
Attention Mechanism, Max-Affine Partition, and Universal Approximation

Hude Liu* Jerry Yao-Chieh Hu*[†] Zhao Song[‡] Han Liu^{†§}

[†]Center for Foundation Models and Generative AI & Department of Computer Science,

[‡]Simons Institute for the Theory of Computing, UC Berkeley, Berkeley, CA 94720, USA

[§]Department of Statistics and Data Science, Northwestern University, Evanston, IL 60208, USA

hudeliu0208@gmail.com, jhu@u.northwestern.edu,
magic.linuxkde@gmail.com, hanliu@northwestern.edu

Abstract

We establish the universal approximation capability of single-layer, single-head self- and cross-attention mechanisms with minimal attached structures. Our key insight is to interpret single-head attention as an input domain-partition mechanism that assigns distinct values to subregions. This allows us to engineer the attention weights such that this assignment imitates the target function. Building on this, we prove that a single self-attention layer, preceded by sum-of-linear transformations, is capable of approximating any continuous function on a compact domain under the L_∞ -norm. Furthermore, we extend this construction to approximate any Lebesgue integrable function under L_p -norm for $1 \leq p < \infty$. Lastly, we also extend our techniques and show that, for the first time, single-head cross-attention achieves the same universal approximation guarantees.

1 Introduction

We establish the universal approximation capability of single-layer, single-head self- and cross-attention mechanisms. Departed from prior studies, our results demonstrate that the expressive power of transformers arises from *only* the (softmax) attention module and an attached linear layer, without additional components such as positional encodings or feed-forward networks (FFNs). More importantly, our proofs show that sequence-to-sequence universal approximation requires only a minimalist configuration: single-layer, single-head attention with linear transformations.

In this era, the power of transformers [Vaswani et al., 2017] is undeniable, given their dominance in modern machine learning. They drive models such as BERT [Devlin, 2018], ChatGPT [Brown et al., 2020, Achiam et al., 2023], and LLaMA [Touvron et al., 2023a,b, Dubey et al., 2024] for language; ViT [Dosovitskiy et al., 2021] and DiT [Peebles and Xie, 2023] for image and video; DNABERT [Ji et al., 2021, Zhou et al., 2023] for genomics; and Moirai [Woo et al., 2024, Liu et al., 2024] for time series, among many others. Central to these successes is the *attention mechanism*. While numerous variants and implementations exist [Tay et al., 2022], the *softmax-based* vanilla attention

*Equal contribution. Version: December 15, 2025. Future updates are on <https://arxiv.org/abs/2504.19901>.

[Vaswani et al., 2017] remains a mainstay in both research and industry communities (e.g., ChatGPT and Llama).

However, despite its practical importance, theoretical insights into why softmax attention is so powerful remain incomplete. Moreover, the extent to which softmax attention alone drives performance is unclear. Empirical [Tay et al., 2022] and theoretical [Keles et al., 2023, Deng et al., 2023, Alman and Yu, 2024] evidence suggests that deviating from softmax attention (e.g., via sub-quadratic approximations) often degrades performance, indicating that softmax attention may be a central engine in Transformer architectures. At the same time, a growing body of work explores its memory capacity [Mahdavi et al., 2023, Kim et al., 2023, Kajitsuka and Sato, 2024], universal approximation properties [Yun et al., 2019, Kajitsuka and Sato, 2023, Jiang and Li, 2023], representation learning [Sanford et al., 2024b, Chen and Li, 2024], and task-specific theoretical performance [Gurevych et al., 2022, Edelman et al., 2022]. However, these studies often rely on additional components, such as feed-forward networks (FFNs) or multi-head setups or customized assumptions, as they target the entire Transformer architecture rather than isolating the role of attention module.

To this end, this work presents attention-only expressiveness results: *softmax-based attention alone* already suffices for universal approximation of sequence-to-sequence functions. We operate under three key premises for investigating the expressiveness of attention:

1. We focus on *softmax*-based attention,
2. We seek a *minimalist* design (a single layer of single-head attention plus a linear transformation),
3. We impose *minimal assumptions* on the data distribution or network architecture (no positional encodings, no multi-head expansions, no FFNs).

We provide new proofs that a *single* self-attention layer approximates any continuous sequence-to-sequence function on a compact domain, in both the L_∞ and L_p norms. Furthermore, we show, for the first time, a parallel result for *cross-attention*, revealing its universal approximation capability under the same minimalist setting.

Contributions. Our contributions are as follows:

- **Interpreting Attention as a Max-Affine Partition.** We show that single-head softmax attention, combined with a linear layer, implicitly partitions the input domain using a max-affine construction. This partitioning allows attention to assign distinct outputs to each partition cell. This perspective clarifies how softmax-based attention enables a powerful piecewise-linear approximation scheme.
- **Single-Layer, Single-Head Self-Attention Universality.** We prove that a single self-attention layer is a universal approximator for continuous sequence-to-sequence functions on compact domains. Our results cover both L_p - and L_∞ -norms guarantees and require minimal assumptions on data and architecture, highlighting the inherent expressive power of attention alone.
- **Single-Head Cross-Attention Universality.** We establish, for the first time, that the same approach also endows a single-layer, single-head *cross-attention* with universal approximation capabilities. This result further underscores that much of a Transformer’s expressiveness can reside solely in its attention block, even when the queries and keys come from distinct input sequences.

Organization. Section 2 presents the ideas we built on. Section 3 shows our interpretation of Attention as a Max-Affine Partition in a simplified setting. Section 4 presents our universal approximation results for single-layer, single-head self- and cross-attentions.

1.1 Related Work

Universal Approximation. Early works of universal approximation theorems focuses on the expressiveness of feed-forward networks (FFN) [Cybenko, 1989, Hornik, 1991, Carroll and Dickinson,

1989]. Since Vaswani et al. [2017] propose the transformer architecture and the scaled dot-product attention module, there is a series of research aiming to explain the expressiveness of transformer. Yun et al. [2019], Kajitsuka and Sato [2023] offer explanation from the perspective of contextual mapping. Among them, Yun et al. [2019] are the first to prove the universal approximation capability of transformer. Yet since the network in [Yun et al., 2019] requires excessive layers ($\mathcal{O}(n(1/\delta)^{dn}/n!)$), Kajitsuka and Sato [2023] make more careful estimation upon the numerical results of contextual mapping and proves that with skip connections, a one-layer transformer is capable of approximating any permutation equivariant continuous function. Takakura and Suzuki [2023] add positional encoding to lift the restriction of permutation equivariance, and demonstrate a one-layer transformer approximates shift-equivariant α -smoothness function with an error independent of input and output dimension. Jiang and Li [2023] give a non-constructive proof using Kolmogorov representation theorem on the Jackson-type approximation rate of a two-layer transformer. While prior works have achieved diverse and extensive result regarding the expressive capability of transformer, their results require the feed-forward network (FFN) to add expressiveness to the attention module in order to achieve universal approximation, which differs from our results derived from attention-only network. Concurrently, Hu et al. [2025a] give an interpolation-based proof that softmax attention alone (no FFN) is a universal approximator for continuous sequence-to-sequence maps on compact domains.

Provable Capabilities of Transformer. Recent theoretical studies also shed light on the practical behavior of attention mechanism. Olsson et al. [2022] show that induction heads help models learn patterns in context. Sanford et al. [2024a] prove that Transformers can do complex computations with few layers because they work in parallel. In contrast, Luo et al. [2022] find that some Transformer designs lose expressivity when using relative positional encodings. Kim and Suzuki [2024], Chen et al. [2025] provide Transformer’s hardness results on learning constrained boolean functions. Building on [Hu et al., 2025a], Hu et al. [2025b] show that a fixed two-attention-layer softmax Transformer is prompt-programmable: it emulates any algorithm implementable by a single attention layer (cf. [Bai et al., 2023]), providing a constructive account of one-model-many-tasks behavior with softmax (not ReLU) Transformers. To add on these ideas, we prove that a single-layer, single-head softmax attention with a simple linear layer can approximate any continuous function on a compact domain. This shows that attention alone can learn arbitrary sequence-to-sequence mappings.

2 Preliminaries

We now present some ideas we built on.

Notation. For a vector v , we denote its i -th entry by v_i and its subvector from the i_1 -th to the i_2 -th entry (inclusive) by $v_{i_1:i_2}$ with $i_1 < i_2$. For a matrix M , we use $M_{i,j}$ for the entry in the i -th row and j -th column, $M_{i,:}$ for the i -th row, and $M_{:,j}$ for the j -th column. The submatrix spanning rows i_1 through i_2 and columns j_1 through j_2 is denoted by $M_{i_1:i_2,j_1:j_2}$ with $i_1 < i_2, j_1 < j_2$. We define $c_{a \times b}$ as an $a \times b$ matrix with constant entries c , and abbreviate $c_{a \times 1}$ as c_a . For norms, we define $\|\cdot\|_\infty$ as the maximum absolute element in a vector or matrix. The p -norms are given by $\|v\|_p = (\sum_i |v_i|^p)^{1/p}$ for a vector v and $\|M\|_p = (\sum_{i,j} |M_{i,j}|^p)^{1/p}$ for a matrix M . For function norms, we define the L_∞ norm as $\|f\|_{L_\infty} := \sup_{x \in X_f} \|f(x)\|_\infty$, where X_f is the input domain of f , and the L_p norm as $\|f\|_{L_p} := (\int_{x \in X_f} |f(x)|_p^p, dx)^{1/p}$ for $1 \leq p < \infty$. For functions, when a function $f : \mathbb{R} \rightarrow \mathbb{R}$ is applied on a vector or a matrix, it means to apply f on every entry of the vector/matrix (i.e., $\exp([a_1, a_2]) := [\exp(a_1), \exp(a_2)]$).

Self-Attention and Cross-Attention Layers. For a self-attention $\text{Attn}_s : \mathbb{R}^{D \times N} \rightarrow \mathbb{R}^{D \times N_{\text{out}}}$, and any input $Z \in \mathbb{R}^{D \times N}$, we define its output as:

$$\text{Attn}_s(Z) = W_V Z \text{Softmax}((W_K Z)^\top W_Q Z) W_O,$$

where $W_K, W_Q \in \mathbb{R}^{d_{\text{Attn}} \times D}$, $W_V \in \mathbb{R}^{D \times D}$, $W_O \in \mathbb{R}^{N \times N_{\text{out}}}$. Here d_{Attn} stands for the hidden size of the attention block. N_{out} stands for the output sequence length.

For a cross-attention $\text{Attn}_c : \mathbb{R}^{D \times N} \times \mathbb{R}^{D \times N} \rightarrow \mathbb{R}^{D \times N_{\text{out}}}$ and any input $Z_K, Z_Q \in \mathbb{R}^{D \times N}$, we define its output as:

$$\text{Attn}_c(Z_K, Z_Q) = W_V Z_K \text{Softmax}((W_K Z_K)^\top W_Q Z_Q) W_O.$$

Here W_K, W_Q, W_V, W_O are defined as those in self-attention.

Since we provide separate discussions for self-attention and cross-attention in this work, we omit the subscript and denote them as Attn when this causes no ambiguity.

Layer of Sum of Linear Transformations. We use $\text{Linear} : \mathbb{R}^{D_1 \times N_1} \rightarrow \mathbb{R}^{D_2 \times N_2}$ to denote a layer of sum of linear transformations. For any input $Z \in \mathbb{R}^{D_1 \times N_1}$, we define its output as follows:

$$\text{Linear}(Z) := \sum_{i=1}^H P_i Z Q_i + R,$$

where $P_i \in \mathbb{R}^{D_2 \times D_1}$, $Q_i \in \mathbb{R}^{N_1 \times N_2}$ for $i \in [H]$, $R \in \mathbb{R}^{D_2 \times N_2}$. Here H is a positive integer which denotes the number of linear transformations to sum.

3 Attention as Max-Affine Value Reassignment

In this section, we introduce a new interpretation of attention as a value reassignment to a max affine function. Essentially, we show that attention prepended with a Linear layer is able to reassign values to a partition generated by a max-affine function. We start with the below definition.

Definition 3.1 (Max-Affine Function). Let $\mathcal{X} \subset \mathbb{R}^{d_x}$ be a domain, and fix a positive integer N_{ma} . For each $i \in [N_{\text{ma}}]$, define an affine function $y_i : \mathcal{X} \rightarrow \mathbb{R}$ for all $x \in \mathcal{X}$:

$$y_i(x) = a_i^\top x + b_i, \quad \text{where } a_i \in \mathbb{R}^{d_x} \text{ and } b_i \in \mathbb{R}.$$

The *max-affine function* $\text{MaxAff} : \mathcal{X} \rightarrow \mathbb{R}$ corresponding to affine functions $\{y_i(\cdot)\}_{i \in [N_{\text{ma}}]}$ is defined as

$$\text{MaxAff}(x) = \max_{i \in [N_{\text{ma}}]} \{a_i^\top x + b_i\}.$$

Intuitively, a max-affine function selects, at each point $x \in \mathcal{X}$, the largest output among N_{ma} affine functions. Geometrically, each affine function $y_i(x) = a_i^\top x + b_i$ defines a hyperplane in $\mathbb{R}^{d_x+1}$. Thus, MaxAff follows the highest hyperplane at each x , forming a piecewise linear, convex surface — the upper envelope of the given affine hyperplanes.

Remark 3.1 (Technical Assumption). For simplicity of presenting our interpretation, we make the following technical assumption for all results in this section:

Assumption 3.1. For any max-affine function MaxAff , we exclude situations where the difference between its largest and second-largest affine components is smaller than a specified threshold. (Please see proofs for explicit definition.)

We do not apply this assumption in other sections.

3.1 Max-Affine Partition

We now show that a max-affine function $\text{MaxAff}(\cdot)$ induces a partition of its input domain $\mathcal{X}$. Specifically, the input domain $\mathcal{X}$ is divided up according to which affine function is the maximum at each point x . To be concrete, we define this partition as follows:

Proposition 3.1 (Max-Affine Partition). Following [Definition 3.1](#), consider a max-affine function $\text{MaxAff}(x) = \max_{i \in [N_{\text{ma}}]} \{a_i^\top x + b_i\}$, and let $\mathcal{X} \subset \mathbb{R}^{d_x}$ be its input domain. Then MaxAff generates a partition on $\mathcal{X}$:

$$P_{\text{ma}} := \{U_i \mid i \in [N_{\text{ma}}]\}, \quad U_i := \{x \in \mathcal{X} \mid \text{MaxAff}(x) = a_i^\top x + b_i\}, \quad i \in [N_{\text{ma}}].$$

We call the partition P_{ma} the *max-affine partition* of $\mathcal{X}$ induced by MaxAff .

Intuitively, U_i is the set of all point x for which the i -th affine function $a_i^\top x + b_i$ achieves the same value as the max-affine output. Since $\text{MaxAff}(\cdot)$ is the *maximum* of all the affine components, the i -th component is (one of) the highest among all components. Hence, the input domain $\mathcal{X}$ becomes partitioned “regions” $\{U_i\}_{i \in [N_{\text{ma}}]}$. That is, if a point x belongs to a region U_i , the corresponding affine function $a_i^\top x + b_i$ is (tied for) the largest. Please see [Appendix D.1](#) for a detailed proof.

Set Overlaps and Boundaries. By construction, every $x \in \mathcal{X}$ lies in at least one of the sets $\{U_i\}$, but it may belong to multiple sets if several affine components attain the same maximal value. Hence, the collection $\{U_i\}$ is generally a “partition” in an informal sense: while each U_i is typically associated with a distinct region, their pairwise intersections are non-empty on boundary hyperplanes. We address these overlaps in detail within our theorems, where boundary regions do not affect the main approximation arguments but require careful handling to ensure mathematical rigor.

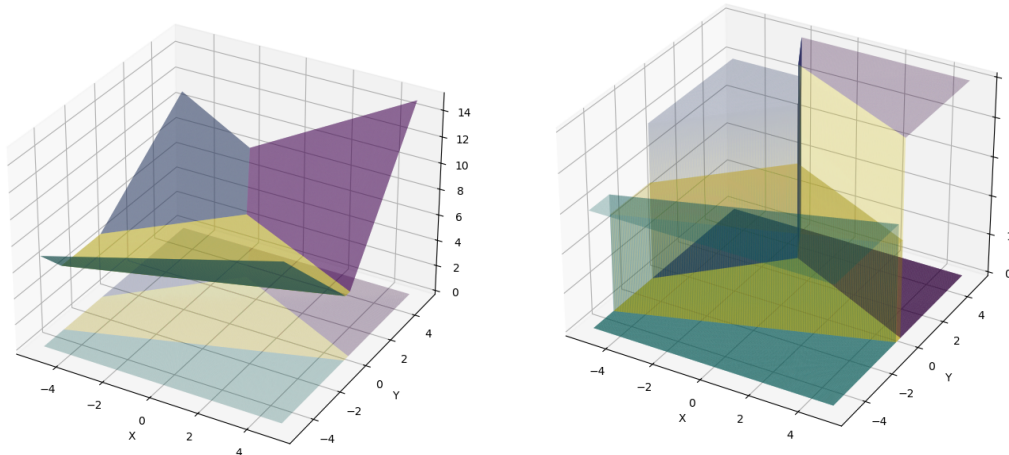
Indicator Encoding of the Partition. For certain analytical and algorithmic tasks, it is helpful to embed the notion of “which affine part is active” into a vector-valued indicator. Formally, we define the indicators for max-affine partitions.

Definition 3.2 (Indicator of Max-Affine Partition). Following the notations in [Proposition 3.1](#), for a max-affine partition $\{U_i | i \in [N_{\text{ma}}]\}$, we define $i_x := \operatorname{argmax}_{i \in [N_{\text{ma}}]} (y_i(x))$ to be the label of the maximal affine component. Then, we define the indicator $E : \mathbb{R}^{d_x} \rightarrow \mathbb{R}^{N_{\text{ma}}}$ as:

$$E(x) = e_{i_x}^{(N_{\text{ma}})},$$

which is a one-hot vector whose only non-zero entry is the i_x -th one.

Namely, each component of $E(x)$ is zero unless it corresponds to an index achieving the maximum, in which it has the value of 1. In [Figure 1a](#), we show an example of the max-affine partition.



(a) **Max-Affine Partition on a 2-D Domain.** Colored regions show where each affine component is active.

(b) **Value Reassignment of Figure 1a.** Each region is reassigned a different affine function.

3.2 Attention Scores Encode Indicators for Max-Affine Partition

We now discuss the connection between self-attention and a max-affine partition. We show that self-attention with a Linear layer attached before it can generate a max-affine partition. Further, for every input token, the attention score matrix approximately indicates which part of the partition it belongs to. We state this result as follows:

Proposition 3.2 (Attention Approximates Indicator of Max-Affine Partition). Let $X = [X_1, X_2, \dots, X_n] \in \mathbb{R}^{d \times n}$ denote any input sequence. We use $\mathcal{X}$ to denote the domain of all $X_i, i \in [n]$. Let MaxAff be any max-affine function on $\mathcal{X}$ with N_{ma} components, and let $\epsilon > 0$ be any positive real number. We define $P_{\text{ma}} = \{U_i | i \in [N_{\text{ma}}]\}$ as the max-affine partition generated by MaxAff as in [Proposition 3.1](#). Then, there exists a Linear layer and a self-attention Attn whose attention matrix satisfies:

$$\|\text{Softmax}((W_K \text{Linear}(X))^{\top} W_Q \text{Linear}(X)) W_O - [E(X_1), E(X_2), \dots, E(X_n)]\|_{\infty} \leq \epsilon,$$

with exception of a region of arbitrarily small Lebesgue measure in $\mathbb{R}^n$. Here W_K, W_Q are the attention weights within Attn . W_O only truncates the irrelevant part of the attention score matrix.

Proposition 3.2 shows that the attention matrix is able to approximate a vector denoting the position of the input token, by indicating which part of the max-affine partition contains the input token.

3.3 Attention Reassign Value to Each Part of the Max-Affine Partition

In the work of [Kim and Kim, 2022], they prove that max-affine functions are universal approximators for convex functions. In order to turn them into universal approximators, a possible solution is to reassign value to each part of the max-affine partition generated by the original max-affine function. In the following theorem, we show that a single-head self-attention is capable of completing this task.

Proposition 3.3 (Attention Reassigns Value to Max-Affine Partition). Following the notation in **Proposition 3.2**, Let $F : \mathbb{R}^d \rightarrow \mathbb{R}_{\text{out}}^d$ be a piece-wise constant function which is separately constant on each $U_i, i \in [N_{\text{ma}}]$. We show that for any $\epsilon > 0$, there exists an self-attention Attn such that

$$\|\text{Attn}(X) - [F(X_1), F(X_2), \dots, F(X_n)]\|_{\infty} \leq \epsilon,$$

for every X in $\mathcal{X}$ with exception of a region of arbitrarily small Lebesgue measure in $\mathbb{R}^n$.

Proposition 3.3 shows that attention is able to output different values according to the indicator generated in **Proposition 3.2**.

We conclude this section with two remarks.

Remark 3.2 (Extension to Function on All Tokens). In this section, for the conciseness in demonstration of method, we adopted a token-wise function F as the example function. Yet since affine functions on all tokens can be easily obtained by adding token-wise affine functions, this simplified version of our method generalizes well on functions taking all tokens as input and leads us to results shown in **Section 4**.

Remark 3.3. Lastly, we emphasize that here the approximation excludes a small area for overall simplicity in this demonstration of our method. We address this issue in the proofs of the universal approximation theorems in the next section.

Figure 1b provides us an example of **Proposition 3.3**.

4 Single-Layer, Single-Head Attention Achieves Universal Sequence-to-Sequence Approximation

In this section, we present our main results:

- A single layer of *single-head self-attention* preceded by one linear layer is a sequence-to-sequence universal approximator for continuous functions on any compact domain.
- A single layer of *single-head cross-attention* preceded by one linear layer is likewise a sequence-to-sequence universal approximator for continuous functions on any compact domain.

Importantly, we achieve attention-only universal approximation for both the L_p -norm and L_{∞} -norm, whereas most existing results apply only to the L_p -norm and require additional auxiliary components in the transformer block (e.g., multiple attention or feed-forward layers). Moreover, our universality result for cross-attention is the first of its kind. Specifically, we present our results for self-attention in **Section 4.1** and for cross-attention in **Section 4.2**.

4.1 Single-Head Self-Attention as a Universal Seq-to-Seq Approximator

We now present our main result: a single-layer, single-head self-attention module, combined with a linear transformation, is sufficient to approximate any continuous map $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ on a compact domain $U \subseteq [-D, D]^{d \times n}$. We present the result first in terms of the L_{∞} norm for continuous f and then extend it to L_p integrable functions.

Theorem 4.1 (L_∞ -Norm Universal Approximation). Let $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ denote any continuous function on a compact domain $U \subset \mathbb{R}^{d \times n}$ and let $\epsilon > 0$ be any positive real number. There exists a self-attention Attn with a prepended Linear layer, such that

$$\|f - \text{Attn} \circ \text{Linear}\|_{L_\infty} \leq \epsilon.$$

Theorem 4.1 indicates that a *single-layer* self-attention block, combined with a linear preprocessing layer Linear, approximates sequence-to-sequence f in the L_∞ -norm.

Overview of Proof Strategy. We adopt a proof strategy based on a key observation: self-attention is capable of approximating target functions via implicit MaxAff operations. Our proof consists of the following 4 steps:

- **Step 1: Partition Input Domain U via MaxAff.** Construct a max-affine function MaxAff over U (i.e., input domain of target function f) such that this MaxAff induces a partition of size- N_{ma} of U .
- **Step 2: Configure Linear and Attn to Imitate MaxAff over U .** Use Linear and W_K, W_Q in Attn to map the input $Z \in U$ to values of the affine components $\{y_i(Z) = a_i^\top \tilde{Z} + b_i\}_{i \in [N_{\text{ma}}]}$ of MaxAff. Here we flatten the input sequence $Z \in \mathbb{R}^{d \times n}$ to $\tilde{Z} \in \mathbb{R}^{dn}$ to compute MaxAff.
- **Step 3: Engineer Attn to Generate an Indicator of Which Partition Cell the Input Belongs To.** Within self-attention Attn, design $K^\top Q$ so that $\text{Softmax}(K^\top Q)$ produces a near-one-hot vector as an indicator to the max-affine partition induced by MaxAff (as defined in **Definition 3.2**). This indicator (approximately an one-hot vector) shows which part (i.e., partitioned cell) of the partition contains the input sequence Z .
- **Step 4: Map the Indicator to the Target Value $f(Z)$.** Map each partition cell's indicator to the corresponding value of f . By continuity of f , refining the partitioned cell ensures $\|f - \text{Attn} \circ \text{Linear}\|_\infty \leq \epsilon$.

Proof Sketch. We elaborate above in detail. Consider a continuous function $f : U \subseteq [-D, D]^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ on a compact domain U . Let $\epsilon > 0$. We aim to construct a *single-layer, single-head* self-attention mechanism Attn (prepended with a linear transformation Linear) such that

$$\|f - \text{Attn} \circ \text{Linear}\|_{L_\infty} \leq \epsilon.$$

Step 1: Partition Input Domain U via MaxAff.

- **Flattening Input.** Each input $Z \in \mathbb{R}^{d \times n}$ is reshaped into a single vector $\tilde{Z} \in \mathbb{R}^{dn}$ by stacking its rows or columns. This unifies the domain as $\tilde{Z} \in [-D, D]^{dn}$.
- **Grid / Max-Affine Construction.** Since f is uniformly continuous on the compact set U , choose $\delta > 0$ such that

$$\|Z_1 - Z_2\|_\infty < \delta \implies \|f(Z_1) - f(Z_2)\|_\infty < \epsilon.$$

We subdivide $[-D, D]^{dn}$ into cubes of side $\leq \delta$, yielding $G = P^{dn}$ grid centers $\{v_j\}_{j=0}^{G-1}$. We treat MaxAff as a piecewise (max-)affine or piecewise-constant partition: for each $\tilde{Z}$, there's a nearest v_j within $\delta/2$.

- **Technical Highlight.** This partition-based approach leverages uniform continuity to discretize U . The number of partitions can be large but finite, ensuring we only need a single-layer of attention to “select” the correct grid cell.

Step 2: Configure Linear and Attn to Imitate MaxAff over U .

- **Sum-of-Linear-Transformations Map Linear.** Design Linear : $\mathbb{R}^{d \times n} \rightarrow \mathbb{R}^M$ (for some dimension M) to capture the dot products $\langle v_j, \tilde{Z} \rangle$. Essentially, Linear(Z) arranges these

$\{v_j^\top \tilde{Z}\}$ in a form accessible to attention. This ensures each grid center v_j can be individually “queried.”

- **Encoding Affine Components.** Observe that $\max_j \{\langle v_j, \tilde{Z} \rangle - \frac{1}{2} \|v_j\|^2\}$ is akin to a max-affine function. We store terms $v_j^\top \tilde{Z}$, plus $-\frac{1}{2} \|v_j\|^2$, into K and Q for later use in $\text{Softmax}(K^\top Q)$.
- **Technical Highlight.** This step demonstrates how we embed $\{\langle v_j, \tilde{Z} \rangle\}$ into a single-head attention setting — no extra feed-forward layers required. The linear map Linear is carefully constructed so that each “component” is individually addressable.

Step 3: Engineer Attn to Generate an Indicator of Which Partition Cell the Input Belongs to.

- **Construct $K^\top Q$.** In the self-attention block, let $K^\top Q \approx R(\langle v_j, \tilde{Z} \rangle - \frac{1}{2} \|v_j\|^2)$, where $R > 0$ is large. This makes $\text{Softmax}(K^\top Q)$ favor the row j^* maximizing

$$\langle v_j, \tilde{Z} \rangle - \frac{1}{2} \|v_j\|^2.$$

- **Near-One-Hot Distribution.** Hence the j^* -th row obtains probability close to 1, effectively identifying which grid center v_{j^*} is nearest to $\tilde{Z}$. We interpret this as a near-one-hot “indicator” vector for the correct partition cell.
- **Technical Highlight.** This is the crux: attention’s softmax can act as a *continuous* $\arg \max$ by scaling the scores with R . As $R \rightarrow \infty$, the distribution becomes more peaked, approximating a hard partition.

Step 4: Map the Indicator to the Target Value $f(Z)$.

- **Assigning Values.** We place $f(v_j)$ in the “value matrix” W_V , so that once row j^* is selected, the attention output is $\approx f(v_{j^*})$. Since Z is within $\delta/2$ of v_{j^*} , uniform continuity implies

$$\|f(Z) - f(v_{j^*})\| \leq \epsilon, \quad (\text{for suitably chosen } \delta).$$

- **Final Reshaping (If Needed).** A small linear projection M can reshape the output back to $\mathbb{R}^{d \times n}$. The essential logic is that the correct $f(v_j)$ is “routed” to the final output via the near-one-hot attention distribution.
- **Technical Highlight.** This reveals how a single-head attention layer, armed with linear preprocessing, suffices to replicate the entire function f . No feed-forward sub-layer or multiple heads are needed to achieve universal approximation.

