbf{X}[j,k]^2 d_{ij} e_{ij} \left(\sum_{\substack{k=1\\k\neq j}}^n d_{ik}\left(1-e_{ik}\right)\right)^2}{\left(\sum_{k=1}^n d_{ik} e_{ik} \mathbf{X}[i] W_D + \mathbf{C}[i]\right)^2 \left(\frac{\mathbf{C}[i]}{\mathbf{X}[i]W_D} + \sum_{k=1}^n d_{ik} e_{ik}\right)^2} \\
&\leq \mathbb{E}\frac{\sum_{j=1}^n \mathbf{X}[j,k]^2 d_{ij} e_{ij} \left(\sum_{\substack{k=1\\k\neq j}}^n d_{ik}\left(1-e_{ik}\right)\right)^2}{4\mathbf{C}[i]^2 \left(\sum_{k=1}^n d_{ik} e_{ik}\right)^4}.
\end{aligned}$$

Finally, the global upper bound for the gradient norm squared of W_V is concluded:

$$\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_Q}\right\|_F^2 \leq \sum_{i=1}^n \sum_{k=1}^d \sigma^2 \|\mathbf{X}[i]\|_F^2 \mathbb{E}\left(\frac{\sum_{j=1}^n \mathbf{X}[j,k]^2 d_{ij} e_{ij} \left(\sum_{\substack{k=1\\k\neq j}}^n d_{ik}\left(1-e_{ik}\right)\right)^2}{4\mathbf{C}[i]^2 \left(\sum_{k=1}^n d_{ik} e_{ik}\right)^4}\right) \triangleq C_Q = O(1). \tag{20}$$

From Eq. equation 18 and Eq. equation 20, we conclude that the complexity of $\mathbb{E}\left\|\frac{\partial \mathbf{Sa}}{\partial W_Q}\right\|_F^2$ is $\Theta(1)$. □