In sum, combining these steps, we see that: (i) A finite grid subdivides U to handle uniform continuity. (ii) Linear encodes $\{\langle v_j, \tilde{Z} \rangle\}$. (iii) Large- R $\text{Softmax}(K^\top Q)$ selects the best anchor v_{j^*} . (iv) A “value matrix” translates that selection into $f(v_{j^*})$. We conclude that a single-layer, single-head self-attention block approximates f within ϵ in the L_∞ norm. Please see [Appendix E.1](#) for a proof. $\square$

Our result in L_∞ norm can be easily extended to L_p norm, where it applies to not just the continuous functions but all Lebesgue integrable functions with compact support. Please see [Corollary E.1.1](#) for more details.

4.2 Single-Head Cross-Attention as a Universal Seq-to-Seq Approximator

Here we extend self-attention universal approximation results from [Section 4.1](#) to cross-attention. Importantly, we establish the first known universal approximation in cross-attention setting. First, we state our main result in L_∞ -norm.

Theorem 4.2 (L_∞ -Norm Universal Approximation). Let $f : U_K \times U_Q \rightarrow \mathbb{R}^{d \times n}$ denote any continuous function on a compact domain $U_K \times U_Q$ and let ϵ be any positive real number. Here $U_K, U_Q \in \mathbb{R}^{d \times n}$ stands for the compact domain of the two input sequences of cross-attention. Then

there exists a cross-attention Attn prepended with a Linear layer such that

$$\|f - \text{Attn} \circ \text{Linear}\|_{L_\infty} \leq \epsilon.$$

Theorem 4.2 indicates that a *single-layer cross-attention* block, prepended with a linear preprocessing layer Linear, approximates $f : U_K \rightarrow U_Q \rightarrow \mathbb{R}^{d \times n}$ in L_∞ -norm.

Proof Sketch. Our proof follows that of **Theorem 4.1** except one additional step: use Attn to aggregate the max-affine functions on U_K, U_Q and merge into a MaxAff function on $U_K \times U_Q$. The proof consists of the following steps:

Step 1: Partition the Input Domain U_K and U_Q with MaxAff $_K$ and MaxAff $_Q$ Respectively. Construct two max-affine function MaxAff $_K$ over U_K and MaxAff $_Q$ over U_Q such that this MaxAff $_K$ induces a partition of size- N_{ma} of U and MaxAff $_Q$ a same size partition on U_Q .

Step 2: Configure Linear and Attn to Imitate MaxAff $_K$, MaxAff $_Q$ over W_K, U_Q Respectively. Use Linear and W_K, W_Q in Attn to map the input $Z_K, Z_Q \in U$ to values of the affine components $\{y_i(Z) = a_i^\top \tilde{Z} + b_i\}_{i \in [N_{\text{ma}}]}$ of MaxAff $_K$ and MaxAff $_Q$ respectively. Here we flatten the input sequence $Z \in \mathbb{R}^{d \times n}$ to $\tilde{Z} \in \mathbb{R}^{dn}$ to express MaxAff concisely.

Step 3: Use Attn to Aggregate MaxAff $_K$ and MaxAff $_Q$ to Form a MaxAff : $U_K \times U_Q \rightarrow \mathbb{R}$ on Both Input Sequences. Use Attn to generate MaxAff(Z_K, Z_Q) := MaxAff $_K$ (Z_K) + MaxAff $_Q$ (Z_Q). This max-affine function merges the partition on U_K and U_Q to generate a unified partition on $U_K \times U_Q$.

Step 4: Use Attn to Indicate the Position of the Both Input Sequence in the MaxAff-Generated Partition. Use Attn to generate an indicator to the max-affine partition generated by MaxAff (as defined in **Definition 3.2**). This indicator (approximately a one-hot vector) shows which part of the MaxAff-generated partition contains the Cartesian product of both input sequences $Z_K \times Z_Q$.

Step 5: Map the indicator to the Corresponding Value of f . Map the indicator to the corresponding value of the target function f by adding terms related to f to Attn.

Please see **Appendix E.2** for a detailed proof. □

5 Concluding Remarks

We introduce a novel interpretation of attention as a mechanism for reassigning values to a partition induced by a max-affine function. This unique perspective allows us to show that prepending a single linear layer before either self-attention or cross-attention enables the network to (i) generate indicator functions representing max-affine partitions (**Proposition 3.2**) and (ii) selectively reassign values to each partition cell (**Proposition 3.3**). As a result, we prove that both single-head self-attention and single-head cross-attention, when combined with a single layer of sum of linear transformations, achieve universal approximation of compactly supported continuous functions under L_∞ norm, or integrable functions under L_p norm. **Numerical validations** backup our theory in **Appendix B**.

Key Insights and Results.

- **Max-Affine Partition.** A max-affine function naturally partitions its input domain, and attention (with appropriate transformations) can approximate the indicator functions of these partitions.
- **Value Reassignment.** Self-attention reassigns output values based on partition indicators, capturing a broad class of piecewise-defined functions.
- **Universal Approximation.** With only a single linear layer and a single-head attention module, one can approximate arbitrary sequence-to-sequence maps in both the L_∞ and L_p senses, for both self-attention (**Theorem 4.1** and **Corollary E.1.1**) and cross-attention (**Theorem 4.2** and **Corollary E.2.1**) architectures.

Limitations. While our results highlight the surprising representational power of single-head attention with linear preprocessing, several limitations warrant discussion:

- **Large Dimensions and Network Size.** Our minimal-assumption design needs many partition regions to cover diverse targets. This follows naturally from the general setting we study. High-dimensional inputs or long sequences then inflate the parameter count and hinder practice. [Appendix A](#) eases the burden but does not eliminate it entirely.
- **Training Complexity.** Our proofs are *constructive* rather than *prescriptive* for training, meaning standard gradient-based methods may not (always) efficiently find the required weight configurations.
- **Data Distribution Shifts.** Like many universal approximation results, our approach does not account for distribution shifts or generalization beyond the compact domain used for training.

Implications and Future Work. Our findings explain why transformers excel at modeling heterogeneous data: attention can create flexible partitions of the input space and assign context-dependent outputs. This perspective raises open questions for future research: Can multi-head or deeper attention layers simplify representational requirements or reduce approximation constants? How might learned partitions or specialized positional encodings improve efficiency in practice? Can adaptive or data-driven strategies automatically discover near-optimal partitions for specific tasks?

Overall, our results establish a theoretical foundation for understanding attention-based architectures as universal function approximators. They illustrate how token-wise information is *partitioned and reassigned* to represent complex sequence-to-sequence functions with minimal assumptions and structural requirements on data and model.

Acknowledgments

The authors thank Mimi Gallagher, Sara Sanchez, Dino Feng and Andrew Chen for useful discussions; and Weimin Wu, Hong-Yu Chen and Jennifer Zhang for collaborations on related topics. JH also thanks the Red Maple Family for support. The authors also thank the anonymous reviewers and program chairs for constructive comments.

Lastly, JH dedicates this work to the memory of his aunt, Lily Cheung, who passed away during its preparation (March 2025). Her loving and caring spirit will always inspire him.

JH is supported by the Walter P. Murphy Fellowship and the Terminal Year Fellowship (Paul K. Richter Memorial Award) of Northwestern University. HL is partially supported by NIH R01LM1372201, NSF AST-2421845, Simons Foundation MPS-AI-00010513, AbbVie, Dolby and Chan Zuckerberg Biohub Chicago Spoke Award. This research was supported in part through the computational resources and staff contributions provided for the Quest high performance computing facility at Northwestern University which is jointly supported by the Office of the Provost, the Office for Research, and Northwestern University Information Technology. The content is solely the responsibility of the authors and does not necessarily represent the official views of the funding agencies.

References

- Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical report. *arXiv preprint arXiv:2303.08774*, 2023.
- Josh Alman and Hantao Yu. Fundamental limitations on subquadratic alternatives to transformers. *arXiv preprint arXiv:2410.04271*, 2024.
- Yu Bai, Fan Chen, Huan Wang, Caiming Xiong, and Song Mei. Transformers as statisticians: Provable in-context learning with in-context algorithm selection. *Advances in neural information processing systems*, 36:57125–57211, 2023.
- Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Gireeja Ranade Sastry, Amanda Askell, et al. Language models are few-shot learners. *Advances in Neural Information Processing Systems*, 33:1877–1901, 2020.

- Carroll and Dickinson. Construction of neural nets using the radon transform. In *International 1989 joint conference on neural networks*, pages 607–611. IEEE, 1989.
- Bo Chen, Zhenmei Shi, Zhao Song, and Jiahao Zhang. Provable failure of language models in learning majority boolean logic via gradient descent. *arXiv preprint arXiv:2504.04702*, 2025.
- Sitan Chen and Yuanzhi Li. Provably learning a multi-head attention layer. *arXiv preprint arXiv:2402.04084*, 2024.
- George Cybenko. Approximation by superpositions of a sigmoidal function. *Mathematics of control, signals and systems*, 2(4):303–314, 1989.
- Yichuan Deng, Zhao Song, and Tianyi Zhou. Superiority of softmax: Unveiling the performance edge over linear attention. *arXiv preprint arXiv:2310.11685*, 2023.
- Jacob Devlin. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv preprint arXiv:1810.04805*, 2018.
- Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, and Neil Houlsby. An image is worth 16x16 words: Transformers for image recognition at scale. In *International Conference on Learning Representations*, 2021.
- Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, Ahmad Al-Dahle, Aiesha Letman, Akhil Mathur, Alan Schelten, Amy Yang, Angela Fan, et al. The llama 3 herd of models. *arXiv preprint arXiv:2407.21783*, 2024.
- Benjamin L Edelman, Surbhi Goel, Sham Kakade, and Cyril Zhang. Inductive biases and variable creation in self-attention mechanisms. In *International Conference on Machine Learning*, pages 5793–5831. PMLR, 2022.
- Iryna Gurevych, Michael Kohler, and Gözde Gül Şahin. On the rate of convergence of a classifier based on a transformer encoder. *IEEE Transactions on Information Theory*, 68(12):8139–8155, 2022.
- Kurt Hornik. Approximation capabilities of multilayer feedforward networks. *Neural networks*, 4(2): 251–257, 1991.
- Jerry Yao-Chieh Hu, Hude Liu, Hong-Yu Chen, Weimin Wu, and Han Liu. Universal approximation with softmax attention. *arXiv preprint arXiv:2504.15956*, 2025a.
- Jerry Yao-Chieh Hu, Hude Liu, Jennifer Yuntong Zhang, and Han Liu. In-context algorithm emulation in fixed-weight transformers. *arXiv preprint arXiv:2508.17550*, 2025b.
- Yanrong Ji, Zhihan Zhou, Han Liu, and Ramana V Davuluri. Dnabert: pre-trained bidirectional encoder representations from transformers model for dna-language in genome. *Bioinformatics*, 37(15):2112–2120, 2021.
- Haotian Jiang and Qianxiao Li. Approximation theory of transformer networks for sequence modeling. *CoRR*, 2023.
- Tokio Kajitsuka and Issei Sato. Are transformers with one layer self-attention using low-rank weight matrices universal approximators? *arXiv preprint arXiv:2307.14023*, 2023.
- Tokio Kajitsuka and Issei Sato. Optimal memorization capacity of transformers. *arXiv preprint arXiv:2409.17677*, 2024.
- Feyza Duman Keles, Pruthuvi Mahesakya Wijewardena, and Chinmay Hegde. On the computational complexity of self-attention. In *International Conference on Algorithmic Learning Theory*, pages 597–619. PMLR, 2023.
- Jinrae Kim and Youdan Kim. Parameterized convex universal approximators for decision-making problems. *IEEE Transactions on Neural Networks and Learning Systems*, 35(2):2448–2459, 2022.

- Junghwan Kim, Michelle Kim, and Barzan Mozafari. Provable memorization capacity of transformers. In *The Eleventh International Conference on Learning Representations*, 2023.
- Juno Kim and Taiji Suzuki. Transformers provably solve parity efficiently with chain of thought. *arXiv preprint arXiv:2410.08633*, 2024.
- Xu Liu, Juncheng Liu, Gerald Woo, Taha Aksu, Yuxuan Liang, Roger Zimmermann, Chenghao Liu, Silvio Savarese, Caiming Xiong, and Doyen Sahoo. Moirai-moe: Empowering time series foundation models with sparse mixture of experts. *arXiv preprint arXiv:2410.10469*, 2024.
- Shengjie Luo, Shanda Li, Shuxin Zheng, Tie-Yan Liu, Liwei Wang, and Di He. Your transformer may not be as powerful as you expect. *Advances in Neural Information Processing Systems*, 35: 4301–4315, 2022.
- Sadeh Mahdavi, Renjie Liao, and Christos Thrampoulidis. Memorization capacity of multi-head attention in transformers. *arXiv preprint arXiv:2306.02010*, 2023.
- Catherine Olsson, Nelson Elhage, Neel Nanda, Nicholas Joseph, Nova DasSarma, Tom Henighan, Ben Mann, Amanda Askell, Yuntao Bai, Anna Chen, et al. In-context learning and induction heads. *arXiv preprint arXiv:2209.11895*, 2022.
- William Peebles and Saining Xie. Scalable diffusion models with transformers. In *Proceedings of the IEEE/CVF International Conference on Computer Vision*, pages 4195–4205, 2023.
- Clayton Sanford, Daniel Hsu, and Matus Telgarsky. Transformers, parallel computation, and logarithmic depth. *arXiv preprint arXiv:2402.09268*, 2024a.
- Clayton Sanford, Daniel J Hsu, and Matus Telgarsky. Representational strengths and limitations of transformers. *Advances in Neural Information Processing Systems*, 36, 2024b.
- Shokichi Takakura and Taiji Suzuki. Approximation and estimation ability of transformers for sequence-to-sequence functions with infinite dimensional input. In *International Conference on Machine Learning*, pages 33416–33447. PMLR, 2023.
- Yi Tay, Mostafa Dehghani, Dara Bahri, and Donald Metzler. Efficient transformers: A survey. *ACM Computing Surveys*, 55(6):1–28, December 2022. ISSN 1557-7341. doi: 10.1145/3530811.
- Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. Llama: Open and efficient foundation language models. *arXiv preprint arXiv:2302.13971*, 2023a.
- Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, et al. Llama 2: Open foundation and fine-tuned chat models. *arXiv preprint arXiv:2307.09288*, 2023b.
- Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Łukasz Kaiser, and Illia Polosukhin. Attention is all you need. *Advances in neural information processing systems*, 30, 2017.
- Gerald Woo, Chenghao Liu, Akshat Kumar, Caiming Xiong, Silvio Savarese, and Doyen Sahoo. Unified training of universal time series forecasting transformers. *arXiv preprint arXiv:2402.02592*, 2024.
- Chulhee Yun, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank J Reddi, and Sanjiv Kumar. Are transformers universal approximators of sequence-to-sequence functions? *arXiv preprint arXiv:1912.10077*, 2019.
- Zhihan Zhou, Yanrong Ji, Weijian Li, Pratik Dutta, Ramana Davuluri, and Han Liu. Dnabert-2: Efficient foundation model and benchmark for multi-species genome. *arXiv preprint arXiv:2306.15006*, 2023.

Appendix

A	Extension to Practical Settings	13
B	Proof-of-Concept Experiments	14
C	Additional Experimental Results	14
C.1	Numerical Justifications for Theoretical Results in Section 3	14
D	Proofs of Results in Section 3	16
D.1	Proof of Proposition 3.1	16
D.2	Proof of Proposition 3.2	16
D.3	Proof of Proposition 3.3	19
E	Proof of Results in Section 4	20
E.1	Proof of Theorem 4.1	20
E.2	Proof of Theorem 4.2	34
F	Proof of Results in Appendix A	47
F.1	Proof of Theorem A.1	47
G	Extended Related Work	55
H	Extension to Transformer Setting	56

Impact Statement

By the formal nature of this work, we do not expect any immediate negative social impact.

A Extension to Practical Settings

In practical scenarios, despite defined on a high dimension input domain ($\mathbb{R}^{d \times n}$), attention is often considered to approximate a function defined upon a small input domain $\mathcal{X} \subset \mathbb{R}^{d \times n}$.

To this end, we extend our method to the approximation rate of L -Lipschitz functions with a relatively small input domain. We state our result as the following theorem.

Theorem A.1. Let $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ denote an L -Lipschitz function (in terms of 2-norm) whose input domain is $\mathcal{X}$. For any $\epsilon > 0$, assume $\mathcal{X}$ is contained in N_x spheres by the radius of $\epsilon/(3L)$ in 2-norm. Then, there exists a Linear layer and a Attn layer such that:

$$\|\text{Attn} \circ \text{Linear} - f\|_{\infty} \leq \epsilon.$$

Furthermore, Attn and Linear have a total number of $\mathcal{O}(dnN_x)$ trainable parameters.

Proof Sketch. This proof only differs from the proof of **Theorem 4.1** on the choice of partition. For universal approximation, we choose a partition that evenly partition the whole space. In this theorem, we change this partition to have each part centered on a different sphere described in the **Theorem A.1**. By characterizing our partition, we achieve a more precise approximation result.

Please see **Appendix F.1** for a detailed proof. □

Theorem A.1 states that when the input domain is contained in N_x spheres of ϵ -level radius, there exists a single-head self-attention layer that approximates the target function with a precision of ϵ .

B Proof-of-Concept Experiments

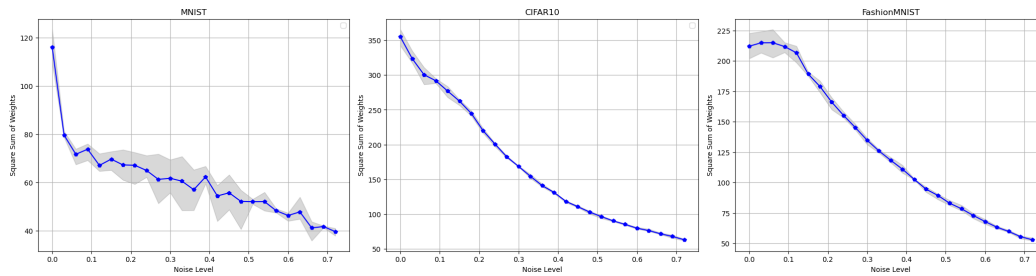


Figure 2: **Scale of Attention Weights vs. Training noise.** For MNIST, CIFAR-10, and Fashion-MNIST we plot the ℓ_2 -norm of W_K and W_Q against the injected label-noise ratio. In all three datasets the weight scale declines monotonically as noise increases, corroborating [Proposition 3.2](#): higher noise hampers precise partitioning, so the model reduces the magnitude of weights that form the attention score matrix.

In [Proposition 3.2](#), we demonstrate domain-partition mechanism of attention. In this mechanism, the temperature of the Softmax function affects the precision of the max-affine partition generated by attention, which is crucial to the complex approximations accomplished in [Theorem 4.1](#) and [Corollary E.1.1](#).

Since the temperature of Softmax is equivalent to the scale of the matrix involved in computing the attention score matrix (W_K, W_Q), our theory suggests the scale of W_K, W_Q decreases when the input data contains more noise, as a result of the rise in difficulty to form a clear partition, and an approximation based on this partition.

To verify this conjecture, we test the correlation between the scale of W_K, W_Q and the noise level in the training data.

Objectives. Examine the relationship between scale of matrix involved in computing the attention score matrix in attention (W_K, W_Q) and the noise level (using Gaussian noise) in the dataset.

Data. We perform separate experiments on the training set of the noised MNIST, CIFAR10 and FashionMNIST datasets with noise level (the coefficient multiplying the standard Gaussian noise) gradually adding from 0 to 0.72 by the step size of 0.03.

Network setups. Our network consists of a single-head self-attention followed by a feed-forward network. Due to the complexity and different characteristics of the selected datasets, the size of the feed-forward network slightly differs between datasets.

Results. [Figure 2](#) presents our results. As the noise level increases, a decrease in the scale of weights in W_K, W_Q becomes evident in all settings. This aligns with our theory.

C Additional Experimental Results

In this section, we present additional experimental results to support our theoretical results.

C.1 Numerical Justifications for Theoretical Results in [Section 3](#)

To validate our results in [Proposition 3.2](#), we conducted the following experiment to examine whether the max-affine function generated within the attention of the form in [Proposition 3.2](#) can learn to separate the input domain according to the values of the target function.

Specifically, we use attention to approximate a step function and observe the max-affine function generated by the weights in K and Q matrices in the attention score matrix. The result of this experiment is shown in [Figure 3](#).

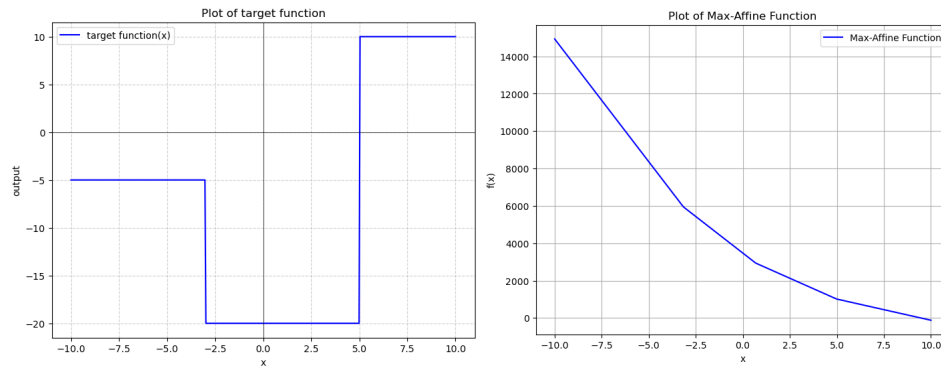


Figure 3: Result of using a single-head attention to approximate a step function. The max-affine function generated in the attention score matrix turns at points close to the switching points in the step function.

The max-affine function generated in the attention score matrix turns at points close to the switching points in the step function. This generates a partition in the input domain that resembles the distribution of the flat parts in the step function. This result aligns with our theory.

D Proofs of Results in Section 3

D.1 Proof of Proposition 3.1

Proposition D.1 (Proposition 3.1 Restated: Max-Affine Partition). Following Definition 3.1, consider a max-affine function $\text{MaxAff}(x) = \max_{i \in [N_{\text{ma}}]} \{a_i^\top x + b_i\}$, and let $\mathcal{X} \subset \mathbb{R}^{d_x}$ be its input domain. Then MaxAff generates a partition on $\mathcal{X}$:

$$P_{\text{ma}} := \{U_i \mid i \in [N_{\text{ma}}]\},$$

$$U_i := \{x \in \mathcal{X} \mid \text{MaxAff}(x) = a_i^\top x + b_i\}, \quad i \in [N_{\text{ma}}].$$

We call the partition P_{ma} the *max-affine partition* of $\mathcal{X}$ induced by MaxAff .

Proof. If an x_0 is not grouped to any U_i , $i \in [N_{\text{MaxAff}}]$. Since MaxAff is define over $\mathcal{X}$ and thus defined on x_0 , we have:

$$\text{MaxAff}(x_0) \neq a_i^\top x_0 + b_i, \quad i \in [N_{\text{MaxAff}}].$$

This is contradictory to the definition of MaxAff .

Since in Section 3 we exclude the discussion on the overlapped regions of the affine components $\{y_i = a_i^\top x + b_i\}$, $\{U_i \mid i \in [N_{\text{MaxAff}}]\}$ form a partition on $\mathcal{X}$. This completes the proof. $\square$

D.2 Proof of Proposition 3.2

Proposition D.2 (Proposition 3.2 Restated: Attention Approximates Indicator of Max-Affine Partition). Let $X = [X_1, X_2, \dots, X_n] \in \mathbb{R}^{d \times n}$ denote any input sequence. We use $\mathcal{X}$ to denote the domain of all X_i , $i \in [n]$. Let MaxAff be any max-affine function on $\mathcal{X}$ with N_{MaxAff} components, and let $\epsilon > 0$ be any positive real number. We define $P_{\text{MaxAff}} = \{U_i \mid i \in [N_{\text{MaxAff}}]\}$ as the max-affine partition generated by MaxAff as in Proposition 3.1. Let E be the indicator of P_{MaxAff} as defined in Definition 3.2. Under the above definitions, there exists a Linear layer and a self-attention Attn whose attention matrix satisfies

$$\|\text{Softmax}((W_K \text{Linear}(X))^\top W_Q \text{Linear}(X)) W_O - [E(X_1), E(X_2), \dots, E(X_n)]\|_\infty \leq \epsilon,$$

with exception of an arbitrarily small region. Here W_K , W_Q are the attention weights within Attn .

Proof. We first denote that according to the premise of Section 3, the intersection region of different affine components are omitted. This means for an arbitrarily small $\delta > 0$, this proposition malfunctions on any points within a δ radius neighborhood of the intersecting lines of max-affine partitions.

Our proof consists of two parts:

1. Construct Linear and Attn .
2. Estimate the error between the attention score matrix of $\text{Attn} \circ \text{Linear}$ and the target indicator.

For the max-affine function MaxAff , we denote it as follows.

Definition D.1 (Max-Affine Function). Let $a_i \in \mathbb{R}^d$, $b_i \in \mathbb{R}$, $i \in [N_{\text{MaxAff}}]$ denote the coefficients of the affine components of MaxAff . In this definition, MaxAff writes out as

$$\text{MaxAff}(Z) = \max_{i \in [N_{\text{MaxAff}}]} \{a_i^\top Z + b_i\}, \quad (\text{D.1})$$

for any $Z \in \mathbb{R}^d$.

Remark D.1. For conciseness of presentation, we assume the top component of MaxAff exceeds the second-largest by a fixed $\Delta > 0$, independent of the input and arbitrarily small.

Construction of Linear. Without loss of generality, assume $N_{\text{MaxAff}} \geq n$. We construct Linear (the layer of linear transformations) to be

$$\text{Linear}(Z) := \begin{bmatrix} I_d \\ 0_{n \times d} \end{bmatrix} Z \begin{bmatrix} I_n & 0_{n \times (N_{\text{MaxAff}} - n)} \end{bmatrix} + \begin{bmatrix} 0_{d \times N_{\text{MaxAff}}} \\ I_{N_{\text{MaxAff}}} \end{bmatrix}.$$

The the output of Linear(X) is

$$\begin{aligned} \text{Linear}(X) &= \begin{bmatrix} I_d \\ 0_{n \times d} \end{bmatrix} X \begin{bmatrix} I_n & 0_{n \times (N_{\text{MaxAff}} - n)} \end{bmatrix} + \begin{bmatrix} 0_{d \times N_{\text{MaxAff}}} \\ I_{N_{\text{MaxAff}}} \end{bmatrix} \\ &= \begin{bmatrix} X & 0_{d \times (N_{\text{MaxAff}} - n)} \\ 0_{n \times n} & 0_{n \times (N_{\text{MaxAff}} - n)} \end{bmatrix} + \begin{bmatrix} 0_{d \times N_{\text{MaxAff}}} \\ I_{N_{\text{MaxAff}}} \end{bmatrix} \\ &= \begin{bmatrix} X & 0_{d \times (N_{\text{MaxAff}} - n)} \\ I_n & 0_{n \times (N_{\text{MaxAff}} - n)} \\ 0_{(N_{\text{MaxAff}} - n) \times n} & I_{N_{\text{MaxAff}} - n} \end{bmatrix}. \end{aligned} \quad (\text{D.2})$$

Construction of Attn. Since we only use the attention score matrix $\text{Softmax}(K^\top Q)$, we only have to construct the W_K and W_Q matrices.

We construct them to be as follows

$$\begin{aligned} W_K &= R \begin{bmatrix} 0_{d \times d} & a_1 & a_2 & \cdots & a_{N_{\text{MaxAff}}} \\ 0 & b_1 & b_2 & \cdots & b_{N_{\text{MaxAff}}} \end{bmatrix} \\ W_Q &= \begin{bmatrix} I_d & 0_{1 \times d} & 0_{1 \times N_{\text{MaxAff}} - d} \\ 0_{1 \times d} & 1_{1 \times d} & 0_{1 \times N_{\text{MaxAff}} - d} \end{bmatrix}, \end{aligned}$$

where R is a coefficient to control the precision of the approximation. Specifically, as R increases, Softmax is closer to maximum function, and the approximation is more precise.

In this construction, we now calculate the K and Q matrices of attention

$$\begin{aligned} K &= W_K \text{Linear}(X) \\ &= R \begin{bmatrix} 0_{d \times d} & a_1 & a_2 & \cdots & a_{N_{\text{MaxAff}}} \\ 0 & b_1 & b_2 & \cdots & b_{N_{\text{MaxAff}}} \end{bmatrix} \cdot \begin{bmatrix} X & 0_{d \times (N_{\text{MaxAff}} - n)} \\ I_n & 0_{n \times (N_{\text{MaxAff}} - n)} \\ 0_{(N_{\text{MaxAff}} - n) \times n} & I_{N_{\text{MaxAff}} - n} \end{bmatrix} \quad (\text{By (D.2)}) \\ &= R \begin{bmatrix} a_1 & a_2 & \cdots & a_{N_{\text{MaxAff}}} \\ b_1 & b_2 & \cdots & b_{N_{\text{MaxAff}}} \end{bmatrix}, \end{aligned}$$

and

$$\begin{aligned} Q &= W_Q \text{Linear}(X) \\ &= \begin{bmatrix} I_d & 0_{1 \times d} & 0_{1 \times N_{\text{MaxAff}} - d} \\ 0_{1 \times d} & 1_{1 \times d} & 0_{1 \times N_{\text{MaxAff}} - d} \end{bmatrix} \cdot \begin{bmatrix} X & 0_{d \times (N_{\text{MaxAff}} - n)} \\ I_n & 0_{n \times (N_{\text{MaxAff}} - n)} \\ 0_{(N_{\text{MaxAff}} - n) \times n} & I_{N_{\text{MaxAff}} - n} \end{bmatrix} \quad (\text{By (D.2)}) \\ &= \begin{bmatrix} X \cdot I_d & 0_{d \times N_{\text{MaxAff}}} \\ 1_{1 \times d} & 0_{1 \times N_{\text{MaxAff}}} \end{bmatrix} \\ &= \begin{bmatrix} X & 0_{d \times N_{\text{MaxAff}}} \\ 1_{1 \times d} & 0_{1 \times N_{\text{MaxAff}}} \end{bmatrix}. \end{aligned}$$

Calculation of $\text{Softmax}(K^\top Q)$. We now calculate the attention score matrix as

$$\begin{aligned} &\text{Softmax}(K^\top Q) \\ &= \text{Softmax} \left(R \begin{bmatrix} a_1 & a_2 & \cdots & a_{N_{\text{MaxAff}}} \\ b_1 & b_2 & \cdots & b_{N_{\text{MaxAff}}} \end{bmatrix}^\top \begin{bmatrix} X & 0_{d \times N_{\text{MaxAff}}} \\ 1_{1 \times d} & 0_{1 \times N_{\text{MaxAff}}} \end{bmatrix} \right) \\ &= \text{Softmax} \left(R \begin{bmatrix} a_1^\top & b_1 \\ a_2^\top & b_2 \\ \vdots & \vdots \\ a_{N_{\text{MaxAff}}}^\top & b_{N_{\text{MaxAff}}} \end{bmatrix} \cdot \begin{bmatrix} X & 0_{d \times N_{\text{MaxAff}}} \\ 1_{1 \times d} & 0_{1 \times N_{\text{MaxAff}}} \end{bmatrix} \right) \end{aligned}$$

$$= \text{Softmax} \left(R \begin{bmatrix} a_1^\top x_1 + b_1 & \cdots & a_1^\top x_n + b_1 & 0_{1 \times (N_{\text{MaxAff}} - d)} \\ a_2^\top x_1 + b_2 & \cdots & a_2^\top x_n + b_2 & 0_{1 \times (N_{\text{MaxAff}} - d)} \\ \vdots & \ddots & \vdots & \vdots \\ a_{N_{\text{MaxAff}}}^\top x_1 + b_{N_{\text{MaxAff}}} & \cdots & a_{N_{\text{MaxAff}}}^\top x_n + b_{N_{\text{MaxAff}}} & 0_{1 \times (N_{\text{MaxAff}} - d)} \end{bmatrix} \right).$$

Estimation of Approximation Error. For $i \in [n]$, we have

$$\begin{aligned} \text{Softmax} (K^\top Q)_{:,i} &= \text{Softmax} \left(R \begin{bmatrix} a_1^\top x_i + b_1 \\ a_2^\top x_i + b_2 \\ \vdots \\ a_{N_{\text{MaxAff}}}^\top x_i + b_{N_{\text{MaxAff}}} \end{bmatrix} \right) \\ &= \frac{1}{\sum_{\eta=1}^{N_{\text{MaxAff}}} \exp(Ra_\eta^\top x_i + Rb_\eta)} \begin{bmatrix} \exp(Ra_1^\top x_i + Rb_1) \\ \exp(Ra_2^\top x_i + Rb_2) \\ \vdots \\ \exp(Ra_{N_{\text{MaxAff}}}^\top x_i + Rb_{N_{\text{MaxAff}}}) \end{bmatrix}. \end{aligned}$$

This yields the entry on the k -th row of $\text{Softmax} K^\top Q_{:,i}$ to be

$$\text{Softmax} (K^\top Q)_{k,i} = \frac{\exp(Ra_k^\top x_i + Rb_k)}{\sum_{\eta=1}^{N_{\text{MaxAff}}} \exp(Ra_\eta^\top x_i + Rb_\eta)}.$$

When $a_k^\top x_i + b_k$ is the maximal affine component and $a_{k'}^\top x_i + b_{k'}$ is the second largest, we have

$$\begin{aligned} \text{Softmax} (K^\top Q)_{k,i} &= 1 - \frac{\sum_{\eta \in [N_{\text{MaxAff}}], \eta \neq k} \exp(Ra_\eta^\top x_i + Rb_\eta)}{\sum_{\eta=1}^{N_{\text{MaxAff}}} \exp(Ra_\eta^\top x_i + Rb_\eta)} \\ &\geq 1 - \frac{\sum_{\eta \in [N_{\text{MaxAff}}], \eta \neq k} \exp(Ra_\eta^\top x_i + Rb_\eta)}{\sum_{\eta=1}^{N_{\text{MaxAff}}} \exp(Ra_k^\top x_i + Rb_k)} \\ &\geq 1 - (N_{\text{MaxAff}} - 1) \frac{\exp(Ra_{k'}^\top x_i + Rb_{k'})}{\exp(Ra_k^\top x_i + Rb_k)} \\ &= 1 - \frac{N_{\text{MaxAff}} - 1}{\exp(Ra_k^\top x_i + Rb_k - (Ra_{k'}^\top x_i + Rb_{k'}))} \\ &\geq 1 - \frac{N_{\text{MaxAff}} - 1}{\exp(R\Delta)}. \end{aligned}$$

Thus when

$$R \geq \Delta \cdot (\ln(N_{\text{MaxAff}} - 1) - \ln \epsilon),$$

we have

$$\frac{N_{\text{MaxAff}} - 1}{\exp(R\Delta)} \leq \epsilon,$$

which means

$$\text{Softmax} K^\top Q_{k,i} \geq 1 - \epsilon. \quad (\text{D.3})$$

Moreover, since the sum of all entries in $\text{Softmax} K^\top Q_{:,i}$ is 1, we have

$$\text{Softmax} (K^\top Q)_{h,i} \leq 1 - \text{Softmax} K^\top Q_{k,i} \leq 1 - (1 - \epsilon) = \epsilon, \quad h \neq k. \quad (\text{D.4})$$

(D.3) and (D.3) are equivalent to

$$\| \text{Softmax} K^\top Q_{k,i} - 1 \|_\infty \leq \epsilon$$

$$\|\text{Softmax } K^\top Q_{h,i} - 0\|_\infty \leq \epsilon, \quad h \neq k.$$

This yields

$$\|\text{Softmax } (K^\top Q)_{:,i} - E(X_i)\|_\infty \leq \epsilon.$$

Thus, by the nature of $\|\cdot\|_\infty$,

$$\|\text{Softmax } (K^\top Q)_{:,i} - [E(X_1), E(X_2), \dots, E(X_n)]\|_\infty \leq \epsilon.$$

We construct W_O to discard $\text{Softmax } K^\top Q_{n+1:N_{\text{MaxAff}},i}$ in $\text{Softmax } K^\top Q$:

$$\begin{bmatrix} I_n \\ 0_{(N_{\text{MaxAff}}-n) \times n} \end{bmatrix}.$$

Thus

$$\begin{aligned} & \|\text{Softmax } (K^\top Q) W_O - [E(X_1), E(X_2), \dots, E(X_n)]\|_\infty \\ &= \|\text{Softmax } (K^\top Q)_{1:n,i} - [E(X_1), E(X_2), \dots, E(X_n)]\|_\infty \\ &\leq \epsilon. \end{aligned}$$

This completes the proof. $\square$

D.3 Proof of Proposition 3.3

Proposition D.3 (Proposition 3.3 Restated: Attention Reassigns Value to Max-Affine Partition). Following the notation in Proposition 3.2, let $F: \mathbb{R}^d \rightarrow \mathbb{R}_{\text{out}}^d$ be a piece-wise constant function which is separately constant on each $U_i, i \in [N_{\text{MaxAff}}]$. We show that for any $\epsilon > 0$, there exists an self-attention Attn such that

$$\|\text{Attn}(X) - [F(X_1), F(X_2), \dots, F(X_n)]\|_\infty \leq \epsilon,$$

for every X in $\mathcal{X}$ with exception of a region of arbitrarily small Lebesgue measure in $\mathbb{R}^n$.

Proof. Let Linear and the W_K , W_Q and W_O matrices be the same as in Appendix D.2. Then by Appendix D.2, we have

$$\|\text{Softmax } (K^\top Q) W_O - [E(X_1), E(X_2), \dots, E(X_n)]\|_\infty \leq \epsilon_0,$$

for any $\epsilon_0 > 0$.

Let V_i denote the value of F on U_i .

Construction of W_V . We construct W_V to be

$$W_V := [0_{1 \times d} \quad V_1 \quad V_2 \quad \dots \quad V_{N_{\text{MaxAff}}}]$$

Thus V equals to

$$\begin{aligned} V &:= W_V \text{Linear}(X) \\ &= [0_{1 \times d} \quad V_1 \quad V_2 \quad \dots \quad V_{N_{\text{MaxAff}}}] \begin{bmatrix} X & 0_{d \times (N_{\text{MaxAff}}-n)} \\ I_n & 0_{n \times (N_{\text{MaxAff}}-n)} \\ 0_{(N_{\text{MaxAff}}-n) \times n} & I_{N_{\text{MaxAff}}-n} \end{bmatrix} \\ &= [V_1 \quad V_2 \quad \dots \quad V_{N_{\text{MaxAff}}}] \end{aligned}$$

Thus we have

$$\begin{aligned} & \|\text{Softmax } (K^\top Q) W_O - [F(X_1), F(X_2), \dots, F(X_n)]\|_\infty \\ &= \|[V_1 \quad V_2 \quad \dots \quad V_{N_{\text{MaxAff}}}] \text{Softmax } (K^\top Q) W_O - [F(X_1), F(X_2), \dots, F(X_n)]\|_\infty \\ &= \|[V_1 \quad V_2 \quad \dots \quad V_{N_{\text{MaxAff}}}] \text{Softmax } (K^\top Q) W_O - [V_1 \quad V_2 \quad \dots \quad V_{N_{\text{MaxAff}}}] [E(X_1), E(X_2), \dots, E(X_n)]\|_\infty \\ &\leq \|V\|_\infty \epsilon_0. \end{aligned}$$

Let $\|V\|_\infty \epsilon_0 \leq \epsilon$ yields the final result. This completes the proof. $\square$

E Proof of Results in Section 4

E.1 Proof of Theorem 4.1

In this section we give the proofs of our universal approximation theorems of self-attention. We first prove the L_∞ norm version whose target function are continuous. Then we combine this result with the well known Lusin's theorem and extend our result to Lebesgue integrable functions in terms of L_p norm.

Theorem E.1 (Theorem 4.1 Restated: L_∞ -Norm Universal Approximation of Self-Attention). Let $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ denote any continuous function on a compact domain $U \subset \mathbb{R}^{d \times n}$ and let $\epsilon > 0$ be any positive real number. Then, there exists a self-attention Attn with a prepended Linear layer, such that

$$\|f - \text{Attn} \circ \text{Linear}\|_{L_\infty} \leq \epsilon.$$

Proof Sketch. Our proof consists of four conceptual steps.

Step 1: Partition Input Domain U via MaxAff.

- **Flattening Input.** Each input $Z \in \mathbb{R}^{d \times n}$ is reshaped into a single vector $\tilde{Z} \in \mathbb{R}^{dn}$ by stacking its rows or columns. This unifies the domain as $\tilde{Z} \in [-D, D]^{dn}$.
- **Grid / Max-Affine Construction.** Since f is uniformly continuous on the compact set U , choose $\delta > 0$ such that

$$\|Z_1 - Z_2\|_\infty < \delta \implies \|f(Z_1) - f(Z_2)\|_\infty < \epsilon.$$

We subdivide $[-D, D]^{dn}$ into cubes of side $\leq \delta$, yielding $G = P^{dn}$ grid centers $\{v_j\}_{j=0}^{G-1}$. We treat MaxAff as a piecewise (max-)affine or piecewise-constant partition: for each $\tilde{Z}$, there's a nearest v_j within $\delta/2$.

Step 2: Configure Linear and Attn to Imitate MaxAff over U .

- **Sum-of-Linear-Transformations Map Linear.** Design Linear : $\mathbb{R}^{d \times n} \rightarrow \mathbb{R}^M$ (for some dimension M) to capture the dot products $\langle v_j, \tilde{Z} \rangle$. Essentially, Linear(Z) arranges these $\{v_j^\top \tilde{Z}\}$ in a form accessible to attention. This ensures each grid center v_j can be individually “queried.”
- **Encoding Affine Components.** Observe that $\max_j \{\langle v_j, \tilde{Z} \rangle - \frac{1}{2}\|v_j\|^2\}$ is akin to a max-affine function. We store terms $v_j^\top \tilde{Z}$, plus $-\frac{1}{2}\|v_j\|^2$, into K and Q for later use in $\text{Softmax}(K^\top Q)$.

Step 3: Enginner Attn to Generate an Indicator of Which Partition Cell the Input Belongs To.

- **Construct $K^\top Q$.** In the self-attention block, let $K^\top Q \approx R(\langle v_j, \tilde{Z} \rangle - \frac{1}{2}\|v_j\|^2)$, where $R > 0$ is large. This makes $\text{Softmax}(K^\top Q)$ favor the row j^* maximizing

$$\langle v_j, \tilde{Z} \rangle - \frac{1}{2}\|v_j\|^2.$$

- **Near-One-Hot Distribution.** Hence the j^* -th row obtains probability close to 1, effectively identifying which grid center v_{j^*} is nearest to $\tilde{Z}$. We interpret this as a near-one-hot “indicator” vector for the correct partition cell.

Step 4: Map the Indicator to the Target Value $f(Z)$.

- **Assigning Values.** We place $f(\tilde{v}_j)$ in the “value matrix” W_V , so that once row j^* is selected, the attention output is $\approx f(\tilde{v}_{j^*})$. Since Z is within $\delta/2$ of v_{j^*} , uniform continuity implies

$$\|f(Z) - f(\tilde{v}_{j^*})\| \leq \epsilon, \text{ (for suitably chosen } \delta).$$

- **Final Reshaping (If Needed).** A small linear projection M can reshape the output back to $\mathbb{R}^{d \times n}$. The essential logic is that the correct $f(\tilde{v}_j)$ is “routed” to the final output via the near-one-hot attention distribution.

Thus, a single-head attention block with a minimal linear layer can approximate any continuous function on the domain. This completes the proof. $\square$

Proof. We divide our proof into two parts:

- **Part 1: Construction of Attn and Linear.** We construct Attn and Linear in accordance with the steps shown in the **proof sketch**, and calculate the precise output of our construction.
- **Part 2: Estimation of Approximation Error between $\text{Attn} \circ \text{Linear}$ and f .** We calculate the difference between the output calculated in previous part and the target function to

Part 1: Construction of Attn and Linear.

We first construct the grid points in $[-D, D]^{dn}$ used in the construction of Linear and Attn.

These grid points are used to construct the max-affine partition. Specifically, the max-affine partition we use is a grid-partition and these points are the center points of these grids.

Construction of Grid Centers in $[-D, D]^{dn}$. Let $Z = [z_1, z_2, \dots, z_n] \in \mathbb{R}^{d \times n}$ denote the input to Linear. Define $\tilde{Z} := [z_1^\top, z_2^\top, \dots, z_n^\top]^\top$. $P \in N_+$ is a parameter that controls the size of the attention block and the error of our approximation.

Definition E.1 (Grid Centers in $[-D, D]^{dn}$). Define $v_{k_1, k_2, \dots, k_{dn}} \in \mathbb{R}^{dn}$ as

$$v_{k_1, k_2, \dots, k_{dn}} := \left[\frac{2Dk_1 - DP}{P}, \frac{2Dk_2 - DP}{P}, \dots, \frac{2Dk_{dn} - DP}{P} \right]^\top,$$

for $k_i \in \{0, 1, 2, \dots, P-1\}$, $i \in [dn]$.

Remark E.1 (Scalar-Labeled Grid Centers). For each multi-index $(k_1, \dots, k_{dn})$ with $k_i \in \{0, \dots, P-1\}$, we define

$$s := \sum_{i=1}^{dn} k_i P^{i-1}, \quad s \in \{0, \dots, P^{dn} - 1\}.$$

This base- P expansion gives a one-to-one map between the tuple and the scalar. This notation allows us to define another representation of the grid center:

$$v_s := v_{k_1, \dots, k_{dn}}.$$

For every $v \in V$, we define

$$\tilde{v} := \underbrace{[v_{1:d}, v_{d+1:2d}, \dots, v_{(n-1)d+1:nd}]}_{d \times n}.$$

We now construct functions E and T . They are linear functions of $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ playing crucial roles in the constructions of W_K and W_Q in $\text{Attn}(\cdot)$.

Construction of E and T . We first show that f is bounded. Because f is continuous within a closed region, its output value is bounded ∞ -norm. Let B_0 denote this bound

$$B_0 := \|f\|_{L_\infty}.$$

We now construct two functions $E(\cdot), T(\cdot)$ related to f . Their sum is a constant while their subtraction is scaled f . For any $Z \in \mathbb{R}^{d \times n}$, we define

$$E(Z) := 1_{d \times n} - \frac{f(Z)}{B_0}, \quad (\text{E.1})$$

$$T(Z) := 1_{d \times n} + \frac{f(Z)}{B_0}, \quad (\text{E.2})$$

and

$$\begin{aligned} (E + T)(Z) &:= E(Z) + T(Z), \\ (E - T)(Z) &:= E(Z) - T(Z). \end{aligned}$$

By the definition of $E(\cdot)$ and $T(\cdot)$, we have

$$(E + T)(Z) \equiv 2_{d \times n} \quad (\text{E.3})$$

$$(E - T)(Z) = \frac{2f(Z)}{B_0}. \quad (\text{E.4})$$

for any $Z \in \mathbb{R}^{d \times n}$.

Construction of the Layer of Sum of Linear Transformations. We now construct the Linear layer to be

$$\text{Linear}(Z) := \sum_{j=0}^{G-1} \left(\sum_{k=0}^{(n-1)} \underbrace{(Ze_{k+1}^{(n)})^\top}_{d \times 1} (v_j)_{kd+1:kd+d} \right) e_1^{(2dG+1)} \sum_{s=0}^{d-1} \left(e_{j+s+1}^{(2dG)} + e_{j+s+dG+1}^{(2dG)} \right)^\top + \begin{bmatrix} 0_{1 \times 2dG} \\ I_{2dG} \end{bmatrix},$$

($e_{j+s+dG+1}^{(2dG)}$ is shifting the 1 in $e_{j+s+1}^{(2dG)}$ down for dG rows.)

where $G = P^{dn}$.

This layer multiplies the flattened input with the grid centers in **Definition E.1** and append a $2dG$ -dimensional identity matrix below the matrix containing these multiplications.

We now express the output of Linear in a simpler form in the following discussion.

First, we show that

$$\begin{aligned} \sum_{k=0}^{(n-1)} \underbrace{(Ze_{k+1}^{(n)})^\top}_{\text{retrieve the } (k+1)\text{-th token}} (v_j)_{kd+1:kd+d} &= \sum_{k=0}^{(n-1)} z_{k+1}^\top (v_j)_{kd+1:kd+d} \\ &= [z_1^\top, z_2^\top, \dots, z_n^\top] v_j \\ &= \tilde{Z}^\top v_j \quad (\text{By } \tilde{Z} \text{ being the flattened input}) \\ &= v_j^\top \tilde{Z} \in \mathbb{R}, \quad j \in \{0, 1, 2, \dots, G-1\}. \end{aligned}$$

This yields

$$\begin{aligned} \text{Linear}(Z) &= \sum_{j=0}^{G-1} v_j^\top \tilde{Z} \sum_{s=0}^{d-1} \left(e_{j+s+1}^{(2dG)} + e_{j+s+dG+1}^{(2dG)} \right)^\top e_1^{(2dG+1)} + \begin{bmatrix} 0_{1 \times 2dG} \\ I_{2dG} \end{bmatrix} \\ &= \begin{bmatrix} X_0 & X_0 \\ I_{dG} & 0_{dG \times dG} \\ 0_{dG \times dG} & I_{dG} \end{bmatrix}. \end{aligned} \quad (\text{E.5})$$

Explicitly, the last line is by

$$\sum_{j=0}^{G-1} v_j^\top \tilde{Z} \sum_{s=0}^{d-1} \left(e_{j+s+1}^{(2dG)} \right)^\top = X_0,$$

which implies

$$\sum_{j=0}^{G-1} v_j^\top \tilde{Z} \sum_{s=0}^{d-1} \left(e_{j+s+1}^{(2dG)} + e_{j+s+dG+1}^{(2dG)} \right)^\top = [X_0 \ X_0].$$

Here

$$X_0 := \begin{bmatrix} v_0^\top \tilde{Z} 1_{1 \times d} & v_1^\top \tilde{Z} 1_{1 \times d} & v_2^\top \tilde{Z} 1_{1 \times d} & \cdots & v_{G-1}^\top \tilde{Z} 1_{1 \times d} \end{bmatrix}.$$

To summarize, in the output of the first layer of linear transformations, the first row consists of linear transformations of the flattened input, while the other rows are together an identity matrix (I_{2dG}).

Construction of K and Q Matrices. We now construct the W_k and W_Q matrices in the self-attention block and calculate the output of Softmax ($K^\top Q$).

We define W_K as follows

$$W_K := \begin{bmatrix} 1 & 0 & \cdots & 0 & 0 & \cdots & 0 \\ 0 & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times d} \\ 0_n & \ln(T(\tilde{v}_0))^\top & \cdots & \ln(T(\tilde{v}_{G-1}))^\top & \ln(E(\tilde{v}_0))^\top & \cdots & \ln(E(\tilde{v}_{G-1}))^\top \end{bmatrix}.$$

The definition of W_K yields that

$$\begin{aligned} K &:= W_K \text{Linear}(Z) \\ &= \begin{bmatrix} 1 & 0 & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 \\ 0 & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_1\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_1\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times d} \\ 0_n & \ln(T(\tilde{v}_0))^\top & \ln(T(\tilde{v}_1))^\top & \cdots & \ln(T(\tilde{v}_{G-1}))^\top & \ln(E(\tilde{v}_0))^\top & \ln(E(\tilde{v}_1))^\top & \cdots & \ln(E(\tilde{v}_{G-1}))^\top \end{bmatrix} \\ &\quad \cdot \begin{bmatrix} X_0 & X_0 \\ I_{dG} & 0_{dG \times dG} \\ 0_{dG \times dG} & I_{dG} \end{bmatrix} \\ &= \begin{bmatrix} v_0^\top \tilde{Z} 1_{1 \times d} & v_1^\top \tilde{Z} 1_{1 \times d} & \cdots & v_{G-1}^\top \tilde{Z} 1_{1 \times d} & v_0^\top \tilde{Z} 1_{1 \times d} & v_1^\top \tilde{Z} 1_{1 \times d} & \cdots & v_{G-1}^\top \tilde{Z} 1_{1 \times d} \\ -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_1\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_1\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times d} \\ \ln(T(\tilde{v}_0))^\top & \ln(T(\tilde{v}_1))^\top & \cdots & \ln(T(\tilde{v}_{G-1}))^\top & \ln(E(\tilde{v}_0))^\top & \ln(E(\tilde{v}_1))^\top & \cdots & \ln(E(\tilde{v}_{G-1}))^\top \end{bmatrix}, \\ &\quad \text{(By (E.5))} \end{aligned}$$

where the last line follows from X_0 being multiplied by 1 and thus appearing in the first row of the output.

Next, we construct W_Q to be

$$W_Q := \begin{bmatrix} 0 & R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ 0 & R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ 0_n & I_n & 0_{n \times (2dG-n)} \end{bmatrix}.$$

This yields that

$$\begin{aligned} Q &= W_Q \text{Linear}(Z) \\ &= \begin{bmatrix} 0 & R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ 0 & R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ 0_n & I_n & 0_{n \times (2dG-n)} \end{bmatrix} \cdot \begin{bmatrix} X_0 & X_0 \\ I_{dG} & 0_{dG \times dG} \\ 0_{dG \times dG} & I_{dG} \end{bmatrix} \\ &= \begin{bmatrix} R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ I_n & 0_{n \times (2dG-n)} \end{bmatrix}. \end{aligned}$$

We now calculate the attention matrix Softmax ($K^\top Q$).

Calculation of $\text{Softmax}(K^\top Q)$. First, $K^\top Q$ writes out as

$$\begin{aligned}
 K^\top Q &= \begin{bmatrix} v_0^\top \tilde{Z} 1_d & \frac{\|v_0\|_2^2}{2} 1_d & \ln(T(\tilde{v}_0)) \\ v_1^\top \tilde{Z} 1_d & \frac{\|v_1\|_2^2}{2} 1_d & \ln(T(\tilde{v}_1)) \\ \vdots & \vdots & \vdots \\ v_{G-1}^\top \tilde{Z} 1_d & \frac{\|v_{G-1}\|_2^2}{2} 1_d & \ln(T(\tilde{v}_{G-1})) \\ v_0^\top \tilde{Z} 1_d & \frac{\|v_0\|_2^2}{2} 1_d & \ln(E(\tilde{v}_0)) \\ v_1^\top \tilde{Z} 1_d & \frac{\|v_1\|_2^2}{2} 1_d & \ln(E(\tilde{v}_1)) \\ \vdots & \vdots & \vdots \\ v_{G-1}^\top \tilde{Z} 1_d & \frac{\|v_{G-1}\|_2^2}{2} 1_d & \ln(E(\tilde{v}_{G-1})) \end{bmatrix} \cdot \begin{bmatrix} R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ R 1_{1 \times n} & 0_{1 \times (2dG-n)} \\ I_n & 0_{n \times (2dG-n)} \end{bmatrix} \\
 &= \begin{bmatrix} R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2}) 1_{d \times n} + \ln(T(\tilde{v}_0)) & 0_{d \times (2dG-n)} \\ R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2}) 1_{d \times n} + \ln(T(\tilde{v}_1)) & 0_{d \times (2dG-n)} \\ \vdots & \vdots \\ R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2}) 1_{d \times n} + \ln(T(\tilde{v}_{G-1})) & 0_{d \times (2dG-n)} \\ R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2}) 1_{d \times n} + \ln(E(\tilde{v}_0)) & 0_{d \times (2dG-n)} \\ R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2}) 1_{d \times n} + \ln(E(\tilde{v}_1)) & 0_{d \times (2dG-n)} \\ \vdots & \vdots \\ R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2}) 1_{d \times n} + \ln(E(\tilde{v}_{G-1})) & 0_{d \times (2dG-n)} \end{bmatrix}, \quad (\text{E.6})
 \end{aligned}$$

where the last line follows from the multiplication of block matrices. This multiplication between $K^\top$ and Q is equivalent to first multiplying the first 2 columns in $K^\top$ with R and then broadcasting their sum to the first n columns, and then adding the result with T and E related blocks. Columns are all filled with 0 except for the first n columns.

Remark E.2 (Interpretation of $K^\top Q$). The non-zero entries of $K^\top Q$ is an aggregation of two matrices

$$\begin{bmatrix} R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})1_{d \times n} \\ R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})1_{d \times n} \\ \vdots \\ R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})1_{d \times n} \\ R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})1_{d \times n} \\ R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})1_{d \times n} \\ \vdots \\ R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})1_{d \times n} \end{bmatrix} \quad (\text{E.7})$$

and

$$\begin{bmatrix} \ln(T(\tilde{v}_0)) \\ \ln(T(\tilde{v}_1)) \\ \vdots \\ \ln(T(\tilde{v}_{G-1})) \\ \ln(E(\tilde{v}_0)) \\ \ln(E(\tilde{v}_1)) \\ \vdots \\ \ln(E(\tilde{v}_{G-1})) \end{bmatrix}. \quad (\text{E.8})$$

In these two matrices, (E.7) is identical between columns and has the precision coefficient R free of our choice. In later discussions, we set R to be sufficiently large so that the Softmax approximates a maximum function, and “selects” the i of the maximal $R(v_i^\top \tilde{Z} - \frac{\|v_i\|_2^2}{2})1_{d \times n}$ for $i \in \{0, 1, \dots, G-1\}$. By “select” we mean only the entries with the selected label has a value not close to 0 in each column of $\text{Softmax}(K^\top Q)$.

(E.8) does not include R related terms. Thus when R is set to be sufficiently large in our later discussions, (E.8) does not affect the selection made by (E.7).

If we exclude the (E.8) in the attention score matrix $\text{Softmax}(K^\top Q)$, the output approximates a matrix whose columns are all-zero except for two sub-vector equal to $1/2d \cdot 1_d$. This writes out as (here we only show the first n non-constant columns)

$$\begin{bmatrix} 0_{(s-1)d \times n} \\ \frac{1}{2d}1_{d \times n} \\ 0_{(G-s)d \times n} \\ 0_{(s-1)d \times n} \\ \frac{1}{2d}1_{d \times n} \\ 0_{(G-s)d \times n} \end{bmatrix}, \quad (\text{E.9})$$

for any $s \in [G]$. The addition of (E.8) change the 1_d in (E.9) to

$$\begin{bmatrix} 0_{(s-1)d \times n} \\ \frac{1}{2d}T(\tilde{v}_{s-1}) \\ 0_{(G-s)d \times n} \\ 0_{(s-1)d \times n} \\ \frac{1}{2d}E(\tilde{v}_{s-1}) \\ 0_{(G-s)d \times n} \end{bmatrix}. \quad (\text{E.10})$$

In later discussion, we use V to transform (E.10) to $T(\tilde{v}_{s-1}) - E(\tilde{v}_{s-1}) = 2f(\tilde{v}_{s-1})/2dB_0$ to obtain the final output.

Now, we divide the calculation of $\text{Softmax}(K^\top Q)$ into two parts: the calculation of $\exp(K^\top Q)$ and the calculation of the denominator of every column of $\text{Softmax}(K^\top Q)$. This denominator explicitly writes out as $\sum_{j=1}^{2dG} \exp(K^\top Q)_{ij}$ for each $i \in [2dG]$.

For $\exp(K^\top Q)$, by (E.6), we have

$$\exp(K^\top Q) = \begin{bmatrix} \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right) T(\tilde{v}_0) & 1_{d \times (2dG-n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right) T(\tilde{v}_1) & 1_{d \times (2dG-n)} \\ \vdots & \vdots \\ \exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right) T(\tilde{v}_{G-1}) & 1_{d \times (2dG-n)} \\ \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right) E(\tilde{v}_0) & 1_{d \times (2dG-n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right) E(\tilde{v}_1) & 1_{d \times (2dG-n)} \\ \vdots & \vdots \\ \exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right) E(\tilde{v}_{G-1}) & 1_{d \times (2dG-n)} \end{bmatrix}. \quad (\text{E.11})$$

For the denominator, we calculate it in columns. Let i denote the column which we calculate the denominator in Softmax. When $i \in \{n+1, n+2, \dots, 2dG\}$, there are $1 \cdot 2dG = 2dG$ columns. And when $i \in [n]$, we denote that

$$\begin{aligned} \sum_{j=1}^{2dG} \exp(K^\top Q)_{i,j} &= \sum_{j=1}^G \left[(1_{1 \times d} T(\tilde{v}_{j-1})_{:,i} + 1_{1 \times d} E(\tilde{v}_{j-1})_{:,i}) \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \right] \\ &\quad (\text{By (E.11)}) \\ &= \sum_{j=1}^G \left[(1_{1 \times d} (E + T)(v_{j-1})_{:,i}) \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \right] \\ &= \sum_{j=1}^G \left[(1_{1 \times d} (2_{d \times n})_{:,i}) \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \right] \\ &= \sum_{j=1}^G 2d \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right), \quad i \in [n]. \end{aligned} \quad (\text{E.12})$$

Observing from (E.12), $\sum_{j=1}^{2dG} \exp(K^\top Q)_{i,j}$ is *invariant* of i for $i \in [n]$. In this case, we define

$$\alpha(Z) := \frac{1}{2d} \sum_{j=1}^{2dG} \exp(K^\top Q)_{i,j} = \sum_{j=1}^G \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \in \mathbb{R}, \quad i \in [n].$$

From (E.11) and (E.12), we have

$$\begin{aligned} &\text{Softmax}(K^\top Q) \\ &= \exp(K^\top Q) \odot \left[\frac{1}{\sum_{j=1}^{2dG} \exp(K^\top Q)_{1j}} 1_{2dG \times n} \quad \frac{1}{2dG} 1_{2dG \times (2dG-n)} \right] \\ &\quad (\text{By } \frac{1}{\sum_{j=1}^{2dG} \exp(K^\top Q)_{ij}} \text{ is invariant of } i \text{ for } i \in [n]) \\ &= \begin{bmatrix} \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right) T(\tilde{v}_0) & 1_{d \times (2dG-n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right) T(\tilde{v}_1) & 1_{d \times (2dG-n)} \\ \vdots & \vdots \\ \exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right) T(\tilde{v}_{G-1}) & 1_{d \times (2dG-n)} \\ \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right) E(\tilde{v}_0) & 1_{d \times (2dG-n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right) E(\tilde{v}_1) & 1_{d \times (2dG-n)} \\ \vdots & \vdots \\ \exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right) E(\tilde{v}_{G-1}) & 1_{d \times (2dG-n)} \end{bmatrix} \odot \begin{bmatrix} \frac{1}{2d\alpha(Z)} 1_{2dG \times n} & \frac{1}{2dG} 1_{2dG \times (2dG-n)} \end{bmatrix} \end{aligned}$$

$$= \frac{1}{2d} \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_0) & \frac{1}{G} \mathbf{1}_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_1) & \frac{1}{G} \mathbf{1}_{d \times (2dG-n)} \\ \vdots & \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_{G-1}) & \frac{1}{G} \mathbf{1}_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_0) & \frac{1}{G} \mathbf{1}_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_1) & \frac{1}{G} \mathbf{1}_{d \times (2dG-n)} \\ \vdots & \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_{G-1}) & \frac{1}{G} \mathbf{1}_{d \times (2dG-n)} \end{bmatrix}. \quad (\text{E.13})$$

Construction of W_V and W_O . We now construct the W_V matrix and calculate the V matrix of the self-attention.

We define W_V as:

$$W_V := [0_d \quad X_1 \quad -X_1]_{d \times (1+2dG)},$$

where

$$X_1 := [I_d \quad I_d \quad \cdots \quad I_d]_{d \times dG},$$

is a matrix formed by stacking G I_d matrix horizontally.

With this definition, we compute V matrix as follows

$$\begin{aligned} V &:= W_V \text{Linear}(Z) \\ &= [0_d \quad X_1 \quad -X_1] \cdot \begin{bmatrix} X_0 & X_0 \\ I_{dG} & 0_{dG \times dG} \\ 0_{dG \times dG} & I_{dG} \end{bmatrix} \\ &= [X_1 \quad -X_1]. \end{aligned} \quad (\text{E.14})$$

After the construction and calculation of V , we go on to construct W_O as:

$$W_O = \begin{bmatrix} dB_0 I_n \\ 0_{(2dG-n) \times n} \end{bmatrix}.$$

The sole purpose of W_O is to extract the non-zero entries of the final output.

Calculation of the Output of $\text{Attn} \circ \text{Linear}$. We now compute the final output of the self-attention block

$$\text{Attn} \circ \text{Linear}(Z)$$

$$\begin{aligned}
&= \frac{1}{2d} [X_1 \quad -X_1] \cdot \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_0) & \frac{1}{G} 1_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_1) & \frac{1}{G} 1_{d \times (2dG-n)} \\ \vdots & \vdots \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_{G-1}) & \frac{1}{G} 1_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_0) & \frac{1}{G} 1_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_1) & \frac{1}{G} 1_{d \times (2dG-n)} \\ \vdots & \vdots \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_{G-1}) & \frac{1}{G} 1_{d \times (2dG-n)} \end{bmatrix} W_O \\
&\quad \text{(By (E.14) and (E.13))} \\
&= \frac{1}{2d} X_1 \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} (T(\tilde{v}_0) - E(\tilde{v}_0)) & 0_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} (T(\tilde{v}_1) - E(\tilde{v}_1)) & 0_{d \times (2dG-n)} \\ \vdots & \vdots \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} (T(\tilde{v}_{G-1}) - E(\tilde{v}_{G-1})) & 0_{d \times (2dG-n)} \end{bmatrix} W_O \\
&\quad \text{(Sum of } X_1 \text{ multiplied by } T \text{ related blocks and } -X_1 \text{ multiplied by } E \text{ related ones)} \\
&= \frac{1}{2d} X_1 \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2f(\tilde{v}_0)}{B_0} & 0_{d \times (2dG-n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2f(\tilde{v}_1)}{B_0} & 0_{d \times (2dG-n)} \\ \vdots & \vdots \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2f(\tilde{v}_{G-1})}{B_0} & 0_{d \times (2dG-n)} \end{bmatrix} W_O. \quad \text{(By (E.3))}
\end{aligned}$$

Let I_d denote the d -dimensional identity matrix. We have

$$X_1 \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_0)}{B_0} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_1)}{B_0} \\ \vdots \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_{G-1})}{B_0} \end{bmatrix}$$

$$\begin{aligned}
&= [I_d \quad I_d \quad \cdots \quad I_d]_{d \times dG} \cdot \underbrace{\begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_0)}{B_0} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_1)}{B_0} \\ \vdots \\ \frac{\exp\left(R(v_{G-1}^\top \tilde{Z} - \frac{\|v_{G-1}\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_{G-1})}{B_0} \end{bmatrix}}_{:=S} \\
&\quad \text{(Equivalent to summing all blocks in } S\text{)} \\
&= \sum_{j=0}^{G-1} I_d \cdot \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_j)}{B_0} \\
&= \sum_{j=0}^{G-1} \frac{1}{\alpha(Z)} \exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right) \frac{2f(\tilde{v}_j)}{B_0}.
\end{aligned}$$

This yields

$$\begin{aligned}
\text{Attn} \circ \text{Linear}(Z) &= \left[\sum_{j=0}^{G-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_j)}{B_0} \quad 0_{d \times (2dG-n)} \right] W_O \\
&= \left[\sum_{j=0}^{G-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_j)}{B_0} \quad 0_{d \times (2dG-n)} \right] \cdot \begin{bmatrix} dB_0 I_n \\ 0_{(2dG-n) \times n} \end{bmatrix} \\
&= \sum_{j=0}^{G-1} \frac{1}{\alpha(Z)} \exp\left(R(v_j^\top \tilde{Z} - \frac{1}{2}\|v_j\|_2^2)\right) f(\tilde{v}_j). \tag{E.15}
\end{aligned}$$

Part 2: Estimation of the Approximation Error between $\text{Attn} \circ \text{Linear}$ and f .

With above calculations of the output of $\text{Attn} \circ \text{Linear}$, we now demonstrate how this output approximates our target function.

Essentially, we demonstrate that each term in the summation of (E.15), given by

$$\frac{1}{\alpha(Z)} \exp\left(R(v_j^\top \tilde{Z} - \frac{1}{2}\|v_j\|_2^2)\right),$$

approximates a max-affine indicator as R becomes sufficiently large. They are each multiplied with $f(\tilde{v}_j)$, which is the value of the target function at the center point of the indicated region.

Definition E.2 (Max-Affine Function on $\tilde{Z}$). Let $\text{Aff}_j \in \mathbb{R}^{dn} \rightarrow \mathbb{R}$ with $j \in \{0, 1, 2, \dots, G-1\}$ denote a group of affine functions defined as:

$$\text{Aff}_j(\tilde{Z}) = v_j^\top \tilde{Z} - \frac{1}{2}\|v_j\|_2^2, \quad j \in \{0, 1, 2, \dots, G-1\}.$$

Then let $\text{MaxAff} \in \mathbb{R}^{dn} \rightarrow \mathbb{R}$ denote a max affine function whose affine components are $\{\text{Aff}_j \mid j \in \{0, 1, 2, \dots, G-1\}\}$. Explicitly defined as:

$$\text{MaxAff}(\tilde{Z}) = \max_{j \in \{0, 1, 2, \dots, G-1\}} \left\{ \text{Aff}_j(\tilde{Z}) \right\}.$$

Because the target function f is a continuous function on a closed domain, the function f is uniformly continuous. Thus for ϵ , there exists a $\delta > 0$ such that for any Z_1, Z_2 , as long as $\|\tilde{Z}_1 - \tilde{Z}_2\|_\infty \leq \delta$, we have $\|f(Z_1) - f(Z_2)\|_\infty \leq \epsilon/3$.

According to this δ , we divide the affine components of MaxAff into three parts:

1. The maximal component, which has the smallest label j_m .

2. All affine components that match the maximal component or fall within δ of it (J_0 as defined below).
3. The remaining Aff_j for $j \in \{0, 1, \dots, G-1\}$ (J_1 as defined below).

We write out the labels of these groups of components as follows

$$\begin{aligned} j_m &:= \min_{j \in \{0, 1, 2, \dots, G-1\}} \{\text{Aff}_j(\tilde{Z}) = \text{MaxAff}(\tilde{Z})\}, \\ J_0 &:= \{j \mid \text{MaxAff}(\tilde{Z}) - \text{Aff}_j(\tilde{Z}) \leq \delta\}, \\ J_1 &:= \{j \mid \text{MaxAff}(\tilde{Z}) - \text{Aff}_j(\tilde{Z}) > \delta\}. \end{aligned}$$

For any pair of $i, j \in \{0, 1, \dots, G-1\}$, we have

$$\begin{aligned} \text{Aff}_i(\tilde{Z}) - \text{Aff}_j(\tilde{Z}) &= v_i^\top \tilde{Z} - \frac{\|v_i\|_2^2}{2} - \left(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2} \right) \\ &= -\frac{\|\tilde{Z}\|_2^2}{2} + v_i^\top \tilde{Z} - \frac{\|v_i\|_2^2}{2} - \left(-\frac{\|\tilde{Z}\|_2^2}{2} + v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2} \right) \\ &= -\frac{1}{2} \|\tilde{Z} - v_i\|_2^2 + \frac{1}{2} \|\tilde{Z} - v_j\|_2^2. \end{aligned}$$

Thus for j_m , we have

$$-\frac{1}{2} \|\tilde{Z} - v_{j_m}\|_2^2 + \frac{1}{2} \|\tilde{Z} - v_j\|_2^2 = \text{Aff}_{j_m}(\tilde{Z}) - \text{Aff}_j(\tilde{Z}) \geq 0, \quad j \in \{0, 1, \dots, G-1\}.$$

This yields

$$\|\tilde{Z} - v_{j_m}\|_2^2 \leq \|\tilde{Z} - v_j\|_2^2,$$

for all $j \in \{0, 1, \dots, G-1\}$.

This denotes j_m is also the label of the closest v_i to $\tilde{Z}$ among all $v_i, i \in \{0, 1, \dots, G-1\}$. Thus we have

$$\|v_{j_m} - \tilde{Z}\|_2 = \min_{i \in \{0, 1, \dots, G-1\}} \{\|v_i - \tilde{Z}\|_2\}. \quad (\text{E.16})$$

Now, we prove v_{j_m} (the grid point nearest to $\tilde{Z}$) has a distance to $\tilde{Z}$ smaller than half of the grid width (e.g., D/g) in infinite norm.

Let $\mathcal{D} := 2D/g \times \{-1, 0, 1\}^{dn}$ denote a set differences to v_{j_m} from the set of all v_i ($i \in \{0, 1, \dots, G-1\}$) neighboring v_{j_m} . For any Δ in $\mathcal{D}$, from (E.16) we have

$$\|v_{j_m} - \tilde{Z}\|_2^2 \leq \|v_{j_m} + \Delta - \tilde{Z}\|_2^2.$$

This yields

$$2\Delta^\top (\tilde{Z} - v_{j_m}) \leq \|\Delta\|_2^2.$$

This means that, for any $k \in [dn]$, by selecting Δ to be $\pm 2D/ge_k^{(dn)}$, we have:

$$\pm 2 \cdot \frac{2D}{g} (\tilde{Z} - v_{j_m})_k = 2\Delta^\top (\tilde{Z} - v_{j_m}) \leq \|\Delta\|_2^2 = \frac{4D^2}{g^2}.$$

Thus we have

$$\left| (\tilde{Z} - v_{j_m})_k \right| \leq \frac{D}{g}, \quad k \in [dn],$$

which implies

$$\|\tilde{Z} - v_{j_m}\|_\infty \leq \frac{D}{g}.$$

Set g to be larger than $2D/\delta$; we have

$$\|\tilde{Z} - v_{j_m}\|_\infty \leq \frac{\delta}{2},$$

thus

$$\|f(Z) - f(\tilde{v}_{j_m})\|_\infty \leq \frac{\epsilon}{3}, \quad (\text{E.17})$$

where the inequality holds by $\delta/2 < \delta$.

Calculation of $\|\text{Attn} \circ \text{Linear} - f\|_\infty$. We now calculate the difference between the output in (E.15) and target function f

$$\begin{aligned} & \|\text{Attn} \circ \text{Linear}(Z) - f(Z)\|_\infty \\ &= \left\| \sum_{j=0}^{G-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} f(\tilde{v}_j) - f(Z) \right\|_\infty \\ &= \left\| \sum_{j=0}^{G-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} (f(\tilde{v}_j) - f(Z)) \right\|_\infty \quad \left(\text{By } \sum_{j=0}^{G-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} = 1 \right) \\ &\leq \sum_{j=0}^{G-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \quad (\text{By property of infinite norm}) \\ &= \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty \\ &\quad + \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\ &\quad + \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty. \end{aligned} \quad (\text{E.18})$$

We now calculate each part in (E.18).

As previously stated, for any Z_1, Z_2 , as long as $\|\tilde{Z}_1 - \tilde{Z}_2\|_\infty \leq \delta$, we have $\|f(Z_1) - f(Z_2)\|_\infty \leq \epsilon/3$. Thus when we designate $\tilde{Z}_1 = v_j$ for any $j \in J_0$ and $\tilde{Z}_2 = v_{j_m}$, along with (E.17) we have

$$\begin{aligned} & \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\ &\leq \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} (\|f(\tilde{v}_j) - f(\tilde{v}_{j_m})\|_\infty + \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty) \\ &\leq \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot \left(\frac{\epsilon}{3} + \frac{\epsilon}{3}\right) \\ &= \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2\epsilon}{3}. \end{aligned} \quad (\text{E.19})$$

For j_m , we have

$$\frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{1}{2}\|v_{j_m}\|_2^2)\right)}{\alpha(Z)} \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty \leq \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{1}{2}\|v_{j_m}\|_2^2)\right)}{\alpha(Z)} \cdot \frac{\epsilon}{3}. \quad (\text{E.20})$$

When R is larger than $\frac{8}{3\delta^2} \ln\left(\frac{3}{2}B_0G\epsilon\right)$, we have

$$\begin{aligned}
& \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\
& \leq \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot 2B_0 \quad (\text{By } \|f\|_{L_\infty} = B_0) \\
& \leq 2B_0 \frac{\sum_{j \in J_1} \exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \\
& < 2B_0 \frac{\sum_{j \in J_1} \exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)} \\
& \quad (\alpha(Z) \text{ is the sum of all } \exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right), \text{ thus larger than } \exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)) \\
& = 2B_0 \sum_{j \in J_1} \exp\left(\frac{R}{2}(\|v_{j_m} - Z\|_2^2 - \|v_j - Z\|_2^2)\right) \\
& \leq 2B_0 \|J_1\| \exp\left(\frac{R}{2} \left[\left(\frac{\delta}{2}\right)^2 - \delta^2\right]\right) \\
& < 2B_0 G \exp\left(\frac{-3R\delta^2}{8}\right) \\
& \leq 2B_0 G \exp\left(\frac{-3\delta^2 \cdot \frac{8 \ln\left(\frac{3}{2}B_0G\epsilon\right)}{3\delta^2}}{8}\right) \quad (\text{By } R \geq \frac{8}{3\delta^2} \ln\left(\frac{3}{2}B_0G\epsilon\right)) \\
& = \frac{\epsilon}{3}. \tag{E.21}
\end{aligned}$$

Combining (E.19) and (E.20) yields

$$\begin{aligned}
& \sum_{j \in J_0 \cup \{j_m\}} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\
& \leq \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2\epsilon}{3} + \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \frac{\epsilon}{3} \quad (\text{By (E.19) and (E.20)}) \\
& \leq \sum_{j \in J_0 \cup \{j_m\}} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2\epsilon}{3} \\
& \leq \frac{2\epsilon}{3}, \tag{E.22}
\end{aligned}$$

where the last line is by $\sum_{j \in J_0 \cup \{j_m\}} \frac{1}{\alpha(Z)} \exp\left(R(v_j^\top \tilde{Z} - \frac{1}{2}\|v_j\|_2^2)\right) \leq 1$.

We plug (E.21) and (E.22) to (E.18) and get

$$\begin{aligned}
\|\text{Attn} \circ \text{Linear}(Z) - f(Z)\|_\infty & \leq \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty \\
& \quad + \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\
& \quad + \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty
\end{aligned}$$

$$\begin{aligned} &\leq \frac{2\epsilon}{3} + \frac{\epsilon}{3} \\ &= \epsilon. \end{aligned}$$

This completes the proof. $\square$

We also extend this L_∞ -Norm result we just proved to L_p -Norm.

Corollary E.1.1 (L_p -Norm Universal Approximation). Let $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ denote any Lebesgue integrable function on a compact domain $U \in \mathbb{R}^{d \times n}$ and let $\epsilon > 0$ be any positive real number. Then, there exists a self-attention Attn prepended with a Linear layer such that

$$\|f - \text{Attn} \circ \text{Linear}\|_{L_p} \leq \epsilon.$$

Proof Sketch. The same partition-based construction applies almost everywhere; outside a negligible set, f is continuous (Lusin's theorem). Thus the L_∞ argument extends. $\square$

Proof. Since f is Lebesgue integrable on a compact set, f is bounded almost every where. Let B_p denote the bound of $\|f\|_p$.

By Lusin's theorem, for f on a compact domain U , there exists a continuous function g which is equal to f in U except for a region D_δ such that $\mu(D_\delta) \leq \Delta$. This can be written as

$$D_\delta = \{Z | f(Z) \neq g(Z)\}, \quad (\text{E.23})$$

$$\mu(D_\delta) \leq \Delta. \quad (\text{E.24})$$

Here μ stands for the Lebesgue measure of a set.

By [Theorem 4.1](#), there exists a net work $\text{Attn} \circ \text{Linear}$, consists of a self-attention Attn and a layer of sum of linear transformation Linear such that

$$\|\text{Attn} \circ \text{Linear} - g\|_{L_\infty} \leq \epsilon_0,$$

for any $\epsilon_0 > 0$.

This denote that for any $Z \in U$

$$\|\text{Attn} \circ \text{Linear}(Z) - g(Z)\|_p \leq (dn \cdot \epsilon^p)^{\frac{1}{p}} = \epsilon_0 (dn)^{\frac{1}{p}}.$$

Combine this with [\(E.23\)](#) and [\(E.24\)](#), we get

$$\begin{aligned} \mu(\{Z | \|\text{Attn} \circ \text{Linear}(Z) - g(Z)\|_\infty > \epsilon_0\}) &\leq \mu(\{f(Z) \neq g(Z)\}) \\ &\leq \Delta, \end{aligned} \quad (\text{E.25})$$

since that $f(Z) = g(Z)$, $\|\text{Attn} \circ \text{Linear}(Z) - g(Z)\| = \|\text{Attn} \circ \text{Linear}(Z) - f(Z)\| \leq \epsilon_0$.

This yields

$$\begin{aligned} \|f - \text{Attn} \circ \text{Linear}\|_{L_p} &= \left(\int_{Z \in U} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx \right)^{\frac{1}{p}} \\ &\leq \left(\int_{Z \in U \setminus D_\delta} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx + \int_{Z \in D_\delta} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx \right)^{\frac{1}{p}} \\ &= \left(\int_{Z \in U \setminus D_\delta} \|g - \text{Attn} \circ \text{Linear}\|_p^p dx + \int_{Z \in D_\delta} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx \right)^{\frac{1}{p}} \\ &\leq (\mu(U \setminus D_\delta) (\epsilon_0 (dn)^{\frac{1}{p}})^p + \Delta \cdot B_p^p)^{\frac{1}{p}} \quad (\text{By (E.25)}) \\ &\leq \epsilon_0 (dn \mu(U))^{\frac{1}{p}} + \Delta^{\frac{1}{p}} B_p. \end{aligned}$$

Set

$$\begin{aligned} \epsilon_0 &\leq \frac{\epsilon}{2(dn \mu(U))^{\frac{1}{p}}} \\ \Delta &\leq \frac{\epsilon^p}{B_p \cdot 2^p}. \end{aligned}$$

We have

$$\begin{aligned}
\|f - \text{Attn} \circ \text{Linear}\|_{L_p} &\leq \epsilon_0 (dn\mu(U))^{\frac{1}{p}} + \Delta^{\frac{1}{p}} B_p \\
&\leq (dn\mu(U))^{\frac{1}{p}} \cdot \frac{\epsilon}{2(dn\mu(U))^{\frac{1}{p}}} + \left(\frac{\epsilon^p}{B_p \cdot 2^p}\right)^{\frac{1}{p}} B_p \\
&= \frac{\epsilon}{2} + \frac{\epsilon}{2} \\
&= \epsilon.
\end{aligned}$$

This completes our proof. $\square$

E.2 Proof of Theorem 4.2

Theorem E.2. Let $U_K \subset \mathbb{R}^{d \times n}$ and $U_Q \subset \mathbb{R}^{d \times n}$ be two compact domains, and let $f : U_K \times U_Q \rightarrow \mathbb{R}^{d \times n}$ be any continuous function that takes input from both domains. We use $Z_K, Z_Q \in \mathbb{R}^{d \times n}$ to denote the two inputs of f from U_K and U_Q respectively. Without loss of generality, suppose both input domains to be $[-D, D]^{d \times n}$, where $D \in \mathbb{R}_+$. Then for any $\epsilon > 0$, there exists a single-head cross-attention Attn and two layers of sum of linear transformations, Linear_K and Linear_Q such that:

$$\|\text{Attn}(\text{Linear}_K(Z_K), \text{Linear}_Q(Z_Q)) - f(Z_K, Z_Q)\|_\infty \leq \epsilon,$$

for any $Z_K, Z_Q \in [-D, D]^{d \times n}$.

Proof. Without loss of generality, assume $U_K = U_Q = [-D, D]^{d \times n}$ for a $D \in \mathbb{R}_+$.

Construction of Grid Centers in U_K, U_Q . Same as in Appendix E.1, we define $\tilde{Z} := [z_1^\top, z_2^\top, \dots, z_n^\top]^\top$. $P \in \mathbb{N}_+$ is a parameter that controls the size of the attention block and the error of our approximation. Define $v_{k_1, k_2, \dots, k_{dn}} \in \mathbb{R}^{dn}$ to be

$$v_{k_1, k_2, \dots, k_{dn}} := \left[\frac{2Dk_1 - DP}{P}, \frac{2Dk_2 - DP}{P}, \dots, \frac{2Dk_{dn} - DP}{P} \right]^\top, \quad k_i \in \{0, 1, 2, \dots, P-1\}, \quad i \in [dn].$$

Let $V := \{v_{k_1, k_2, \dots, k_{dn}} \mid k_i \in \{0, 1, 2, \dots, P-1\}, i \in [dn]\}$ be the set of all $v_{k_1, k_2, \dots, k_{dn}}$. We also define another way to refer to a vector in V , denoted as

$$v_{\sum_{i=1}^{dn} k_i P^{(i-1)}} := v_{k_1, k_2, \dots, k_{dn}}.$$

Please see Remark E.1 for the reason for the feasibility of such expression.

Following the notation in Appendix E.1, for every $v \in V$, we define

$$\tilde{v} := \underbrace{[v_{1:d}, v_{d+1:2d}, \dots, v_{(n-1)d+1, nd}]}_{d \times n}$$

as a $d \times n$ matrix-form representation of v .

Construction of f Related Function E and T . The continuity of f within a closed region guarantees it to be bounded in ∞ -norm. Let B_0 denote this bound. For any $a_K, a_Q \in \mathbb{R}^{d \times n}$, we define

$$\begin{aligned}
E(a_K, a_Q) &:= 1_{d \times n} - \frac{f(a_K, a_Q)}{B_0} \\
T(a_K, a_Q) &:= 1_{d \times n} + \frac{f(a_K, a_Q)}{B_0}.
\end{aligned}$$

We define $(E + T)(a_K, a_Q) = E(a_K, a_Q) + T(a_K, a_Q)$. By the definition of E and T , $(E + T)(a_K, a_Q) \equiv 2_{d \times n}$ for any $a_K, a_Q \in \mathbb{R}^{d \times n}$.

Remark E.3 (Intuition behind E and T). E and T are constructed to satisfy 3 conditions:

- $T(Z_k, Z_Q) + E(Z_K, Z_Q) \equiv 2$.
- $T(Z_k, Z_Q) - E(Z_K, Z_Q) = 2f(Z_K, Z_Q)/B_0$.
- $T, E > 0$ for any input.

The first condition is used to configure the denominator in the Softmax expression of attention to a constant value. The second condition is used to form the value of f in the

For simplicity, same as in [Appendix E.1](#), define

$$G := P^{dn}.$$

We now construct the Linear_K and Linear_Q layers to be

$$\begin{aligned} \text{Linear}_K(Z_K) &:= \sum_{j=0}^{G-1} \left(\sum_{k=0}^{(n-1)} (Z_K e_{k+1}^{(n)})^\top (v_j)_{kd+1:kd+d} \right) e_{2dG^2+j+1}^{(2dG^2+G)} \sum_{s=0}^{dG-1} \left(e_{j+s+1}^{(2dG^2)} + e_{j+s+dG^2+1}^{(2dG^2)} \right)^\top \\ &\quad + \begin{bmatrix} I_{2dG^2} \\ 0_{G \times 2dG^2} \end{bmatrix}, \\ \text{Linear}_Q(Z_Q) &:= \sum_{j=0}^{G-1} \left(\sum_{k=0}^{(n-1)} (Z_Q e_{k+1}^{(n)})^\top (v_j)_{kd+1:kd+d} \right) e_{j+1}^{(n+G)} [1_{1 \times n} \quad 0_{1 \times (2dG^2-n)}] \\ &\quad + \begin{bmatrix} 0_{G \times n} & 0_{G \times (2dG^2-n)} \\ I_n & 0_{n \times (2dG^2-n)} \end{bmatrix}. \end{aligned}$$

Same as that in [Theorem E.1](#), we have

$$\sum_{k=0}^{(n-1)} (Z_K e_{k+1}^{(n)})^\top (v_j)_{kd+1:kd+d} = v_j^\top \tilde{Z}_K, \quad (\text{E.26})$$

$$\sum_{k=0}^{(n-1)} (Z_Q e_{k+1}^{(n)})^\top (v_j)_{kd+1:kd+d} = v_j^\top \tilde{Z}_Q, \quad (\text{E.27})$$

for $j \in \{0, 1, 2, \dots, G-1\}$.

We now calculate the output of Linear_K and Linear_Q .

For Linear_K , we have

$$\begin{aligned} \text{Linear}_K(Z_K) &= \sum_{j=0}^{G-1} v_j^\top \tilde{Z}_K e_{2dG^2+j+1}^{(2dG^2+G)} \sum_{s=0}^{dG-1} \left(e_{j+s+1}^{(2dG^2)} + e_{j+s+dG^2+1}^{(2dG^2)} \right)^\top + \begin{bmatrix} I_{2dG^2} \\ 0_{G \times 2dG^2} \end{bmatrix} \\ &= \begin{bmatrix} I_{2dG^2} \\ \sum_{j=0}^{G-1} v_j^\top \tilde{Z}_K \sum_{s=0}^{dG-1} \left(e_{j+s+1}^{(2dG^2)} + e_{j+s+dG^2+1}^{(2dG^2)} \right)^\top \end{bmatrix} \quad (\text{by (E.26)}) \\ &= \begin{bmatrix} I_{dG^2} & 0_{dG^2 \times dG^2} \\ \sum_{j=0}^{G-1} v_j^\top \tilde{Z}_K \sum_{s=0}^{dG-1} \left(e_{j+s+1}^{(2dG^2)} \right)^\top & \sum_{j=0}^{G-1} v_j^\top \tilde{Z}_K \sum_{s=0}^{dG-1} \left(e_{j+s+1}^{(2dG^2)} \right)^\top \end{bmatrix} \\ &= \begin{bmatrix} I_{dG^2} & 0_{dG^2 \times dG^2} \\ 0_{dG^2 \times dG^2} & I_{dG^2} \end{bmatrix}, \quad (\text{E.28}) \\ \text{Linear}_Q(Z_Q) &= \sum_{j=0}^{G-1} v_j^\top \tilde{Z}_Q e_{j+1}^{(n+G)} [1_{1 \times n} \quad 0_{1 \times (2dG^2-n)}] + \begin{bmatrix} 0_{G \times n} & 0_{G \times (2dG^2-n)} \\ I_n & 0_{n \times (2dG^2-n)} \end{bmatrix} \end{aligned}$$

$$\begin{aligned}
&= \begin{bmatrix} \sum_{j=0}^{G-1} v_j^\top \tilde{Z}_Q e_{j+1}^{(2dG^2+G)} 1_{1 \times n} & 0_{1 \times (2dG^2-n)} \\ I_n & 0_{n \times (2dG^2-n)} \end{bmatrix} \quad (\text{by (E.27)}) \\
&= \begin{bmatrix} X_Q & 0_{G \times (2dG^2-n)} \\ I_n & 0_{n \times (2dG^2-n)} \end{bmatrix}, \quad (\text{E.29})
\end{aligned}$$

in which X_K and X_Q are defined as

$$\begin{aligned}
X_K &:= \underbrace{\begin{bmatrix} v_0^\top \tilde{Z}_K 1_{1 \times dG} & v_1^\top \tilde{Z}_K 1_{1 \times dG} & v_2^\top \tilde{Z}_K 1_{1 \times dG} & \cdots & v_{G-1}^\top \tilde{Z}_K 1_{1 \times dG} \end{bmatrix}}_{1 \times dG^2}, \\
X_Q &:= \underbrace{\begin{bmatrix} v_0^\top \tilde{Z}_Q 1_{1 \times n} \\ v_1^\top \tilde{Z}_Q 1_{1 \times n} \\ v_2^\top \tilde{Z}_Q 1_{1 \times n} \\ \vdots \\ v_{G-1}^\top \tilde{Z}_Q 1_{1 \times n} \end{bmatrix}}_{G \times n}.
\end{aligned}$$

We now construct the W_k and W_Q matrices in the self-attention block and calculate the output of $\text{Softmax}(K^\top Q)$.

In the following, we define W_K in parts. First, we present it as a block matrix

$$W_K := \begin{bmatrix} 0_{1 \times dG^2} & 0_{1 \times dG^2} & 1 \\ W_0 & W_0 & 0 \\ W_1 & W_1 & 0 \\ W_T & W_E & 0 \end{bmatrix}. \quad (\text{E.30})$$

We then define the submatrices in (E.30) as follows

$$\begin{aligned}
W_0 &:= \begin{bmatrix} -\frac{\|v_0\|_2^2}{2} 1_{1 \times dG} + \bar{W}_0 & -\frac{\|v_1\|_2^2}{2} 1_{1 \times dG} + \bar{W}_0 & -\frac{\|v_2\|_2^2}{2} 1_{1 \times dG} + \bar{W}_0 & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times dG} + \bar{W}_0 \end{bmatrix}, \\
W_T &:= \begin{bmatrix} W_T^{(0)} & W_T^{(1)} & \cdots & W_T^{(G-1)} \end{bmatrix}, \\
W_E &:= \begin{bmatrix} W_E^{(0)} & W_E^{(1)} & \cdots & W_E^{(G-1)} \end{bmatrix}, \\
W_1 &:= [\bar{W}_1 \quad \bar{W}_1 \quad \bar{W}_1 \quad \cdots \quad \bar{W}_1]_{G \times dG^2},
\end{aligned}$$

in which

$$\begin{aligned}
\bar{W}_0 &:= \begin{bmatrix} -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_1\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_2\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{G-1}\|_2^2}{2} 1_{1 \times d} \end{bmatrix} \\
W_T^{(j)} &:= \underbrace{[\ln(T(\tilde{v}_j, \tilde{v}_0))^\top \quad \ln(T(\tilde{v}_j, \tilde{v}_1))^\top \quad \cdots \quad \ln(T(\tilde{v}_j, \tilde{v}_{G-1}))^\top]}_{d \times Gn}, \quad j \in \{0, 1, 2, \dots, G-1\}, \\
W_E^{(j)} &:= \underbrace{[\ln(E(\tilde{v}_j, \tilde{v}_0))^\top \quad \ln(E(\tilde{v}_j, \tilde{v}_1))^\top \quad \cdots \quad \ln(E(\tilde{v}_j, \tilde{v}_{G-1}))^\top]}_{d \times Gn}, \quad j \in \{0, 1, 2, \dots, G-1\}, \\
\bar{W}_1 &:= \underbrace{[Re_1^{(G)} 1_{1 \times d} \quad Re_2^{(G)} 1_{1 \times d} \quad \cdots \quad Re_G^{(G)} 1_{1 \times d}]}_{G \times d}.
\end{aligned}$$

The definition of W_K yields that

$$\begin{aligned}
K &:= W_K \text{Linear}_K(Z_K) \\
&= \begin{bmatrix} 0_{1 \times dG^2} & 0_{1 \times dG^2} & 1 \\ W_0 & W_0 & 0 \\ W_1 & W_1 & 0 \\ W_T & W_E & 0 \end{bmatrix} \cdot \begin{bmatrix} I_{dG^2} & 0_{dG^2 \times dG^2} \\ 0_{dG^2 \times dG^2} & I_{dG^2} \\ X_K & X_K \end{bmatrix} \quad (\text{By (E.28)}) \\
&= \begin{bmatrix} X_K & X_K \\ W_0 & W_0 \\ W_1 & W_1 \\ W_T & W_E \end{bmatrix}.
\end{aligned}$$

Next, we construct the W_Q matrix as

$$W_Q := \begin{bmatrix} 0_{1 \times G} & R1_{1 \times n} \\ 0_{1 \times G} & R1_{1 \times n} \\ I_G & 0_{1 \times n} \\ 0_{1 \times G} & I_n \end{bmatrix}.$$

In this definition, the Q matrix in attention can be calculated as follows

$$\begin{aligned} Q &:= W_Q \text{Linear}_Q(Z_Q) \\ &= \begin{bmatrix} 0_{1 \times G} & R1_{1 \times n} \\ 0_{1 \times G} & R1_{1 \times n} \\ I_G & 0_{1 \times n} \\ 0_{1 \times G} & I_n \end{bmatrix} \cdot \begin{bmatrix} X_Q & 0_{G \times (2dG^2-n)} \\ I_n & 0_{n \times (2dG^2-n)} \end{bmatrix} \quad (\text{By (E.29)}) \\ &= \begin{bmatrix} R1_{1 \times n} & 0_{1 \times (2dG^2-n)} \\ R1_{1 \times n} & 0_{1 \times (2dG^2-n)} \\ X_Q & 0_{G \times (2dG^2-n)} \\ I_n & 0_{n \times (2dG^2-n)} \end{bmatrix}. \end{aligned}$$

Now we calculate the attention matrix $\text{Softmax}(K^\top Q)$.

$K^\top Q$ can be calculated as follows

$$\begin{aligned} K^\top Q &= \begin{bmatrix} X_K & X_K \\ W_0 & W_0 \\ W_1 & W_1 \\ W_T & W_E \end{bmatrix}^\top \begin{bmatrix} R1_{1 \times n} & 0_{1 \times (2dG^2-n)} \\ R1_{1 \times n} & 0_{1 \times (2dG^2-n)} \\ X_Q & 0_{G \times (2dG^2-n)} \\ I_n & 0_{n \times (2dG^2-n)} \end{bmatrix} \\ &= \begin{bmatrix} (RX_K^\top + RW_0^\top)1_{1 \times n} + W_1^\top X_Q + W_T^\top & 0_{dG^2 \times (2dG^2-n)} \\ (RX_K^\top + RW_0^\top)1_{1 \times n} + W_1^\top X_Q + W_E^\top & 0_{dG^2 \times (2dG^2-n)} \end{bmatrix}. \end{aligned}$$

The $W_1^\top X_Q$ in the expression of $K^\top Q$ matrix is further calculated as

$$\begin{aligned} W_1^\top X_Q &= [\bar{W}_1 \quad \bar{W}_1 \quad \bar{W}_1 \quad \cdots \quad \bar{W}_1]_{G \times dG^2}^\top X_Q \\ &= \begin{bmatrix} \bar{W}_1^\top X_Q \\ \bar{W}_1^\top X_Q \\ \vdots \\ \bar{W}_1^\top X_Q \end{bmatrix}_{dG^2 \times G}. \end{aligned}$$

We define $Q_1 := \bar{W}_1^\top X_Q$, then $W_1^\top X_Q$ can be denoted as stacking this block vertically for G times.

In this definition, Q_1 matrix can be expressed as

$$\begin{aligned} Q_1 &:= \bar{W}_1^\top X_Q \\ &= \begin{bmatrix} Re_1^{(G)} 1_{1 \times d} & Re_2^{(G)} 1_{1 \times d} & \cdots & Re_G^{(G)} 1_{1 \times d} \end{bmatrix}^\top \begin{bmatrix} v_0^\top \tilde{Z}_Q 1_{1 \times n} \\ v_1^\top \tilde{Z}_Q 1_{1 \times n} \\ v_2^\top \tilde{Z}_Q 1_{1 \times n} \\ \vdots \\ v_{G-1}^\top \tilde{Z}_Q 1_{1 \times n} \end{bmatrix} \\ &= \begin{bmatrix} Re_1^{(G)} 1_d \\ Re_2^{(G)} 1_d \\ \vdots \\ Re_G^{(G)} 1_d \end{bmatrix} \cdot \begin{bmatrix} v_0^\top \tilde{Z}_Q 1_{1 \times n} \\ v_1^\top \tilde{Z}_Q 1_{1 \times n} \\ v_2^\top \tilde{Z}_Q 1_{1 \times n} \\ \vdots \\ v_{G-1}^\top \tilde{Z}_Q 1_{1 \times n} \end{bmatrix} \end{aligned}$$

$$= \begin{bmatrix} Rv_0^\top \tilde{Z}_Q 1_{d \times n} \\ Rv_1^\top \tilde{Z}_Q 1_{d \times n} \\ Rv_2^\top \tilde{Z}_Q 1_{d \times n} \\ \vdots \\ Rv_{G-1}^\top \tilde{Z}_Q 1_{d \times n} \end{bmatrix}. \quad (\text{E.31})$$

The calculation of $\text{Softmax}(K^\top Q)$ can be disassembled into two parts, the numerator $\exp(\text{Softmax}(K^\top Q))$ in the expression of Softmax and the denominator of every column of $\text{Softmax}(K^\top Q)$, as in the expression of Softmax , explicitly written out as $\sum_{j=1}^{2dG} \exp(K^\top Q)_{ij}$ for each $i \in [2dG]$.

We calculate $\exp(K^\top Q)$ as follows

$$\exp(K^\top Q) = \begin{bmatrix} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_T^\top) & 1_{dG^2 \times (2dG^2 - n)} \\ \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_E^\top) & 1_{dG^2 \times (2dG^2 - n)} \end{bmatrix}. \quad (\text{E.32})$$

For the denominator, we calculate it in columns. Let i denote the column which we calculate the denominator in Softmax . When $i \in \{n+1, n+2, \dots, 2dG^2\}$, the i -th column has 1 in every entry. Thus the sum of all entries in this column equals to $1 \cdot 2dG = 2dG$.

And when $i \in [n]$, we have

$$\begin{aligned} & \sum_{j=1}^{2dG^2} \exp(K^\top Q)_{i,j} \\ &= \sum_{j_1=1}^G \sum_{j_2=1}^G \left[(1_{1 \times d} T(\tilde{v}_{j_1-1}, \tilde{v}_{j_2-1})_{:,i} + 1_{1 \times d} E(\tilde{v}_{j_1-1}, \tilde{v}_{j_2-1})_{:,i}) \right. \\ & \quad \cdot \exp\left(R \left(v_{j_1-1}^\top \tilde{Z}_K - \frac{\|v_{j_1-1}\|_2^2}{2} + v_{j_2-1}^\top \tilde{Z}_Q - \frac{\|v_{j_2-1}\|_2^2}{2} \right)\right) \Big] \\ &= \sum_{j_1=1}^G \sum_{j_2=1}^G \left[1_{1 \times d} (E + T)(v_{j_1-1}, v_{j_2-1})_{:,i} \cdot \exp\left(R \left(v_{j_1-1}^\top \tilde{Z}_K - \frac{\|v_{j_1-1}\|_2^2}{2} + v_{j_2-1}^\top \tilde{Z}_Q - \frac{\|v_{j_2-1}\|_2^2}{2} \right)\right) \right] \\ &= \sum_{j_1=1}^G \sum_{j_2=1}^G \left[(1_{1 \times d} (2d \times n)_{:,i}) \cdot \exp\left(R \left(v_{j_1-1}^\top \tilde{Z}_K - \frac{\|v_{j_1-1}\|_2^2}{2} + v_{j_2-1}^\top \tilde{Z}_Q - \frac{\|v_{j_2-1}\|_2^2}{2} \right)\right) \right] \\ &= \sum_{j_1=1}^G \sum_{j_2=1}^G 2d \cdot \exp\left(R \left(v_{j_1-1}^\top \tilde{Z}_K - \frac{\|v_{j_1-1}\|_2^2}{2} + v_{j_2-1}^\top \tilde{Z}_Q - \frac{\|v_{j_2-1}\|_2^2}{2} \right)\right), \quad i \in [n]. \quad (\text{E.33}) \end{aligned}$$

We observe from (E.33), that $\sum_{j=1}^{2dG^2} \exp(K^\top Q)_{ij}$ is **invariant** of i for $i \in [n]$. In this case, we define

$$\begin{aligned} \alpha(Z_K, Z_Q) &:= \frac{1}{2d} \sum_{j=1}^{2dG^2} \exp(K^\top Q)_{i,j} \\ &= \sum_{j_1=1}^G \sum_{j_2=1}^G \exp\left(R \left(v_{j_1-1}^\top \tilde{Z}_K - \frac{\|v_{j_1-1}\|_2^2}{2} + v_{j_2-1}^\top \tilde{Z}_Q - \frac{\|v_{j_2-1}\|_2^2}{2} \right)\right) \end{aligned}$$

to denote the $1/2d$ of this value invariant of i for simplicity.

Because

$$\alpha(Z_K, Z_Q) = \frac{1}{2d} \sum_{j=1}^{2dG^2} \exp(K^\top Q)_{i,j},$$

from (E.32) and (E.33) we have

$$\begin{aligned}
& \text{Softmax}(K^\top Q) \\
&= \underbrace{\exp(K^\top Q)}_{\text{nominator of Softmax}} \odot \underbrace{\left[\frac{1}{\sum_{j=1}^{2dG^2} \exp(K^\top Q)_{1j}} 1_{2dG \times n} \quad \frac{1}{2dG^2} 1_{2dG \times (2dG-n)} \right]}_{\text{denominator of Softmax}} \\
&\quad \left(\text{By } \sum_{j=1}^{2dG} \frac{1}{\exp(K^\top Q)_{ij}} \text{ is invariant of } i \text{ for } i \in [n] \right) \\
&= \exp(K^\top Q) \odot \left[\frac{1}{2d\alpha(Z_K, Z_Q)} 1_{2dG \times n} \quad \frac{1}{2dG^2} 1_{2dG \times (2dG-n)} \right] \\
&= \begin{bmatrix} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_T^\top) & 1_{dG^2 \times (2dG^2-n)} \\ \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_E^\top) & 1_{dG^2 \times (2dG^2-n)} \end{bmatrix} \\
&\quad \odot \underbrace{\left[\frac{1}{2d\alpha(Z_K, Z_Q)} 1_{2dG \times n} \quad \frac{1}{2dG^2} 1_{2dG \times (2dG-n)} \right]}_{\text{denominator in Softmax}} \quad (\text{By (E.32)}) \\
&= \begin{bmatrix} \frac{1}{2d\alpha(Z_K, Z_Q)} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_T^\top) & \frac{1}{2dG^2} 1_{dG^2 \times (2dG^2-n)} \\ \frac{1}{2d\alpha(Z_K, Z_Q)} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_E^\top) & \frac{1}{2dG^2} 1_{dG^2 \times (2dG^2-n)} \end{bmatrix}.
\end{aligned}$$

Now we've defined and calculated the attention score matrix $\text{Softmax}(K^\top Q)$, we go on to construct the W_V matrix and calculate the result of multiplying $V = W_V \text{Linear}(Z_K)$ to the attention score matrix.

We define W_V as

$$W_V := \underbrace{[X_2 \quad -X_2 \quad 0_d]}_{d \times (2dG^2+1)},$$

where

$$X_2 = \underbrace{[I_d \quad I_d \quad \cdots \quad I_d]}_{d \times dG^2}.$$

This yields the V matrix to be

$$\begin{aligned}
V &= W_V \text{Linear}(Z_K) \\
&= \underbrace{[X_2 \quad -X_2 \quad 0_d]}_{d \times (2dG^2+1)} \cdot \underbrace{\begin{bmatrix} I_{dG^2} & 0_{dG^2 \times dG^2} \\ 0_{dG^2 \times dG^2} & I_{dG^2} \\ X_K & X_K \end{bmatrix}}_{(2dG^2+1) \times 2dG^2} \\
&= \underbrace{[X_2 \quad -X_2]}_{d \times 2dG^2} \cdot \underbrace{\begin{bmatrix} I_{dG^2} & 0_{dG^2 \times dG^2} \\ 0_{dG^2 \times dG^2} & I_{dG^2} \end{bmatrix}}_{2dG^2 \times 2dG^2} \quad (\text{since } X_K \text{ is multiplied by } 0) \\
&= [X_2 \quad -X_2].
\end{aligned}$$

With V , we compute the output of $V \text{Softmax}(K^\top Q)$ as follows

$$\begin{aligned}
& V \text{Softmax}(K^\top Q) \\
&= [X_2 \quad -X_2] \cdot \begin{bmatrix} \frac{1}{2d\alpha(Z_K, Z_Q)} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_T^\top) & \frac{1}{2dG^2} 1_{dG^2 \times (2dG^2-n)} \\ \frac{1}{2d\alpha(Z_K, Z_Q)} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_E^\top) & \frac{1}{2dG^2} 1_{dG^2 \times (2dG^2-n)} \end{bmatrix} \\
&= X_2 \left[\frac{1}{2d\alpha(Z_K, Z_Q)} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_T^\top) \quad \frac{1}{2dG^2} 1_{dG^2 \times (2dG^2-n)} \right] \\
&\quad \underbrace{[-X_2]}_{-X_2 \text{ in } [X_2 - X_2]} \left[\frac{1}{2d\alpha(Z_K, Z_Q)} \exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot \exp(W_E^\top) \quad \frac{1}{2dG^2} 1_{dG^2 \times (2dG^2-n)} \right]
\end{aligned}$$

$$= \frac{1}{2d\alpha(Z_K, Z_Q)} X_2 [\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot [\exp(W_T^\top) - \exp(W_E^\top)] \quad 0_{dG^2 \times (2dG^2 - n)}] . \quad (\text{E.34})$$

To further calculate $V \text{Softmax}(K^\top Q)$, we now calculate the result of its non-trivial part (the part beside $0_{dG^2 \times (2dG^2 - n)}$)

$$X_2 [\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot [\exp(W_T^\top) - \exp(W_E^\top)]] . \quad (\text{E.35})$$

We now calculate each part in (E.35)

$$\begin{aligned} & \exp(W_T^\top) - \exp(W_E^\top) \\ &= (\exp\left(\begin{bmatrix} W_T^{(0)} & W_T^{(1)} & \dots & W_T^{(G-1)} \end{bmatrix}\right) - \exp\left(\begin{bmatrix} W_E^{(0)} & W_E^{(1)} & \dots & W_E^{(G-1)} \end{bmatrix}\right))^\top \\ &= \begin{bmatrix} \exp(W_T^{(0)})^\top - \exp(W_E^{(0)})^\top \\ \exp(W_T^{(1)})^\top - \exp(W_E^{(1)})^\top \\ \vdots \\ \exp(W_T^{(G-1)})^\top - \exp(W_E^{(G-1)})^\top \end{bmatrix} . \end{aligned} \quad (\text{E.36})$$

In (E.36), we have

$$\begin{aligned} \exp(W_T^{(i)})^\top - \exp(W_E^{(i)})^\top &= \begin{bmatrix} \exp(\ln(T(\tilde{v}_i, v_0))) - \exp(\ln(E(\tilde{v}_i, v_0))) \\ \exp(\ln(T(\tilde{v}_i, v_1))) - \exp(\ln(E(\tilde{v}_i, v_0))) \\ \vdots \\ \exp(\ln(T(\tilde{v}_i, v_{G-1}))) - \exp(\ln(E(\tilde{v}_i, v_0))) \end{bmatrix} \\ &= \begin{bmatrix} T(\tilde{v}_i, v_0) - E(\tilde{v}_i, v_0) \\ T(\tilde{v}_i, v_1) - E(\tilde{v}_i, v_0) \\ \vdots \\ T(\tilde{v}_i, v_{G-1}) - E(\tilde{v}_i, v_0) \end{bmatrix} \\ &= \begin{bmatrix} \frac{2f(\tilde{v}_i, v_0)}{B_0} \\ \frac{2f(\tilde{v}_i, v_1)}{B_0} \\ \vdots \\ \frac{2f(\tilde{v}_i, v_{G-1})}{B_0} \end{bmatrix} . \end{aligned}$$

Thus (E.36) is equal to

$$\left(\exp(W_T^{(i)})^\top - \exp(W_E^{(i)})^\top \right)_{(i-1)G+1:iG,:} = \begin{bmatrix} \frac{2f(\tilde{v}_{i-1}, v_0)}{B_0} \\ \frac{2f(\tilde{v}_{i-1}, v_1)}{B_0} \\ \vdots \\ \frac{2f(\tilde{v}_{i-1}, v_{G-1})}{B_0} \end{bmatrix}, \quad i \in [G]. \quad (\text{E.37})$$

We also calculate the other part $\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q)$ in separate parts

$$\begin{aligned} \exp((RX_K^\top + RW_0^\top)1_{1 \times n})_{idG+jd+1:idG+(j+1)d,:} &= \begin{bmatrix} \exp\left(v_0^\top \tilde{Z}_K - \frac{\|v_0\|_2^2}{2}\right)1_{dG \times n} \\ \exp\left(v_1^\top \tilde{Z}_K - \frac{\|v_1\|_2^2}{2}\right)1_{dG \times n} \\ \vdots \\ \exp\left(v_{G-1}^\top \tilde{Z}_K - \frac{\|v_{G-1}\|_2^2}{2}\right)1_{dG \times n} \end{bmatrix}_{idG+jd+1:idG+(j+1)d,:} \\ &= \exp\left(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2}\right)1_{d \times n}, \end{aligned}$$

and

$$\begin{aligned} \exp((RW_1^\top X_Q)1)_{idG+jd+1:idG+(j+1)d,:} &= \begin{bmatrix} Q_1 \\ Q_1 \\ \vdots \\ Q_1 \end{bmatrix}_{idG+jd+1:idG+(j+1)d,:} \\ &\quad \text{(This is a stack of } G \text{ } Q_1 \text{ in (E.31))} \\ &= (Q_1)_{jd+1:(j+1)d,:} \\ &= v_j^\top \tilde{Z}_Q 1_{d \times n}. \end{aligned}$$

Thus

$$\begin{aligned} &\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q)_{idG+jd+1:idG+(j+1)d,:} \\ &= \exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right)1_{d \times n}, \quad i, j \in \{0, 1, \dots, G-1\}. \end{aligned} \quad (\text{E.38})$$

Combing (E.37) and (E.38), we have

$$\begin{aligned} &[\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot [\exp(W_T^\top) - \exp(W_E^\top)]]_{idG+(j-1)d+1:idG+jd,:} \\ &= \exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right)1_{d \times n} \odot \frac{2f(\tilde{v}_{i-1}, v_{j-1})}{B_0}, \quad i, j \in \{0, 1, \dots, G-1\}. \end{aligned}$$

Thus we compute (E.35) as

$$\begin{aligned} &(X_2 [\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot [\exp(W_T^\top) - \exp(W_E^\top)]] \\ &= \sum_{i=0}^{G-1} \sum_{j=0}^{G-1} (X_2)_{:,idG+jd+1:idG+(j+1)d} \\ &\quad \cdot R [\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot [\exp(W_T^\top) - \exp(W_E^\top)]]_{idG+(j-1)d+1:idG+jd,:} \\ &= \sum_{i=0}^{G-1} \sum_{j=0}^{G-1} I_d \cdot \exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right)1_{d \times n} \odot \frac{2f(\tilde{v}_{i-1}, v_{j-1})}{B_0} \\ &\quad \text{(Because } X_2 \text{ is a horizontal stack of } I_d \text{)} \\ &= \sum_{i=0}^{G-1} \sum_{j=0}^{G-1} \exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right)1_{d \times n} \odot \frac{2f(\tilde{v}_{i-1}, v_{j-1})}{B_0}. \end{aligned}$$

We now put back the $1/2d\alpha(Z_K, Z_Q)$ in (E.34) and calculate the final output as

$$\begin{aligned} &V \text{ Softmax } K^\top Q \\ &= \frac{1}{2d\alpha(Z_K, Z_Q)} X_2 [\exp((RX_K^\top + RW_0^\top)1_{1 \times n} + RW_1^\top X_Q) \odot [\exp(W_T^\top) - \exp(W_E^\top)]]_{0_{dG^2 \times (2dG^2-n)}} \\ &= \frac{1}{2d\alpha(Z_K, Z_Q)} \sum_{i=0}^{G-1} \sum_{j=0}^{G-1} \left[\exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right)1_{d \times n} \odot \underbrace{\frac{2f(\tilde{v}_{i-1}, v_{j-1})}{B_0}}_{\exp(W_T^\top) - \exp(W_E^\top)} \right]_{0_{d \times (2dG^2-n)}} \\ &= \left[\frac{1}{dB_0} \sum_{i=0}^{G-1} \sum_{j=0}^{G-1} \frac{\exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right)1_{d \times n} \odot \frac{f(\tilde{v}_{i-1}, v_{j-1})}{B_0}}{\alpha(Z_K, Z_Q)} \right]_{0_{d \times (2dG^2-n)}}. \end{aligned}$$

Next, we construct W_O to be

$$W_O := \begin{bmatrix} dB_0 I_n \\ 0_{(2dG^2-n) \times n} \end{bmatrix}.$$

This yields the final output of $\text{Attn} \circ \text{Linear}$ to be

$$\begin{aligned}
& \text{Attn} \circ \text{Linear}(Z) \\
&= V \text{Softmax } K^\top Q W_O \\
&= \left[\frac{1}{dB_0} \sum_{i=0}^{G-1} \sum_{j=0}^{G-1} \frac{\exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right) 1_{d \times n} \odot \frac{f(\tilde{v}_{i-1}, v_{j-1})}{B_0}}{\alpha(Z_K, Z_Q)} \right]_{0_{d \times (2dG^2-n)}} \cdot \underbrace{\begin{bmatrix} dB_0 I_n \\ 0_{(2dG^2-n) \times n} \end{bmatrix}}_{W_O} \\
&= \sum_{i=0}^{G-1} \sum_{j=0}^{G-1} \frac{\exp\left(R(v_i^\top \tilde{Z}_K - \frac{\|v_i\|_2^2}{2} - \frac{\|v_j\|_2^2}{2} + v_j^\top \tilde{Z}_Q)\right) 1_{d \times n} \odot \frac{f(\tilde{v}_{i-1}, v_{j-1})}{B_0}}{\alpha(Z_K, Z_Q)}. \tag{E.39}
\end{aligned}$$

Estimation of Error between $\text{Attn} \circ \text{Linear}$ and f We now calculate the loss between the result in (E.39) and the target function f . For simplicity, we first define $\tilde{Z} := [[\tilde{Z}_K^\top, \tilde{Z}_Q^\top]^\top]$ to accommodate to the expression of affine functions.

Definition E.3 (Max-Affine Function on $\tilde{Z}$). Let $\text{Aff}_{i,j} \in \mathbb{R}^{dn} \rightarrow \mathbb{R}$, $j \in \{0, 1, 2, \dots, G-1\}$ denote a group of affine functions defined as

$$\text{Aff}_{i,j}(\tilde{Z}) = v_i^\top \tilde{Z}_K + v_j^\top \tilde{Z}_Q - \frac{1}{2}\|v_i\|_2^2 - \frac{1}{2}\|v_j\|_2^2, \quad i, j \in \{0, 1, 2, \dots, G-1\}.$$

Then let $\text{MaxAff} \in \mathbb{R}^{dn} \rightarrow \mathbb{R}$ denote a max affine function whose affine components are $\{\text{Aff}_{i,j} | i, j \in \{0, 1, 2, \dots, G-1\}\}$. Explicitly defined as:

$$\text{MaxAff}(\tilde{Z}) = \max_{i,j \in \{0,1,2,\dots,G-1\}} \left\{ \text{Aff}_{i,j}(\tilde{Z}) \right\}.$$

In the following discussion, we use $\eta \in \{0, 1, \dots, G-1\}^2$ to refer to a pair of coefficients (i, j) , and denote $A_{i,j}$ as A_η for the corresponding η . Furthermore, we denote the two labels encapsulated in η as i_η and j_η

Because the target function f is a continuous function on a closed domain, the function f is uniformly continuous. Thus for ϵ , there exists a $\delta > 0$ such that for any $Z^{(1)} = [Z_K^{(1)}, Z_Q^{(1)}]$, $Z^{(2)} = [Z_K^{(2)}, Z_Q^{(2)}]$, as long as $\|Z^{(1)} - Z^{(2)}\|_\infty \leq \delta$, we have $\|f(Z^{(1)}) - f(Z^{(2)})\|_\infty \leq \epsilon/3$.

According to this δ , we divide the affine components of MaxAff into three parts, the maximal component (and also with the smallest label on both entry), whose label is denoted as η_m , the group of affine components equal to the maximal component or smaller than it by no more than δ , and finally, the other Aff_η . We write out the labels of these groups of components as follows

$$\eta_m := \min_{\eta \in \{0,1,2,\dots,G-1\}^2} \{ \text{Aff}_\eta(\tilde{Z}) = \text{MaxAff}(\tilde{Z}) \},$$

$$E_0 := \{ \eta \mid \text{MaxAff}(\tilde{Z}) - \text{Aff}_\eta(\tilde{Z}) \leq \delta \},$$

$$E_1 := \{ \eta \mid \text{MaxAff}(\tilde{Z}) - \text{Aff}_\eta(\tilde{Z}) > \delta \}.$$

For any pair of $\eta_1, \eta_2 \in \{0, 1, \dots, G-1\}^2$, we denote that

$$\begin{aligned}
& \text{Aff}_{\eta_1}(\tilde{Z}) - \text{Aff}_{\eta_2}(\tilde{Z}) \\
&= v_{i_{\eta_1}}^\top \tilde{Z}_K - \frac{\|v_{i_{\eta_1}}\|_2^2}{2} + v_{j_{\eta_1}}^\top \tilde{Z}_Q - \frac{\|v_{j_{\eta_1}}\|_2^2}{2} - \left(v_{i_{\eta_2}}^\top \tilde{Z}_K - \frac{\|v_{i_{\eta_2}}\|_2^2}{2} + v_{j_{\eta_2}}^\top \tilde{Z}_Q - \frac{\|v_{j_{\eta_2}}\|_2^2}{2} \right) \\
&= -\frac{\|\tilde{Z}_K\|_2^2}{2} + v_{i_{\eta_1}}^\top \tilde{Z}_K - \frac{\|v_{i_{\eta_1}}\|_2^2}{2} - \frac{\|\tilde{Z}_Q\|_2^2}{2} + v_{j_{\eta_1}}^\top \tilde{Z}_Q - \frac{\|v_{j_{\eta_1}}\|_2^2}{2} \\
&\quad - \left(-\frac{\|\tilde{Z}_K\|_2^2}{2} + v_{i_{\eta_2}}^\top \tilde{Z}_K - \frac{\|v_{i_{\eta_2}}\|_2^2}{2} - \frac{\|\tilde{Z}_Q\|_2^2}{2} + v_{j_{\eta_2}}^\top \tilde{Z}_Q - \frac{\|v_{j_{\eta_2}}\|_2^2}{2} \right) \\
&= -\frac{1}{2}\|\tilde{Z}_K - v_{i_{\eta_1}}\|_2^2 - \frac{1}{2}\|\tilde{Z}_Q - v_{j_{\eta_1}}\|_2^2 + \frac{1}{2}\|\tilde{Z}_K - v_{i_{\eta_2}}\|_2^2 + \frac{1}{2}\|\tilde{Z}_Q - v_{j_{\eta_2}}\|_2^2
\end{aligned} \tag{E.40}$$

$$= \frac{1}{2} \|\tilde{Z} - \begin{bmatrix} v_{i_{\eta_2}} \\ v_{j_{\eta_2}} \end{bmatrix}\|_2^2 - \frac{1}{2} \|\tilde{Z} - \begin{bmatrix} v_{i_{\eta_1}} \\ v_{j_{\eta_1}} \end{bmatrix}\|_2^2. \quad (\text{E.41})$$

Let $v_\eta := [v_{i_\eta}^\top, v_{j_\eta}^\top]^\top$, denote a flatten stack of v_{i_η} and v_{j_η} . Same as v_i , define $\tilde{v}_\eta := [\tilde{v}_{i_\eta}, \tilde{v}_{j_\eta}]$. Then the above expression denotes η_m is also the label of the v_η closest to $\tilde{Z}$ among all v_η , $\eta \in \{0, 1, \dots, G-1\}^2$. Thus we have

$$\|v_{\eta_m} - \tilde{Z}\|_2 = \min_{\eta \in \{0, 1, \dots, G-1\}^2} \{\|v_\eta - \tilde{Z}\|_2\}. \quad (\text{E.42})$$

This means that v_{η_m} is the grid center closest to $\tilde{Z}$ in 2-norm.

We now prove this closest grid center has a distance to $\tilde{Z}$ smaller than half of the grid width (D/g) in infinite norm.

Let $\mathcal{D} := 2D/g \times \{-1, 0, 1\}^{dn}$ denote a set of differences to v_{η_m} of all the v_i ($i \in \{0, 1, \dots, G-1\}$) neighboring v_{η_m} . For any Δ in $\mathcal{D}$, from (E.42) we have

$$\|v_{\eta_m} - \tilde{Z}\|_2^2 \leq \|v_{\eta_m} + \Delta - \tilde{Z}\|_2^2.$$

This yields

$$2\Delta^\top (\tilde{Z} - v_{\eta_m}) \leq \|\Delta\|_2^2,$$

which means for any $k \in [dn]$, by selecting Δ to be $\pm \frac{2D}{g} \cdot e_k^{(dn)}$, we have

$$\pm 2 \times \frac{2D}{g} (\tilde{Z} - v_{\eta_m})_k = 2\Delta^\top (\tilde{Z} - v_{\eta_m}) \leq \|\Delta\|_2^2 = \frac{4D^2}{g^2}.$$

Thus we have

$$(|\tilde{Z} - v_{\eta_m}|)_k \leq \frac{D}{g}, \quad k \in [dn].$$

This is equivalent to

$$\|\tilde{Z} - v_{\eta_m}\|_\infty \leq \frac{D}{g}, \quad k \in [dn].$$

Set g to be larger than $2D/\delta$, we have

$$\|\tilde{Z} - v_{\eta_m}\|_\infty \leq \frac{\delta}{2},$$

thus

$$\|f(Z) - f(\tilde{v}_{\eta_m})\|_\infty \leq \frac{\epsilon}{3}. \quad (\text{because } \delta/2 < \delta)$$

Calculation of $\|\text{Attn} \circ \text{Linear} - f\|_{L_\infty}$. We now calculate the difference between the output in (E.39) and target function f

$$\begin{aligned} \|\text{Attn} \circ \text{Linear}(Z) - f(Z)\|_\infty &= \left\| \sum_{\eta=0}^{G-1} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} f(\tilde{v}_\eta) - f(Z) \right\|_\infty \\ &= \left\| \sum_{\eta=0}^{G-1} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} (f(\tilde{v}_\eta) - f(Z)) \right\| \\ &\quad \left(\text{By } \sum_{\eta=0}^{G-1} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} = 1 \right) \end{aligned}$$

$$\begin{aligned}
&\leq \sum_{\eta=0}^{G-1} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta}) - f(Z)\|_{\infty} \\
&\quad \text{(By property of infinite norm)} \\
&= \frac{\exp\left(R(v_{\eta_m}^{\top} \tilde{Z} - \frac{\|v_{\eta_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta_m}) - f(Z)\|_{\infty} \\
&\quad + \sum_{\eta \in \eta_0} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta}) - f(Z)\|_{\infty} \\
&\quad + \sum_{\eta \in \eta_1} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta}) - f(Z)\|_{\infty}. \quad (\text{E.43})
\end{aligned}$$

The last row is simply a separation of the summation in the row above.

We now calculate each part in (E.43).

As previously stated, for any Z_1, Z_2 , as long as $\|\tilde{Z}_1 - \tilde{Z}_2\|_{\infty} \leq \delta$, we have $\|f(Z_1) - f(Z_2)\|_{\infty} \leq \epsilon/3$. Thus when we designate $\tilde{Z}_1 = v_{\eta}$ for any $\eta \in \eta_0$ and $Z_2 = v_{\eta_m}$, along with (E.40) we have

$$\begin{aligned}
&\sum_{\eta \in \eta_0} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta}) - f(Z)\|_{\infty} \\
&\leq \sum_{\eta \in \eta_0} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} (\|f(\tilde{v}_{\eta}) - f(\tilde{v}_{\eta_m})\|_{\infty} + \|f(\tilde{v}_{\eta_m}) - f(Z)\|_{\infty}) \\
&\leq \sum_{\eta \in \eta_0} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \cdot \left(\frac{\epsilon}{3} + \frac{\epsilon}{3}\right) \\
&= \sum_{\eta \in \eta_0} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2\epsilon}{3}. \quad (\text{E.44})
\end{aligned}$$

For any η_m , we have

$$\frac{\exp\left(R(v_{\eta_m}^{\top} \tilde{Z} - \frac{\|v_{\eta_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta_m}) - f(Z)\|_{\infty} \leq \frac{\exp\left(R(v_{\eta_m}^{\top} \tilde{Z} - \frac{\|v_{\eta_m}\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{\epsilon}{3}. \quad (\text{E.45})$$

When R is larger than $8 \ln(3/2 \cdot B_0 G \epsilon) / (3\delta^2)$, we have

$$\begin{aligned}
\sum_{\eta \in \eta_1} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta}) - f(Z)\|_{\infty} &\leq \sum_{\eta \in \eta_1} \frac{\exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \cdot 2B_0 \\
&\quad \text{(By that } f \text{ is bounded)} \\
&\leq 2B_0 \frac{\sum_{\eta \in \eta_1} \exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\alpha(Z)} \\
&< 2B_0 \frac{\sum_{\eta \in \eta_1} \exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right)}{\exp\left(R(v_{\eta_m}^{\top} \tilde{Z} - \frac{\|v_{\eta_m}\|_2^2}{2})\right)} \\
&\quad \left(\alpha(Z) \text{ is the sum of all } \exp\left(R(v_{\eta}^{\top} \tilde{Z} - \frac{\|v_{\eta}\|_2^2}{2})\right), \text{ larger than any element in the sum}\right) \\
&= 2B_0 \sum_{\eta \in \eta_1} \exp\left(\frac{R}{2} (\|v_{\eta_m} - Z\|_2^2 - \|v_{\eta} - Z\|_2^2)\right)
\end{aligned}$$

$$\begin{aligned}
&\leq 2B_0\|\eta_1\| \exp\left(\frac{R}{2}\left[\left(\frac{\delta}{2}\right)^2 - \delta^2\right]\right) \\
&< 2B_0G \exp\left(\frac{-3R\delta^2}{8}\right) \\
&= 2B_0G \exp\left(\frac{-3\delta^2 \cdot \frac{8\ln(\frac{2}{3}B_0G\epsilon)}{3\delta^2}}{8}\right) \\
&= \frac{\epsilon}{3}.
\end{aligned} \tag{E.46}$$

Combing (E.44) and (E.45) yields

$$\begin{aligned}
&\sum_{\eta \in \eta_0 \cup \{\eta_m\}} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_\eta) - f(Z)\|_\infty \\
&\leq \sum_{\eta \in \eta_0} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2\epsilon}{3} + \frac{\exp\left(R(v_{\eta_m}^\top \tilde{Z} - \frac{\|v_{\eta_m}\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{\epsilon}{3} \quad (\text{By (E.44) and (E.45)}) \\
&\leq \sum_{\eta \in \eta_0 \cup \{\eta_m\}} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2\epsilon}{3} \\
&\leq \frac{2\epsilon}{3},
\end{aligned} \tag{E.47}$$

where the last line is by $\sum_{\eta \in E_0 \cup \{\eta_m\}} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} \leq 1$.

By (E.47) and (E.46), we have

$$\begin{aligned}
\|\text{Attn} \circ \text{Linear}(Z) - f(Z)\|_\infty &\leq \frac{\exp\left(R(v_{\eta_m}^\top \tilde{Z} - \frac{\|v_{\eta_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{\eta_m}) - f(Z)\|_\infty \\
&\quad + \sum_{\eta \in E_0} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_\eta) - f(Z)\|_\infty \\
&\quad + \sum_{\eta \in E_1} \frac{\exp\left(R(v_\eta^\top \tilde{Z} - \frac{\|v_\eta\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_\eta) - f(Z)\|_\infty \\
&\leq \frac{2\epsilon}{3} + \frac{\epsilon}{3} \\
&= \epsilon.
\end{aligned}$$

This completes the proof. $\square$

Theorem 4.2 can be easily extended to Lebesgue integrable functions in L_p norm in the following result.

Corollary E.2.1 (L_p -Norm Universal Approximation). Let $f : U_K \times U_Q \rightarrow \mathbb{R}^{d \times n}$ denote any Lebesgue integrable function on a compact domain $U_K \times U_Q$ and let ϵ be any positive real number. Here $U_K, U_Q \in \mathbb{R}^{d \times n}$ stands for the compact domain of the two input sequences of cross-attention. Then, there exists a cross-attention Attn prepended with a Linear layer such that

$$\|f - \text{Attn} \circ \text{Linear}\|_{L_p} \leq \epsilon.$$

Proof. Without loss of generality, assume $U_K = U_Q = [-D, D]^{d \times n}$ for a $D \in \mathbb{R}_+$.

Since f is Lebesgue integrable on a compact set, f is bounded almost every where. Let B_p denote the bound of $\|f\|_p$.

By Lusin's theorem, for f on a compact domain U , there exists a continuous function g which is equal to f in U except for a region D_δ such that $\mu(D_\delta) \leq \Delta$. This can be written as

$$D_\delta = \{Z | f(Z) \neq g(Z)\}, \quad (\text{E.48})$$

$$\mu(D_\delta) \leq \Delta, \quad (\text{E.49})$$

where μ stands for the Lebesgue measure of a set.

By [Theorem 4.2](#), there exists a network $\text{Attn} \circ \text{Linear}$, consists of a cross-attention Attn and a layer of sum of linear transformation Linear such that

$$\|\text{Attn} \circ \text{Linear} - g\|_{L_\infty} \leq \epsilon_0,$$

for any $\epsilon_0 > 0$.

This denote that for any $Z \in U \times U$

$$\|\text{Attn} \circ \text{Linear}(Z) - g(Z)\|_p \leq (dn \cdot \epsilon^p)^{\frac{1}{p}} = \epsilon_0 (dn)^{\frac{1}{p}}.$$

Combing this with [\(E.48\)](#) and [\(E.49\)](#), we get

$$\mu(\{Z | \|\text{Attn} \circ \text{Linear}(Z) - g(Z)\|_\infty > \epsilon_0\}) \leq \mu(\{f(Z) \neq g(Z)\}) \leq \Delta, \quad (\text{E.50})$$

since if $f(Z) = g(Z)$, $\|\text{Attn} \circ \text{Linear}(Z) - g(Z)\| = \|\text{Attn} \circ \text{Linear}(Z) - f(Z)\| \leq \epsilon_0$

This yields

$$\begin{aligned} \|f - \text{Attn} \circ \text{Linear}\|_{L_p} &= \left(\int_{Z \in U \times U} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx \right)^{\frac{1}{p}} \\ &\leq \left(\int_{Z \in U \times U \setminus D_\delta} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx + \int_{Z \in D_\delta} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx \right)^{\frac{1}{p}} \\ &= \left(\int_{Z \in U \times U \setminus D_\delta} \|g - \text{Attn} \circ \text{Linear}\|_p^p dx + \int_{Z \in D_\delta} \|f - \text{Attn} \circ \text{Linear}\|_p^p dx \right)^{\frac{1}{p}} \\ &\leq (\mu(U \times U \setminus D_\delta) (\epsilon_0 (dn)^{\frac{1}{p}})^p + \Delta \cdot B_p^p)^{\frac{1}{p}} \\ &\leq \epsilon_0 (dn \mu(U \times U))^{\frac{1}{p}} + \Delta^{\frac{1}{p}} B_p. \end{aligned}$$

Set

$$\begin{aligned} \epsilon_0 &\leq \frac{\epsilon}{2(dn \mu(U \times U))^{\frac{1}{p}}} \\ \Delta &\leq \frac{\epsilon^p}{B_p \cdot 2^p}. \end{aligned}$$

We have

$$\begin{aligned} \|f - \text{Attn} \circ \text{Linear}\|_{L_p} &\leq \epsilon_0 (dn \mu(U \times U))^{\frac{1}{p}} + \Delta^{\frac{1}{p}} B_p \\ &\leq (dn \mu(U \times U))^{\frac{1}{p}} \cdot \frac{\epsilon}{2(dn \mu(U \times U))^{\frac{1}{p}}} + \left(\frac{\epsilon^p}{B_p \cdot 2^p} \right)^{\frac{1}{p}} B_p \\ &= \frac{\epsilon}{2} + \frac{\epsilon}{2} \\ &= \epsilon. \end{aligned}$$

This completes the proof. □

F Proof of Results in Appendix A

F.1 Proof of Theorem A.1

Theorem F.1 (Theorem A.1 Restated). Let $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ denote an L -Lipschitz function (in terms of 2-norm) whose input domain is $\mathcal{X}$. For any $\epsilon > 0$, assume $\mathcal{X}$ is contained in N_x sphere by the radius of $\epsilon/(3L)$ in 2-norm. Then, there exists a Linear layer and a Attn layer such that:

$$\|\text{Attn} \circ \text{Linear} - f\|_\infty \leq \epsilon.$$

Furthermore, Attn and Linear have a total number of $\mathcal{O}(dnN_x)$ trainable parameters.

Proof sketch. This proof is identical with Theorem 4.1, except for an alteration on the set of v_i . $\square$

Proof. We follow the proof of Theorem 4.1.

Notation of Sphere Centers. Let $Z = [z_1, z_2, \dots, z_n] \in \mathbb{R}^{d \times n}$ denote the input to Linear. Define $\tilde{Z} := [z_1^\top, z_2^\top, \dots, z_n^\top]^\top$. $P \in N_+$ is a parameter that controls the size of the attention block and the error of our approximation.

Let $v_i, i \in [N_x]$ denote the centers of the N_x spheres that covers $\mathcal{X}$. Let $V := \{v_i | i \in [N_x]\}$ denote the set of all v_i .

For every $v \in V$, we define $\tilde{v} := [v_{1:d}^\top, v_{d+1:2d}^\top, \dots, v_{(n-1)d+1:nd}^\top]^\top$.

Construction of f Related Functions. Because f is continuous within a closed region, its output value is bounded in ∞ -norm. Let B_0 denote this bound, we now construct two functions that. For any $a \in \mathbb{R}^{d \times n}$, we define $E(a) := 1_{d \times n} - f(a)/B_0$ and $T(a) = 1_{d \times n} + f(a)/B_0$. We define $(E + T)(a) = E(a) + T(a)$. By the definition of E and T , $(E + T)(a) \equiv 2_{d \times n}$ for any $a \in \mathbb{R}^{d \times n}$.

Construction of the Layer of Sum of Linear Transformations. We now construct the Linear layer to be

$$\text{Linear}(Z) := \sum_{j=0}^{N_x-1} \left(\sum_{k=0}^{(n-1)} (Ze_{k+1}^{(n)})^\top (v_j)_{kd+1:kd+d} \right) e_1^{(2dN_x+1)} \sum_{s=0}^{d-1} \left(e_{j+s+1}^{(2dN_x)} + e_{j+s+dN_x+1}^{(2dN_x)} \right)^\top + \begin{bmatrix} 0_{1 \times 2dN_x} \\ I_{2dN_x} \end{bmatrix},$$

where $N_x = P^{dn}$.

We now express the output of Linear in a simpler form in the following discussion. First, we show that

$$\begin{aligned} \sum_{k=0}^{(n-1)} (Ze_{k+1}^{(n)})^\top (v_j)_{kd+1:kd+d} &= \sum_{k=0}^{(n-1)} z_{k+1}^\top (v_j)_{kd+1:kd+d} \\ &= [z_1^\top, z_2^\top, \dots, z_n^\top] v_j \\ &= v_j^\top \tilde{Z} \in \mathbb{R}, j \in \{0, 1, 2, \dots, N_x - 1\}. \end{aligned}$$

This yields

$$\begin{aligned} \text{Linear}(Z) &= \sum_{j=0}^{N_x-1} v_j^\top \tilde{Z} \sum_{s=0}^{d-1} \left(e_{j+s+1}^{(2dN_x)} + e_{j+s+dN_x+1}^{(2dN_x)} \right)^\top e_1^{(2dN_x+1)} + \begin{bmatrix} 0_{1 \times 2dN_x} \\ I_{2dN_x} \end{bmatrix} \\ &= \begin{bmatrix} X_0 & X_0 \\ I_{dN_x} & 0_{dN_x \times dN_x} \\ 0_{dN_x \times dN_x} & I_{dN_x} \end{bmatrix}, \end{aligned}$$

in which X_0 is defined as follows

$$X_0 := \begin{bmatrix} v_0^\top \tilde{Z} 1_{1 \times d} & v_1^\top \tilde{Z} 1_{1 \times d} & v_2^\top \tilde{Z} 1_{1 \times d} & \dots & v_{N_x-1}^\top \tilde{Z} 1_{1 \times d} \end{bmatrix}.$$

Construction of K and Q Matrices. We now construct the W_k and W_Q matrices in the self-attention block and calculate the output of Softmax ($K^\top Q$).

We define W_K as follows:

$$W_K := \begin{bmatrix} 1 & 0_{1 \times d} & \cdots & 0_{1 \times d} & 0_{1 \times d} & \cdots & 0_{1 \times d} \\ 0 & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} \\ 0 & \ln(T(\tilde{v}_0))^\top & \cdots & \ln(T(\tilde{v}_{N_x-1}))^\top & \ln(E(\tilde{v}_0))^\top & \cdots & \ln(E(\tilde{v}_{N_x-1}))^\top \end{bmatrix}.$$

The definition of W_K yields

$$\begin{aligned} K &:= W_K \text{Linear}(Z) \\ &= \begin{bmatrix} 1 & 0_{1 \times d} & \cdots & 0_{1 \times d} & 0_{1 \times d} & \cdots & 0_{1 \times d} \\ 0 & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} \\ 0 & \ln(T(\tilde{v}_0))^\top & \cdots & \ln(T(\tilde{v}_{N_x-1}))^\top & \ln(E(\tilde{v}_0))^\top & \cdots & \ln(E(\tilde{v}_{N_x-1}))^\top \end{bmatrix} \cdot \begin{bmatrix} X_0 & X_0 \\ I_{dN_x} & 0_{dN_x \times dN_x} \\ 0_{dN_x \times dN_x} & I_{dN_x} \end{bmatrix} \\ &= \begin{bmatrix} v_0^\top \tilde{Z} 1_{1 \times d} & \cdots & v_{N_x-1}^\top \tilde{Z} 1_{1 \times d} & v_0^\top \tilde{Z} 1_{1 \times d} & \cdots & v_{N_x-1}^\top \tilde{Z} 1_{1 \times d} \\ -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} & -\frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -\frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} \\ \ln(T(\tilde{v}_0))^\top & \cdots & \ln(T(\tilde{v}_{N_x-1}))^\top & \ln(E(\tilde{v}_0))^\top & \cdots & \ln(E(\tilde{v}_{N_x-1}))^\top \end{bmatrix}. \end{aligned}$$

Next, we construct W_Q to be

$$W_Q := \begin{bmatrix} 0 & R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ 0 & R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ 0_n & I_n & 0_{n \times (2dN_x-n)} \end{bmatrix}.$$

This yields that

$$\begin{aligned} Q &= W_Q \text{Linear}(Z) \\ &= \begin{bmatrix} 0 & R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ 0 & R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ 0_n & I_n & 0_{n \times (2dN_x-n)} \end{bmatrix} \cdot \begin{bmatrix} X_0 & X_0 \\ I_{dN_x} & 0_{dN_x \times dN_x} \\ 0_{dN_x \times dN_x} & I_{dN_x} \end{bmatrix} \\ &= \begin{bmatrix} R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ I_n & 0_{n \times (2dN_x-n)} \end{bmatrix}. \end{aligned}$$

We now calculate the attention matrix Softmax ($K^\top Q$).

Calculation of Softmax($K^\top Q$). First, $K^\top Q$ can be expressed as follows

$$K^\top Q = \begin{bmatrix} v_0^\top \tilde{Z} 1_d & \frac{\|v_0\|_2^2}{2} 1_d & \ln(T(\tilde{v}_0)) \\ v_1^\top \tilde{Z} 1_d & \frac{\|v_1\|_2^2}{2} 1_d & \ln(T(\tilde{v}_1)) \\ \vdots & \vdots & \vdots \\ v_{N_x-1}^\top \tilde{Z} 1_d & \frac{\|v_{N_x-1}\|_2^2}{2} 1_d & \ln(T(\tilde{v}_{N_x-1})) \\ v_0^\top \tilde{Z} 1_d & \frac{\|v_0\|_2^2}{2} 1_d & \ln(E(\tilde{v}_0)) \\ v_1^\top \tilde{Z} 1_d & \frac{\|v_1\|_2^2}{2} 1_d & \ln(E(\tilde{v}_1)) \\ \vdots & \vdots & \vdots \\ v_{N_x-1}^\top \tilde{Z} 1_d & \frac{\|v_{N_x-1}\|_2^2}{2} 1_d & \ln(E(\tilde{v}_{N_x-1})) \end{bmatrix} \cdot \begin{bmatrix} R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ I_n & 0_{n \times (2dN_x-n)} \end{bmatrix}$$

$$= \begin{bmatrix} R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})1_{d \times n} + \ln(T(\tilde{v}_0)) & 0_{d \times (2dN_x - n)} \\ R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})1_{d \times n} + \ln(T(\tilde{v}_1)) & 0_{d \times (2dN_x - n)} \\ \vdots & \vdots \\ R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})1_{d \times n} + \ln(T(\tilde{v}_{N_x-1})) & 0_{d \times (2dN_x - n)} \\ R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})1_{d \times n} + \ln(E(\tilde{v}_0)) & 0_{d \times (2dN_x - n)} \\ R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})1_{d \times n} + \ln(E(\tilde{v}_1)) & 0_{d \times (2dN_x - n)} \\ \vdots & \vdots \\ R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})1_{d \times n} + \ln(E(\tilde{v}_{N_x-1})) & 0_{d \times (2dN_x - n)} \end{bmatrix}.$$

Now, we divide the calculation of $\text{Softmax}(K^\top Q)$ into two counterparts, the calculation of $\exp(K^\top Q)$ and the calculation of the denominator of every column of $\text{Softmax}(K^\top Q)$, as in the expression of Softmax , explicitly written out as $\sum_{j=1}^{2dN_x} \exp(K^\top Q)_{ij}$ for each $i \in [2dN_x]$.

For $\exp(K^\top Q)$, we have

$$\exp(K^\top Q) = \begin{bmatrix} \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)T(\tilde{v}_0) & 1_{d \times (2dN_x - n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)T(\tilde{v}_1) & 1_{d \times (2dN_x - n)} \\ \vdots & \vdots \\ \exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)T(\tilde{v}_{N_x-1}) & 1_{d \times (2dN_x - n)} \\ \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)E(\tilde{v}_0) & 1_{d \times (2dN_x - n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)E(\tilde{v}_1) & 1_{d \times (2dN_x - n)} \\ \vdots & \vdots \\ \exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)E(\tilde{v}_{N_x-1}) & 1_{d \times (2dN_x - n)} \end{bmatrix} \quad (\text{F.1})$$

$$= \begin{bmatrix} \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)T(\tilde{v}_0) & 1_{d \times (2dN_x - n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)T(\tilde{v}_1) & 1_{d \times (2dN_x - n)} \\ \vdots & \vdots \\ \exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)T(\tilde{v}_{N_x-1}) & 1_{d \times (2dN_x - n)} \\ \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)E(\tilde{v}_0) & 1_{d \times (2dN_x - n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)E(\tilde{v}_1) & 1_{d \times (2dN_x - n)} \\ \vdots & \vdots \\ \exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)E(\tilde{v}_{N_x-1}) & 1_{d \times (2dN_x - n)} \end{bmatrix}. \quad (\text{F.2})$$

For the denominator, we calculate it in columns. Let i denote the column which we calculate the denominator in Softmax . When $i \in \{n+1, n+2, \dots, 2dN_x\}$, it obviously equals to $1 \cdot 2dN_x = 2dN_x$. And when $i \in [n]$, we denote that

$$\begin{aligned} \sum_{j=1}^{2dN_x} \exp(K^\top Q)_{ij} &= \sum_{j=1}^{N_x} \left[(1_{1 \times d} T(\tilde{v}_{j-1})_{:,i} + 1_{1 \times d} E(\tilde{v}_{j-1})_{:,i}) \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \right] \\ &= \sum_{j=1}^{N_x} \left[(1_{1 \times d} (E + T)(v_{j-1})_{:,i}) \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \right] \\ &= \sum_{j=1}^{N_x} \left[(1_{1 \times d} (2d \times n)_{:,i}) \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \right] \end{aligned}$$

$$= \sum_{j=1}^{N_x} 2d \cdot \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right), \quad i \in [n]. \quad (\text{F.3})$$

We observe from (F.3), that $\sum_{j=1}^{2dN_x} \exp(K^\top Q)_{ij}$ is invariant of i for $i \in [n]$. In this case, we define

$$\alpha(Z) := \frac{1}{2d} \sum_{j=1}^{2dN_x} \exp(K^\top Q)_{ij} = \sum_{j=1}^{N_x} \exp\left(R\left(v_{j-1}^\top \tilde{Z} - \frac{\|v_{j-1}\|_2^2}{2}\right)\right) \in \mathbb{R}, \quad i \in [n].$$

From (F.1) and (F.3) we have

$$\begin{aligned} & \text{Softmax}(K^\top Q) \\ &= \exp(K^\top Q) \odot \left[\frac{1}{\sum_{j=1}^{2dN_x} \exp(K^\top Q)_{1j}} \mathbf{1}_{2dN_x \times n} \quad \frac{1}{2dN_x} \mathbf{1}_{2dN_x \times (2dN_x - n)} \right] \\ & \quad \left(\text{By } 1/\sum_{j=1}^{2dN_x} \exp(K^\top Q)_{i,j} \text{ is invariant of } i \text{ for } i \in [n] \right) \\ &= \begin{bmatrix} \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right) T(\tilde{v}_0) & \mathbf{1}_{d \times (2dN_x - n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right) T(\tilde{v}_1) & \mathbf{1}_{d \times (2dN_x - n)} \\ \dots & \dots \\ \exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right) T(\tilde{v}_{N_x-1}) & \mathbf{1}_{d \times (2dN_x - n)} \\ \exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right) E(\tilde{v}_0) & \mathbf{1}_{d \times (2dN_x - n)} \\ \exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right) E(\tilde{v}_1) & \mathbf{1}_{d \times (2dN_x - n)} \\ \dots & \dots \\ \exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right) E(\tilde{v}_{N_x-1}) & \mathbf{1}_{d \times (2dN_x - n)} \end{bmatrix} \odot \left[\frac{1}{2d\alpha(Z)} \mathbf{1}_{2dN_x \times n} \quad \frac{1}{2dN_x} \mathbf{1}_{2dN_x \times (2dN_x - n)} \right] \\ &= \frac{1}{2d} \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_0) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_1) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \dots & \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_{N_x-1}) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_0) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_1) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \dots & \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_{N_x-1}) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \end{bmatrix}. \end{aligned}$$

Construction of W_V and W_O . We now construct the W_V matrix and calculate the V matrix of the self-attention.

We define W_V as

$$W_V := [0_d \quad X_1 \quad -X_1],$$

where

$$X_1 := [I_d \quad I_d \quad \dots \quad I_d]_{d \times dN_x},$$

is a matrix formed by stacking N_x I_d matrices horizontally.

In this definition, V matrix can be calculated as follows:

$$V := W_V \text{Linear}(Z)$$

$$\begin{aligned}
&= [0_d \quad X_1 \quad -X_1] \begin{bmatrix} X_0 & X_0 \\ I_{dN_x} & 0_{dN_x \times dN_x} \\ 0_{dN_x \times dN_x} & I_{dN_x} \end{bmatrix} \\
&= [X_1 \quad -X_1].
\end{aligned}$$

After the construction and calculation of V , we go on to construct W_O as

$$W_O = \begin{bmatrix} dB_0 I_n \\ 0_{(2dN_x - n) \times n} \end{bmatrix}.$$

The sole purpose of W_O is to extract the non-zero entries of the final output.

Calculation of the Output of $\text{Attn} \circ \text{Linear}$. We now calculate the final output of the self-attention block.

$$\begin{aligned}
\text{Attn} \circ \text{Linear}(Z) &= \frac{1}{2d} [X_1 \quad -X_1] \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_0) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_1) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \dots & \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} T(\tilde{v}_{N_x-1}) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_0) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_1) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \\ \dots & \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} E(\tilde{v}_{N_x-1}) & \frac{1}{N_x} \mathbf{1}_{d \times (2dN_x - n)} \end{bmatrix} W_O \\
&= \frac{1}{2d} X_1 \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} (T(\tilde{v}_0) - E(\tilde{v}_0)) & 0_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} (T(\tilde{v}_1) - E(\tilde{v}_1)) & 0_{d \times (2dN_x - n)} \\ \dots & \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} (T(\tilde{v}_{N_x-1}) - E(\tilde{v}_{N_x-1})) & 0_{d \times (2dN_x - n)} \end{bmatrix} W_O \\
&= \frac{1}{2d} X_1 \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_0)}{B_0} & 0_{d \times (2dN_x - n)} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_1)}{B_0} & 0_{d \times (2dN_x - n)} \\ \dots & \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_{N_x-1})}{B_0} & 0_{d \times (2dN_x - n)} \end{bmatrix} W_O.
\end{aligned}$$

We have

$$X_1 \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_0)}{B_0} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_1)}{B_0} \\ \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_{N_x-1})}{B_0} \end{bmatrix} = [I_d \quad I_d \quad \dots \quad I_d]_{d \times dN_x} \cdot \begin{bmatrix} \frac{\exp\left(R(v_0^\top \tilde{Z} - \frac{\|v_0\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_0)}{B_0} \\ \frac{\exp\left(R(v_1^\top \tilde{Z} - \frac{\|v_1\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_1)}{B_0} \\ \dots \\ \frac{\exp\left(R(v_{N_x-1}^\top \tilde{Z} - \frac{\|v_{N_x-1}\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_{N_x-1})}{B_0} \end{bmatrix}$$

$$\begin{aligned}
&= \sum_{j=0}^{N_x-1} I_d \cdot \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_j)}{B_0} \\
&= \sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_j)}{B_0}.
\end{aligned}$$

This yields

$$\begin{aligned}
\text{Attn} \circ \text{Linear}(Z) &= \left[\sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_j)}{B_0} \quad 0_{d \times (2dN_x-n)} \right] W_O \\
&= \left[\sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \frac{2f(\tilde{v}_j)}{B_0} \quad 0_{d \times (2dN_x-n)} \right] \begin{bmatrix} dB_0 I_n \\ 0_{(2dN_x-n) \times n} \end{bmatrix} \\
&= \sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} f(\tilde{v}_j). \tag{F.4}
\end{aligned}$$

Estimation of the Error between $\text{Attn} \circ \text{Linear}(Z)$ and $f(Z)$. After the above calculations of the output of the network, we can now demonstrate how this output approximates our target function.

Definition F.1 (Max-Affine Function on $\tilde{Z}$). Let $\text{Aff}_j \in \mathbb{R}^{dn} \rightarrow \mathbb{R}$, $j \in \{0, 1, 2, \dots, N_x - 1\}$ denote a group of affine functions defined as

$$\text{Aff}_j(\tilde{Z}) = v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2}, \quad j \in \{0, 1, 2, \dots, N_x - 1\}.$$

Then let $\text{MaxAff} \in \mathbb{R}^{dn} \rightarrow \mathbb{R}$ denote a max affine function whose affine components are $\{\text{Aff}_j \mid j \in \{0, 1, 2, \dots, N_x - 1\}\}$. Explicitly defined as

$$\text{MaxAff}(\tilde{Z}) = \max_{j \in \{0, 1, 2, \dots, N_x - 1\}} \{\text{Aff}_j(\tilde{Z})\}.$$

Because the target function f is a continuous function on a closed domain, the function f is uniformly continuous. Thus for ϵ , there exists a $\delta > 0$ such that for any Z_1, Z_2 , as long as $\|\tilde{Z}_1 - \tilde{Z}_2\|_\infty \leq \delta$, we have $\|f(Z_1) - f(Z_2)\|_\infty \leq \epsilon/3$.

According to this δ , we divide the affine components of MaxAff into three parts, the maximal component (and also with the smallest label), whose label is denoted as j_m , the group of affine components equal to the maximal component or smaller than it by no more than δ , and finally, the other Aff_j , $j \in \{0, 1, 2, \dots, N_x - 1\}$. We write out the labels of these groups of components as follows

$$\begin{aligned}
j_m &:= \min_{j \in \{0, 1, 2, \dots, N_x - 1\}} \{\text{Aff}_j(\tilde{Z}) = \text{MaxAff}(\tilde{Z})\}, \\
J_0 &:= \{j \mid \text{MaxAff}(\tilde{Z}) - \text{Aff}_j(\tilde{Z}) \leq \delta\}, \\
J_1 &:= \{j \mid \text{MaxAff}(\tilde{Z}) - \text{Aff}_j(\tilde{Z}) > \delta\}.
\end{aligned}$$

For any pair of $i, j \in \{0, 1, \dots, N_x - 1\}$, we have

$$\begin{aligned}
\text{Aff}_i(\tilde{Z}) - \text{Aff}_j(\tilde{Z}) &= v_i^\top \tilde{Z} - \frac{\|v_i\|_2^2}{2} - \left(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2} \right) \\
&= -\frac{\|\tilde{Z}\|_2^2}{2} + v_i^\top \tilde{Z} - \frac{\|v_i\|_2^2}{2} - \left(-\frac{\|\tilde{Z}\|_2^2}{2} + v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2} \right) \\
&= -\frac{1}{2} \|\tilde{Z} - v_i\|_2^2 + \frac{1}{2} \|\tilde{Z} - v_j\|_2^2.
\end{aligned}$$

This denotes j_m is also the label of the closest v_i to $\tilde{Z}$ among all v_i , $i \in \{0, 1, \dots, N_x - 1\}$. Thus we have

$$\|v_{j_m} - \tilde{Z}\|_2 = \min_{i \in \{0, 1, \dots, N_x - 1\}} \{\|v_i - \tilde{Z}\|_2\}. \tag{F.5}$$

Thus, when considering the Z in the input domain of f , which by definition is contained in N_x spheres, the closest center to Z is the sphere containing Z . This gives

$$\|Z - \tilde{v}_{j_m}\|_2 \leq \frac{\epsilon}{3L}. \quad (\text{F.6})$$

Then, with the L Lipschitzness of L we have

$$\|f(Z) - f(\tilde{v}_{j_m})\|_\infty \leq \frac{\epsilon}{3L} \cdot L = \frac{\epsilon}{3}. \quad (\text{F.7})$$

Difference between Attn $\circ$ Linear and f . We now calculate the difference between the output in (F.4) and target function f

$$\begin{aligned} & \|\text{Attn} \circ \text{Linear}(Z) - f(Z)\|_\infty \\ &= \left\| \sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} f(\tilde{v}_j) - f(Z) \right\|_\infty \\ &= \left\| \sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} (f(\tilde{v}_j) - f(Z)) \right\|_\infty \quad \left(\sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} = 1 \right) \\ &\leq \sum_{j=0}^{N_x-1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \quad (\text{property of infinite norm}) \\ &= \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty \\ &\quad + \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\ &\quad + \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty. \end{aligned} \quad (\text{F.8})$$

We now calculate each part in (F.8).

For the L -Lipschitzness of f , for any Z_1, Z_2 , as long as $\|\tilde{Z}_1 - \tilde{Z}_2\|_\infty \leq \frac{\epsilon}{3L}$, we have $\|f(Z_1) - f(Z_2)\|_\infty \leq \epsilon/3$. Thus when we designate $Z_1 = v_j$ for any $j \in J_0$ and $Z_2 = v_{j_m}$, along with (F.7) we have:

$$\begin{aligned} & \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \quad (\text{F.9}) \\ &\leq \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} (\|f(\tilde{v}_j) - f(\tilde{v}_{j_m})\|_\infty + \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty) \\ &\leq \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot \left(\frac{\epsilon}{3} + \frac{\epsilon}{3}\right) \\ &= \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2\epsilon}{3}. \end{aligned} \quad (\text{F.10})$$

For j_m , we have

$$\frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty \leq \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{\epsilon}{3}. \quad (\text{F.11})$$

When R is larger than $\frac{8}{3\delta^2} \ln\left(\frac{3}{2} \cdot B_0 N_x \epsilon\right)$, we have:

$$\begin{aligned}
& \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\
& \leq \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot 2B_0 \quad (\text{by the bounded nature of } f) \\
& \leq 2B_0 \frac{\sum_{j \in J_1} \exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \\
& < 2B_0 \frac{\sum_{j \in J_1} \exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)} \\
& \quad (\alpha(Z) \text{ is the sum of all } \exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right), \text{ thus larger than any element within the summation}) \\
& = 2B_0 \sum_{j \in J_1} \exp\left(\frac{R}{2} (\|v_{j_m} - Z\|_2^2 - \|v_j - Z\|_2^2)\right) \\
& \leq 2B_0 \|J_1\| \exp\left(\frac{R}{2} \left[\left(\frac{\delta}{2}\right)^2 - \delta^2\right]\right) \\
& < 2B_0 N_x \exp\left(\frac{-3R\delta^2}{8}\right) \\
& = 2B_0 N_x \exp\left(\frac{-3\delta^2 \cdot \frac{8 \ln\left(\frac{3}{2} B_0 N_x \epsilon\right)}{3\delta^2}}{8}\right) \\
& = \frac{\epsilon}{3}. \tag{F.12}
\end{aligned}$$

Combing (F.10) and (F.11) yields

$$\begin{aligned}
& \sum_{j \in J_0 \cup \{j_m\}} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\
& \leq \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2\epsilon}{3} + \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{\epsilon}{3} \quad (\text{By (F.10) and (F.11)}) \\
& \leq \sum_{j \in J_0 \cup \{j_m\}} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \cdot \frac{2\epsilon}{3} \\
& \leq \frac{2\epsilon}{3}, \tag{F.13}
\end{aligned}$$

where the last line is by $\sum_{j \in J_0 \cup \{j_m\}} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \leq 1$.

We plug (F.12) and (F.13) to (F.8) and get

$$\begin{aligned}
\|\text{Attn} \circ \text{Linear}(Z) - f(Z)\|_\infty & \leq \frac{\exp\left(R(v_{j_m}^\top \tilde{Z} - \frac{\|v_{j_m}\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_{j_m}) - f(Z)\|_\infty \\
& \quad + \sum_{j \in J_0} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty
\end{aligned}$$

$$\begin{aligned}
& + \sum_{j \in J_1} \frac{\exp\left(R(v_j^\top \tilde{Z} - \frac{\|v_j\|_2^2}{2})\right)}{\alpha(Z)} \|f(\tilde{v}_j) - f(Z)\|_\infty \\
& \leq \frac{2\epsilon}{3} + \frac{\epsilon}{3} \\
& = \epsilon.
\end{aligned}$$

This concludes our result on the approximation error.

Estimation of the Number of Trainable Parameters. We now estimate the number of trainable parameter in the network we constructed to verify our claim on number of trainable parameters in the main text of this theorem.

Remark F.1 (Meaning of Trainable Parameters). By trainable parameters we denote the parameters that differs according to f . This includes the parameters related to the input domain of $\mathcal{X}$, and excludes the constants (i.e., 0 and 1) in the network.

We estimate the number of trainable parameters by each layer in the network.

First, we do the estimation for the Linear layer. It consists of a sum over $N_x v_j^\top \tilde{Z}$, $j \in [N_x]$, and thus contain $dn \cdot N_x$ trainable parameters.

Then we do the estimation for W_K and W_Q . We restate the construction of W_K and W_Q :

$$\begin{aligned}
W_K &:= \begin{bmatrix} R & 0_{1 \times d} & \cdots & 0_{1 \times d} & 0_{1 \times d} & \cdots & 0_{1 \times d} \\ 0 & -R \frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -R \frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} & -R \frac{\|v_0\|_2^2}{2} 1_{1 \times d} & \cdots & -R \frac{\|v_{N_x-1}\|_2^2}{2} 1_{1 \times d} \\ 0 & \ln(T(\tilde{v}_0))^\top & \cdots & \ln(T(\tilde{v}_{N_x-1}))^\top & \ln(E(\tilde{v}_0))^\top & \cdots & \ln(E(\tilde{v}_{N_x-1}))^\top \end{bmatrix}, \\
W_Q &:= \begin{bmatrix} 0 & R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ 0 & R 1_{1 \times n} & 0_{1 \times (2dN_x-n)} \\ 0_n & I_n & 0_{n \times (2dN_x-n)} \end{bmatrix}.
\end{aligned}$$

From this, we observe they combined together have $2d \cdot N_x + 2dn \cdot N_x$ trainable parameters.

Finally, For W_V and W_O , we restate their definition:

$$\begin{aligned}
W_V &:= [0_d \quad X_1 \quad -X_1], \\
W_O &:= \begin{bmatrix} dB_0 I_n \\ 0_{(2dG-n) \times n} \end{bmatrix},
\end{aligned}$$

where

$$X_1 := [I_d \quad I_d \quad \cdots \quad I_d]_{d \times dG}.$$

W_O contains n trainable parameters (dB_0).

In conclusion, the whole network contains a total of

$$dnN_x + 2dN_x + 2dnN_x + n = 4dnN_x + 2dN_x + n,$$

trainable parameters, which is of $\mathcal{O}(dnN_x)$ level.

This completes the proof. $\square$

G Extended Related Work

Recent empirical studies also shed light on the practical behavior of attention mechanism. [Olsson et al. \[2022\]](#) show that induction heads help models learn patterns in context. [Sanford et al. \[2024a\]](#) prove that Transformers can do complex computations with few layers because they work in parallel. In contrast, [Luo et al. \[2022\]](#) find that some Transformer designs lose expressivity when using relative positional encodings. Our work builds on these ideas. We prove that a single-layer, single-head softmax attention with a simple linear layer can approximate any continuous function on a compact domain. This shows that attention alone can learn arbitrary sequence-to-sequence mappings.

H Extension to Transformer Setting

In this section, we demonstrate how our proof technique in attention extends to the transformer setting. Specifically, we show it is possible to use a three-layer multi-head attention-only network to achieve universal approximation in L_p norm.

Lemma H.1 (Attention Simulate Column-Wise Transformation). For an input $X \in \mathbb{R}^{d \times n}$. Let $l(X) := AXB$, $A \in \mathbb{R}^{d_{\text{output}} \times d}$, $B \in \mathbb{R}^{n \times n}$ be the linear operation (both token-wise and sequence-wise included) we wish to get. Without loss of generality, suppose B has positive entries (since subtraction of positive matrices yields all matrix). We use an all-zero padding token. Let I_{n+1} be the positional encoding below X . Then for any $\epsilon > 0$, there exists a single-head attention Attn such that

$$\|\text{Attn}\left(\begin{bmatrix} X & 0_d \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix}\right) - \begin{bmatrix} l(X) & 0_{d_{\text{output}}} \end{bmatrix}\|_{\infty} \leq \epsilon.$$

Proof. Let s_i be the sum of all entries of $B_{:,i}$ (i -th column) and $M := \max_{i \in [n]} s_i$. Define $S = [s_1 \cdots s_n]$. Construct $W_V := 3M * [A \quad 0_{d_{\text{output}} \times (n+1)}]$, $W_K := [0_{n \times d} \quad \ln(B^{\top}) \quad \ln(3M \cdot 1_n - S^{\top})]$ ($\ln$ is entry-wise), and $W_Q := [0_{n \times d} \quad I_n \quad T \cdot 1_n]$ (T will be turned to arbitrarily large), then the output of attention is $3MA[X \quad 0_d] \text{Softmax}(\begin{bmatrix} \ln(B) & T \cdot H_1 \\ \ln(3M \cdot 1_{1 \times n} - S) & T \cdot H_2 \end{bmatrix})^{\top} [I_n \quad T \cdot 1_n]$.

This equals

$$3MA[X \quad 0_d] \text{Softmax}\left(\begin{bmatrix} \ln(B) & T \cdot H_1 \\ \ln(3M \cdot 1_{1 \times n} - S) & T \cdot H_2 \end{bmatrix}\right),$$

in which H_1, H_2 are the sum of all columns in $\ln(B), \ln(3M \cdot 1_{1 \times n} - S)$ respectively.

This further equals to

$$3MA[X \quad 0_d] \begin{bmatrix} \frac{B}{3M} & a_0 \\ 1_{1 \times n} - \frac{S}{3M} & a_1 \end{bmatrix} = [AXB \quad C], ([a_0 \quad a_1]^{\top} \text{ is the } T\text{-related column}),$$

in which $C = 3MAXa_0$, when $T \rightarrow +\infty$, $a_0 \rightarrow 0_{d_{\text{output}}}$ and the padding token is preserved as well. □

Lemma H.2 (Preservation of Identity Matrix). For any $\epsilon > 0$ and $n \in \mathbb{N}^+$, there exists an attention head Attn that satisfies

$$\|\text{Attn}(I_n) - I_n\|_{\infty} \leq \epsilon.$$

Proof. Construct the W_K, W_Q, W_V matrices of this attention head as

$$\begin{aligned} W_K &:= RI_n \\ W_Q &:= I_n \\ W_V &:= I_n. \end{aligned}$$

The output of this layer is

$$\text{Softmax}(RI_n)$$

Hence when R is sufficiently large, the output is within an arbitrarily small error to I_n . □

Corollary H.0.1. For any $\epsilon > 0$ and input of form

$$\begin{bmatrix} A \\ I_n \end{bmatrix},$$

where $A \in \mathbb{R}^{m \times n}$ denotes any matrix, there exists an attention head Attn such that

$$\|\text{Attn}\left(\begin{bmatrix} A \\ I_n \end{bmatrix}\right) - \begin{bmatrix} 0_{m \times n} \\ I_n \end{bmatrix}\|_{\infty} \leq \epsilon.$$

The proof is obvious. We only have to zero out A in W_K, W_Q, W_V and do the rest as [Lemma H.2](#).

We now prove the universal approximation result in the transformer setting.

Theorem H.1. Let $X \in \mathbb{R}^{d \times n}$ denote the input sequence. Let f be a continuous function on a compact support. For any $\eta > 0$, there exists a three-layer multi-head attention $\text{Attn}^{(i)}, i \in [3]$ such that

$$\|\text{Attn}^{(3)} \circ \text{Attn}^{(2)} \circ \text{Attn}^{(1)} \left(\begin{bmatrix} X & 0_d \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix} \right)_{:,1:n} - f(X)\|_{L_p} \leq \eta.$$

The First Layer

Let $v_i, i \in [P^{dn}]$ be as defined in [Remark E.1](#).

Let $\tilde{X}$ represent the flattened input X and let $\tilde{v}$ represents the $\mathbb{R}^{d \times n}$ sequence form of $v \in \mathbb{R}^{dn}$.

Let $\delta_i, i \in [d]$ be defined as

$$\delta_i := \begin{bmatrix} 0_{i-1} \\ \frac{1}{P} \\ 0_{d-i} \end{bmatrix} \in \mathbb{R}^d.$$

Let $\text{Attn}_h^{(1)}, h \in [n]$ denote the h -th head of $\text{Attn}^{(1)}$. According to [Lemma H.1](#), for any $\epsilon_0 > 0$, there exists such set of Attn_h such that

$$\|\text{Attn}_h^{(1)} \left(\begin{bmatrix} X & 0_d \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix} \right) - [l_h(X) \quad 0_{(d+1)n}]\|_{\infty} \leq \epsilon_0,$$

in which

$$l_h(X) := \begin{bmatrix} 0_{d(h-1) \times n} \\ x_h \cdot 1_{1 \times n} \\ 0_{[d(n-h)+n] \times n} \end{bmatrix}, h \in [n]$$

And construct the $n+1$ -th head to preserve the identity matrix using [Corollary H.0.1](#) (A having the dimension of $dn \times (n+1)$ and the identity matrix preserved being I_{n+1} in this case). So the output approximates

$$\begin{bmatrix} \tilde{X} \cdot 1_{1 \times n} & 0_{dn} \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix} \quad (\text{H.1})$$

to an arbitrarily small error in the infinite norm.

The first attention layer is then defined as

$$\text{Attn}^{(1)} := \sum_{h=1}^{n+1} \text{Attn}_h^{(1)}$$

The Second Layer

Label the heads in the second layer with (v, g, s) pair, $v \in [P^{dn}], g \in [n], s \in \{\pm 1\}$. Construct parameters in $\text{Attn}_{(v,g,s)}^{(2)}$ to be

$$W_Q := \begin{bmatrix} 0_{n \times (g-1)d} & D & 0_{n \times (n-g)d} & -D \cdot (\tilde{v}_v)_{:,g} \cdot 1_{1 \times n} & 0 \\ 0_{1 \times (g-1)d} & 0_{1 \times d} & 0_{1 \times (n-g)d} & s \cdot \frac{1}{2P^2} \cdot 1_{1 \times n} & 0 \end{bmatrix}$$

$$W_K := R \begin{bmatrix} 0_{n \times dn} & I_n & 0_n \\ 0_{1 \times dn} & 1_{1 \times n} & 0 \end{bmatrix},$$

in which D is

$$D := \begin{bmatrix} \delta_1^\top \\ \vdots \\ \delta_n^\top \end{bmatrix}$$

and $R \in \mathbb{R}^+$ is a parameter that will be set in later process.

Then the attention score matrix of $\text{Attn}_{(v,g,s)}^{(2)}$ is

$$\begin{aligned} & \text{Softmax} \left(R \begin{bmatrix} I_n & 0_n \\ 1_{1 \times n} & 0 \end{bmatrix}^\top \begin{bmatrix} D(x_g - (\tilde{v}_v)_{:,g}) \cdot 1_{1 \times n} & 0_n \\ s \cdot \frac{1}{2P^2} \cdot 1_{1 \times n} & 0 \end{bmatrix} \right) \\ &= \text{Softmax} \left(R \begin{bmatrix} D(x_g - (\tilde{v}_v)_{:,g}) \cdot 1_{1 \times n} + s \cdot \frac{1}{2P^2} \cdot 1_{n \times n} & 0_n \\ 0_{1 \times n} & 0 \end{bmatrix} \right) \\ &= \text{Softmax} \left(R \begin{bmatrix} D(x_g - (\tilde{v}_v)_{:,g}) \cdot 1_{1 \times n} & 0_n \\ -s \cdot \frac{1}{2P^2} \cdot 1_{1 \times n} & 0 \end{bmatrix} \right) \end{aligned}$$

When R is taken sufficiently large, for any given $\epsilon_1 > 0$ and an arbitrary $\Delta_s > 0$ invariant of ϵ_1 and R , if

$$\delta_i^\top (x_g - (\tilde{v}_v)_{:,g}) > \frac{1}{2P^2} + \Delta_s$$

for a specific i , then in the attention score matrix of $\text{Attn}_{(v,g,1)}^{(2)}$, the i -th row should be larger than the last row by Δ_s , and this difference after amplified by R makes the last row to be lesser than the given ϵ_1 .

Similarly, when

$$\delta_i^\top (x_g - (\tilde{v}_v)_{:,g}) < -\frac{1}{2P^2} - \Delta_s$$

for a specific i , the $(n+1, j)$ entries in $\text{Attn}_{(v,g,-1)}^{(2)}$ ($j = 1, \dots, n$) are smaller than ϵ_1 when setting R to be sufficiently large. And the sum the rest of the j -th column is larger than $1 - \epsilon_1$.

Finally, when $|\delta_i^\top (x_g - (\tilde{v}_v)_{:,g})| < \frac{1}{2P^2} - \Delta_s$, for all $i \in [n]$, it makes the last row largest in every entry (except the last column). Thus there exists a sufficiently large R , such that the last row of the attention score matrix is larger than $1 - \epsilon_1$ in every entry. This also makes the sum of the rest of the rows less than or equal to ϵ_1 in every column.

We show that the last situation is equivalent to the input token x_g falling into the grid centered at $(\tilde{v}_v)_{:,g}$ in $\mathbb{R}^d$. (notice v_v is a grid point in $\mathbb{R}^{dn}$ and its column is a grid point in $\mathbb{R}^d$)

$$\begin{aligned} \delta_i^\top (x_g - (\tilde{v}_v)_{:,g}) - \frac{1}{2P^2} &= \delta_i^\top (x_g - (\tilde{v}_v)_{:,g}) - \frac{1}{2} \|\delta_i\|_2^2 \\ &= \frac{1}{2} (\|x_g - (\tilde{v}_v)_{:,g}\|_2^2 - \|x_g - ((\tilde{v}_v)_{:,g} + \delta_i)\|_2^2) \\ -\delta_i^\top (x_g - (\tilde{v}_v)_{:,g}) - \frac{1}{2P^2} &= -\delta_i^\top (x_g - (\tilde{v}_v)_{:,g}) - \frac{1}{2} \|\delta_i\|_2^2 \\ &= \frac{1}{2} (\|x_g - (\tilde{v}_v)_{:,g}\|_2^2 - \|x_g - ((\tilde{v}_v)_{:,g} - \delta_i)\|_2^2) \end{aligned}$$

Therefore

$$|\delta_i^\top (x_g - (\tilde{v}_v)_{:,g})| < \frac{1}{2P^2} - \Delta_s$$

is equivalent to x_g being closer to $(\tilde{v}_v)_{:,g}$ than its neighboring grid points in $\mathbb{R}^d$ (which are $\{(\tilde{v}_v)_{:,g} \pm \delta_i | i \in [d]\}$), this concludes it to be within the grid centered at $(\tilde{v}_v)_{:,g}$.

This means that when x_g is within the grid centered at $\tilde{v}_v$, both heads in $\text{Attn}_{(v,g,s)}^{(2)}$, $s \in [\pm 1]$ has their last row in the attention score matrix larger than $1 - \epsilon_1$ (which makes their sum larger than $2 - 2\epsilon_1$) and if x_g is not in the grid, their sum would be smaller than $1 + \epsilon_1$ (because at least one is smaller ϵ and all entries should be smaller than 1)

Let W_V of head labeled (v, g, s) be

$$\begin{bmatrix} 0_{s_v \times dn} & 0_{s_v \times n} & 0_{s_v} \\ 0_{1 \times dn} & 1_{1 \times n} & 0 \\ 0_{t_v \times dn} & 0_{t_v \times n} & 0_{t_v} \end{bmatrix}$$

in which $s_v := vd + (g - 1)$, $t_v = P^{dn}n - s_v + n - 1$. We note that here head $(v, g, 1)$ and $(v, g, -1)$ have the same head.

Then V is

$$\begin{aligned} V &:= W_V \begin{bmatrix} \tilde{X} \cdot 1_{1 \times n} & 0_{dn} \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix} \\ &= \begin{bmatrix} 0_{s_v \times dn} & 0_{s_v \times n} \\ 0_{n \times dn} & 1_{1 \times n} \\ 0_{t_v \times dn} & 0_{t_v \times n} \end{bmatrix} \begin{bmatrix} \tilde{X} \cdot 1_{1 \times n} & 0_{dn} \\ I_n & 0_n \end{bmatrix} \\ &= \begin{bmatrix} 0_{s_v \times n} & 0 \\ 1_{1 \times n} & 0 \\ 0_{t_v \times n} & 0 \end{bmatrix} \in \mathbb{R}^{(P^{dn}n+n) \times (n+1)} \end{aligned}$$

The output of the (v, g, s) -th head in the second attention layers is

$$V \cdot S_a^{(v,g,s)} = \begin{bmatrix} 0_{s_v \times n} & 0_{s_v} \\ 1_{1 \times n} - (S_a^{(v,g,s)})_{n+1,1:n} & \frac{n}{n+1} \\ 0_{t_v \times (n+1)} & 0_{t_v} \end{bmatrix},$$

in which

$$S_a^{(v,g,s)} := \text{Softmax} \left(R \begin{bmatrix} D(x_g - (\tilde{v}_v)_{:,g}) \cdot 1_{1 \times n} & 0_n \\ -s \cdot \frac{1}{2P^2} \cdot 1_{1 \times n} & 0 \end{bmatrix} \right)$$

is the previously constructed attention score of the (v, g, s) head.

Finally, add a head $\text{Attn}_I^{(2)}$ to preserve the identity matrix as that done in the first layer using [Corollary H.0.1](#).

This head outputs (with an arbitrarily small error)

$$\begin{bmatrix} 0_{P^{dn}n \times n} & 0_{P^{dn}n \times 1} \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix}.$$

Define $\text{Attn}^{(2)}$ as the sum of previously defined heads

$$\text{Attn}^{(2)} := \sum_{v,g,s} \text{Attn}_{(v,g,s)}^{(2)} + \text{Attn}_I^{(2)}$$

Then we have that when the input is

$$\begin{bmatrix} \tilde{X} \cdot 1_{1 \times n} & 0_{dn} \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix},$$

the output of this layer is within an arbitrary small error to

$$\begin{bmatrix} 2_{1 \times n} - S(1, 1) & \frac{n}{n+1} \\ \vdots & \vdots \\ 2_{1 \times n} - S(1, n) & \frac{n}{n+1} \\ \vdots & \vdots \\ 2_{1 \times n} - S(P^{dn}, n) & \frac{n}{n+1} \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix}, \quad (\text{H.2})$$

in which

$$S(v, g) := (S_a^{(v, g, -1)})_{n+1, 1:n} + (S_a^{(v, g, 1)})_{n+1, 1:n}.$$

We note that only when input is within the grid centered at v , $2_{1 \times n} - S(v, g)$ is smaller than $2 - (2 - 2\epsilon_1) = 2\epsilon_1$ for every g in all entries.

The Third Layer

The third layer consists of P^{dn} blocks, the v -th block identifies if the input falls inside the v -th grid.

For the v -th block, construct its W_K, W_Q as

$$W_K := \begin{bmatrix} 0_{n \times (v-1)n} & 0_{n \times n} & 0_{n \times (P^{dn}-v)n} & \frac{1}{2}I_n & 0_n \\ 0_{1 \times (v-1)n} & 1_{1 \times n} & 0_{1 \times (P^{dn}-v)n} & 0_{1 \times n} & -\frac{P^{dn}n^2}{n+1} \end{bmatrix}$$

$$W_Q := R_1 \begin{bmatrix} 0_{(n+1) \times P^{dn}n} & I_{n+1} \end{bmatrix},$$

in which R_1 is a scaler whose size we will determine in later process.

When the input has the form of that in (H.2). The K and Q matrices are

$$K := W_K \begin{bmatrix} 2_{1 \times n} - S(1, 1) & \frac{n}{n+1} \\ \vdots & \vdots \\ 2_{1 \times n} - S(1, n) & \frac{n}{n+1} \\ \vdots & \vdots \\ 2_{1 \times n} - S(P^{dn}, n) & \frac{n}{n+1} \\ I_n & 0_n \\ 0_{1 \times n} & 1 \end{bmatrix}$$

$$= \begin{bmatrix} n \cdot 2_{1 \times n} - \sum_{g \in [n]} S(v, g) & 0_n \\ 0 & 0 \end{bmatrix} \in \mathbb{R}^{(n+1) \times (n+1)}$$

$$Q := R_1 \cdot I_{n+1}.$$

This yields the attention score matrix to be

$$\text{Softmax}(K^\top Q) = \text{Softmax}\left(R_1 \begin{bmatrix} n \cdot 2_{1 \times n} - \sum_{g \in [n]} S(v, g) & 0_n \\ 0 & 0 \end{bmatrix}\right)$$

By $n \cdot 2_{1 \times n} - \sum_{g \in [n]} S(v, g)$ is smaller than $2n\epsilon_1$ if input is in the grid centered at v and larger than $1 - \epsilon_1$ if not. Set $\epsilon_1 = 1/4n$, we get that for any $\epsilon_2 > 0$, when R_1 is sufficiently large,

$$\|\text{Softmax}(K^\top Q) - \begin{bmatrix} I_n & \frac{1}{n+1} \cdot 1_n \\ 0_{1 \times n} & \frac{1}{n+1} \end{bmatrix}\|_\infty \leq \epsilon_2,$$

when input is within the grid centered at v .

And when the input is not in the grid centered at v , we have

$$\|\text{Softmax}(K^\top Q) - \begin{bmatrix} 0_{n \times n} & \frac{1}{n+1} \cdot 1_n \\ 1_{1 \times n} & \frac{1}{n+1} \end{bmatrix}\|_\infty \leq \epsilon_2$$

Construct W_V as

$$\begin{bmatrix} 0_{d \times P^{dn}n} & \frac{1}{2}f(\tilde{v}_v) & 0_d \end{bmatrix}$$

This makes the V matrix

$$V = [f(\tilde{v}_v) \quad 0_d],$$

when input has the form in (H.2).

Thus the third layer's v -th block outputs

$$V \text{ Softmax}(K^\top Q) = [f(\tilde{v}_v) \quad 0_n] \cdot \text{Softmax}(R_1 \begin{bmatrix} n \cdot 2_{1 \times n} - \sum_{g \in [n]} S(v, g) & 0_n \\ 0 & 0 \end{bmatrix}).$$

Then for any $\epsilon_3 > 0$, there exists an R_1 such that the output of the third layer satisfies

$$\|V \text{ Softmax}(K^\top Q) - [f(\tilde{v}_v) \quad *]\|_\infty \leq \epsilon_3,$$

when the input falls inside the grid centered at v_v .

And

$$\|V \text{ Softmax}(K^\top Q) - [0_{d \times n} \quad *]\|_\infty \leq \epsilon_3,$$

when the input does not fall inside the grid centered at v_v . Here $*$ denotes the padded column that is not considered in the final output and is hence omitted.

Now we sum all these heads and get the final output of $\text{Attn}^{(3)}$. The final output is within an error of $P^{dn}\epsilon_3$ to

$$[f(\tilde{v}_v) \quad *] + [(P^{dn} - 1) \cdot 0_{d \times n} \quad *]$$

with v_v being the center of the grid that has the input sequence in it.

Analysis of Total Error

Let Ω be the compact support of f with finite measure $\mu(\Omega) = V$.

Let $F(x) = (\text{Attn}^{(3)} \circ \text{Attn}^{(2)} \circ \text{Attn}^{(1)})(x)$ denote the output of the network given ideal inputs Z_i , and let $F^*(x)$ denote the output given perturbed inputs Z_i^* (which are the actual inputs).

We have formerly proven the following conditions for any $\epsilon > 0$:

- **Ideal Approximation:** $\|F(x) - f(x)\|_\infty < \epsilon$.
- **Perturbed Inputs:** The input to the third layer, $Z_3^*(x)$, satisfies $\|Z_3^*(x) - Z_3(x)\|_\infty \leq \epsilon$ on a set $\Omega \setminus B_\delta$, where B_δ is a region of arbitrarily small measure $\mu(B_\delta) < \delta$. On B_δ , the error exceeds ϵ but is still bounded.

Given the conditions above, for any precision $\eta > 0$ and any $p \in [1, \infty)$, the actual output F^* approximates the target function f in the L_p norm such that $\|F^* - f\|_p < \eta$.

We aim to bound the L_p error $\|F^* - f\|_p$. By the Minkowski inequality (triangle inequality for L_p norms), we can separate the error into an approximation component and a stability component:

$$\|F^* - f\|_p \leq \|F^* - F\|_p + \|F - f\|_p. \quad (\text{H.3})$$

We analyze these two terms separately.

1. Bounding the Approximation Error

From the problem statement, the ideal network approximates f uniformly with error ϵ . Using the definition of the L_p norm on the domain Ω :

$$\|F - f\|_p = \left(\int_\Omega \|F(x) - f(x)\|^p d\mu(x) \right)^{1/p} \leq \left(\int_\Omega \epsilon^p d\mu(x) \right)^{1/p} = \epsilon V^{1/p}. \quad (\text{H.4})$$

Since ϵ can be chosen arbitrarily small, this term converges to 0 as $\epsilon \rightarrow 0$.

2. Bounding the Stability Error

Consider the term $\|F^* - F\|_p$, which represents the deviation caused by the perturbed intermediate inputs. Recall that $F(x) = \text{Attn}^{(3)}(Z_3(x))$ and $F^*(x) = \text{Attn}^{(3)}(Z_3^*(x))$. To evaluate the integral over Ω , we partition the domain into the “good” set $S = \Omega \setminus B_\delta$ and the “bad” set B_δ :

$$\|F^* - F\|_p^p = \int_S \|\text{Attn}^{(3)}(Z_3^*) - \text{Attn}^{(3)}(Z_3)\|^p d\mu + \int_{B_\delta} \|\text{Attn}^{(3)}(Z_3^*) - \text{Attn}^{(3)}(Z_3)\|^p d\mu. \quad (\text{H.5})$$

Analysis on S (Lipschitz Continuity): The Multi-Head Attention layer $\text{Attn}^{(3)}$ consists of linear projections and the Softmax function, which are smooth and differentiable operations. Consequently, $\text{Attn}^{(3)}$ is locally Lipschitz continuous on compact domains. Let K be the Lipschitz constant for $\text{Attn}^{(3)}$. On the set S , we are given that $\|Z_3^* - Z_3\| \leq \epsilon$. Therefore:

$$\|\text{Attn}^{(3)}(Z_3^*) - \text{Attn}^{(3)}(Z_3)\| \leq K\|Z_3^* - Z_3\| \leq K\epsilon. \quad (\text{H.6})$$

The integral over S is bounded by:

$$\int_S \|\text{Attn}^{(3)}(Z_3^*) - \text{Attn}^{(3)}(Z_3)\|^p d\mu \leq \mu(S)(K\epsilon)^p \leq V(K\epsilon)^p. \quad (\text{H.7})$$

Analysis on B_δ (Uniform Boundedness): On the region B_δ , the Lipschitz bound fails. However, since Ω is compact and the functions comprising the network are continuous, the image of the network is bounded. There exists a constant $M > 0$ such that $\|F(x)\| \leq M$ and $\|F^*(x)\| \leq M$ for all $x \in \Omega$. By the triangle inequality, the pairwise difference is bounded by $2M$. Thus:

$$\int_{B_\delta} \|\text{Attn}^{(3)}(Z_3^*) - \text{Attn}^{(3)}(Z_3)\|^p d\mu \leq \int_{B_\delta} (2M)^p d\mu = \delta(2M)^p. \quad (\text{H.8})$$

Combining these results, the stability error satisfies:

$$\|F^* - F\|_p \leq (V(K\epsilon)^p + \delta(2M)^p)^{1/p}. \quad (\text{H.9})$$

3. Conclusion

Substituting the bounds back into the original inequality, we obtain:

$$\|F^* - f\|_p \leq \epsilon V^{1/p} + (VK^p\epsilon^p + \delta(2M)^p)^{1/p}. \quad (\text{H.10})$$

To ensure $\|F^* - f\|_p < \eta$, we select parameters as follows:

- Choose ϵ sufficiently small such that both $\epsilon V^{1/p}$ and $V^{1/p}K\epsilon$ are smaller than $\eta/3$.
- Choose the region of perturbation B_δ sufficiently small such that $\delta < (\eta/3)^p/(2M)^p$.

Since ϵ and δ can be made arbitrarily small, for any $\eta > 0$, the condition holds, and we get the global L_p approximation error converges to zero.

NeurIPS Paper Checklist

The checklist is designed to encourage best practices for responsible machine learning research, addressing issues of reproducibility, transparency, research ethics, and societal impact. Do not remove the checklist: **The papers not including the checklist will be desk rejected.** The checklist should follow the references and follow the (optional) supplemental material. The checklist does NOT count towards the page limit.

Please read the checklist guidelines carefully for information on how to answer these questions. For each question in the checklist:

- You should answer [Yes], [No], or [NA].
- [NA] means either that the question is Not Applicable for that particular paper or the relevant information is Not Available.
- Please provide a short (1–2 sentence) justification right after your answer (even for NA).

The checklist answers are an integral part of your paper submission. They are visible to the reviewers, area chairs, senior area chairs, and ethics reviewers. You will be asked to also include it (after eventual revisions) with the final version of your paper, and its final version will be published with the paper.

The reviewers of your paper will be asked to use the checklist as one of the factors in their evaluation. While "[Yes]" is generally preferable to "[No]", it is perfectly acceptable to answer "[No]" provided a proper justification is given (e.g., "error bars are not reported because it would be too computationally expensive" or "we were unable to find the license for the dataset we used"). In general, answering "[No]" or "[NA]" is not grounds for rejection. While the questions are phrased in a binary way, we acknowledge that the true answer is often more nuanced, so please just use your best judgment and write a justification to elaborate. All supporting evidence can appear either in the main paper or the supplemental material, provided in appendix. If you answer [Yes] to a question, in the justification please point to the section(s) where related material for the question can be found.

IMPORTANT, please:

- **Delete this instruction block, but keep the section heading “NeurIPS Paper Checklist”,**
- **Keep the checklist subsection headings, questions/answers and guidelines below.**
- **Do not modify the questions and only use the provided macros for your answers.**

1. Claims

Question: Do the main claims made in the abstract and introduction accurately reflect the paper’s contributions and scope?

Answer: [Yes]

Justification: The Abstract and Introduction explicitly list the three main contributions — Max-Affine interpretation, self-attention universality, and cross-attention universality — and no additional claims are made elsewhere.

Guidelines:

- The answer NA means that the abstract and introduction do not include the claims made in the paper.
- The abstract and/or introduction should clearly state the claims made, including the contributions made in the paper and important assumptions and limitations. A No or NA answer to this question will not be perceived well by the reviewers.
- The claims made should match theoretical and experimental results, and reflect how much the results can be expected to generalize to other settings.
- It is fine to include aspirational goals as motivation as long as it is clear that these goals are not attained by the paper.

2. Limitations

Question: Does the paper discuss the limitations of the work performed by the authors?

Answer: [Yes]

Justification: Sec 5 “Concluding Remarks”, paragraph “Limitations” (lines 336–350) details assumptions on partition granularity, boundary effects, training difficulty, and distribution shift.

Guidelines:

- The answer NA means that the paper has no limitation while the answer No means that the paper has limitations, but those are not discussed in the paper.
- The authors are encouraged to create a separate "Limitations" section in their paper.
- The paper should point out any strong assumptions and how robust the results are to violations of these assumptions (e.g., independence assumptions, noiseless settings, model well-specification, asymptotic approximations only holding locally). The authors should reflect on how these assumptions might be violated in practice and what the implications would be.
- The authors should reflect on the scope of the claims made, e.g., if the approach was only tested on a few datasets or with a few runs. In general, empirical results often depend on implicit assumptions, which should be articulated.
- The authors should reflect on the factors that influence the performance of the approach. For example, a facial recognition algorithm may perform poorly when image resolution is low or images are taken in low lighting. Or a speech-to-text system might not be used reliably to provide closed captions for online lectures because it fails to handle technical jargon.
- The authors should discuss the computational efficiency of the proposed algorithms and how they scale with dataset size.
- If applicable, the authors should discuss possible limitations of their approach to address problems of privacy and fairness.
- While the authors might fear that complete honesty about limitations might be used by reviewers as grounds for rejection, a worse outcome might be that reviewers discover limitations that aren't acknowledged in the paper. The authors should use their best judgment and recognize that individual actions in favor of transparency play an important role in developing norms that preserve the integrity of the community. Reviewers will be specifically instructed to not penalize honesty concerning limitations.

3. Theory assumptions and proofs

Question: For each theoretical result, does the paper provide the full set of assumptions and a complete (and correct) proof?

Answer: [Yes]

Justification: All assumptions are stated next to each theorem in Section 3-4; complete formal proofs are given in Appendices C–D (pp. 16–48).

Guidelines:

- The answer NA means that the paper does not include theoretical results.
- All the theorems, formulas, and proofs in the paper should be numbered and cross-referenced.
- All assumptions should be clearly stated or referenced in the statement of any theorems.
- The proofs can either appear in the main paper or the supplemental material, but if they appear in the supplemental material, the authors are encouraged to provide a short proof sketch to provide intuition.
- Inversely, any informal proof provided in the core of the paper should be complemented by formal proofs provided in appendix or supplemental material.
- Theorems and Lemmas that the proof relies upon should be properly referenced.

4. Experimental result reproducibility

Question: Does the paper fully disclose all the information needed to reproduce the main experimental results of the paper to the extent that it affects the main claims and/or conclusions of the paper (regardless of whether the code and data are provided or not)?

Answer: [Yes]

Justification: Appendix B specifies datasets, noise-injection protocol, model size, and training procedure; code will be released anonymously with the supplementary material.

Guidelines:

- The answer NA means that the paper does not include experiments.
- If the paper includes experiments, a No answer to this question will not be perceived well by the reviewers: Making the paper reproducible is important, regardless of whether the code and data are provided or not.
- If the contribution is a dataset and/or model, the authors should describe the steps taken to make their results reproducible or verifiable.
- Depending on the contribution, reproducibility can be accomplished in various ways. For example, if the contribution is a novel architecture, describing the architecture fully might suffice, or if the contribution is a specific model and empirical evaluation, it may be necessary to either make it possible for others to replicate the model with the same dataset, or provide access to the model. In general, releasing code and data is often one good way to accomplish this, but reproducibility can also be provided via detailed instructions for how to replicate the results, access to a hosted model (e.g., in the case of a large language model), releasing of a model checkpoint, or other means that are appropriate to the research performed.
- While NeurIPS does not require releasing code, the conference does require all submissions to provide some reasonable avenue for reproducibility, which may depend on the nature of the contribution. For example
 - (a) If the contribution is primarily a new algorithm, the paper should make it clear how to reproduce that algorithm.
 - (b) If the contribution is primarily a new model architecture, the paper should describe the architecture clearly and fully.
 - (c) If the contribution is a new model (e.g., a large language model), then there should either be a way to access this model for reproducing the results or a way to reproduce the model (e.g., with an open-source dataset or instructions for how to construct the dataset).
 - (d) We recognize that reproducibility may be tricky in some cases, in which case authors are welcome to describe the particular way they provide for reproducibility. In the case of closed-source models, it may be that access to the model is limited in some way (e.g., to registered users), but it should be possible for other researchers to have some path to reproducing or verifying the results.

5. Open access to data and code

Question: Does the paper provide open access to the data and code, with sufficient instructions to faithfully reproduce the main experimental results, as described in supplemental material?

Answer: [Yes]

Justification: All datasets (MNIST, CIFAR-10, Fashion-MNIST) are public; an anonymized PyTorch implementation and run scripts will be included in the supplemental ZIP.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.

- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. Experimental setting/details

Question: Does the paper specify all the training and test details (e.g., data splits, hyper-parameters, how they were chosen, type of optimizer, etc.) necessary to understand the results?

Answer: [\[Yes\]](#)

Justification: Appendix B lists optimizer, batch size, epochs, and random-seed protocol for each dataset.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The experimental setting should be presented in the core of the paper to a level of detail that is necessary to appreciate the results and make sense of them.
- The full details can be provided either with the code, in appendix, or as supplemental material.

7. Experiment statistical significance

Question: Does the paper report error bars suitably and correctly defined or other appropriate information about the statistical significance of the experiments?

Answer: [\[Yes\]](#)

Justification: Figure 2 (page 14) shows mean $\pm$ 1s.d.v. over five random seeds for each noise ratio; the caption clarifies what the shaded region represents.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).
- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error of the mean.
- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. Experiments compute resources

Question: For each experiment, does the paper provide sufficient information on the computer resources (type of compute workers, memory, time of execution) needed to reproduce the experiments?

Answer: [\[No\]](#)

Justification: The proof-of-concept experiments run on a single commodity GPU, but exact hardware specifications and wall-clock times are not reported.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The paper should indicate the type of compute workers CPU or GPU, internal cluster, or cloud provider, including relevant memory and storage.
- The paper should provide the amount of compute required for each of the individual experimental runs as well as estimate the total compute.
- The paper should disclose whether the full research project required more compute than the experiments reported in the paper (e.g., preliminary or failed experiments that didn't make it into the paper).

9. Code of ethics

Question: Does the research conducted in the paper conform, in every respect, with the NeurIPS Code of Ethics <https://neurips.cc/public/EthicsGuidelines>?

Answer: [Yes]

Justification: The work is purely theoretical/empirical on public data; no ethical concerns were identified (Impact Statement, line 361).

Guidelines:

- The answer NA means that the authors have not reviewed the NeurIPS Code of Ethics.
- If the authors answer No, they should explain the special circumstances that require a deviation from the Code of Ethics.
- The authors should make sure to preserve anonymity (e.g., if there is a special consideration due to laws or regulations in their jurisdiction).

10. Broader impacts

Question: Does the paper discuss both potential positive societal impacts and negative societal impacts of the work performed?

Answer: [Yes]

Justification: The Impact Statement (lines 361–363) argues that the work is foundational and poses no immediate societal risk.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.
- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. Safeguards

Question: Does the paper describe safeguards that have been put in place for responsible release of data or models that have a high risk for misuse (e.g., pretrained language models, image generators, or scraped datasets)?

Answer: [NA]

Justification: No high-risk models or new datasets are released; only small proof-of-concept code is provided.

Guidelines:

- The answer NA means that the paper poses no such risks.
- Released models that have a high risk for misuse or dual-use should be released with necessary safeguards to allow for controlled use of the model, for example by requiring that users adhere to usage guidelines or restrictions to access the model or implementing safety filters.
- Datasets that have been scraped from the Internet could pose safety risks. The authors should describe how they avoided releasing unsafe images.
- We recognize that providing effective safeguards is challenging, and many papers do not require this, but we encourage authors to take this into account and make a best faith effort.

12. Licenses for existing assets

Question: Are the creators or original owners of assets (e.g., code, data, models), used in the paper, properly credited and are the license and terms of use explicitly mentioned and properly respected?

Answer: [Yes]

Justification: Standard datasets are cited in Appendix B; each dataset carries a permissive academic license.

Guidelines:

- The answer NA means that the paper does not use existing assets.
- The authors should cite the original paper that produced the code package or dataset.
- The authors should state which version of the asset is used and, if possible, include a URL.
- The name of the license (e.g., CC-BY 4.0) should be included for each asset.
- For scraped data from a particular source (e.g., website), the copyright and terms of service of that source should be provided.
- If assets are released, the license, copyright information, and terms of use in the package should be provided. For popular datasets, paperswithcode.com/datasets has curated licenses for some datasets. Their licensing guide can help determine the license of a dataset.
- For existing datasets that are re-packaged, both the original license and the license of the derived asset (if it has changed) should be provided.
- If this information is not available online, the authors are encouraged to reach out to the asset's creators.

13. New assets

Question: Are new assets introduced in the paper well documented and is the documentation provided alongside the assets?

Answer: [NA]

Justification: The work does not introduce new datasets, models, or benchmarks.

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.

- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. Crowdsourcing and research with human subjects

Question: For crowdsourcing experiments and research with human subjects, does the paper include the full text of instructions given to participants and screenshots, if applicable, as well as details about compensation (if any)?

Answer: [NA]

Justification: No human subjects or crowdsourcing involved.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Including this information in the supplemental material is fine, but if the main contribution of the paper involves human subjects, then as much detail as possible should be included in the main paper.
- According to the NeurIPS Code of Ethics, workers involved in data collection, curation, or other labor should be paid at least the minimum wage in the country of the data collector.

15. Institutional review board (IRB) approvals or equivalent for research with human subjects

Question: Does the paper describe potential risks incurred by study participants, whether such risks were disclosed to the subjects, and whether Institutional Review Board (IRB) approvals (or an equivalent approval/review based on the requirements of your country or institution) were obtained?

Answer: [NA]

Justification: No human-subject study carried out.

Guidelines:

- The answer NA means that the paper does not involve crowdsourcing nor research with human subjects.
- Depending on the country in which research is conducted, IRB approval (or equivalent) may be required for any human subjects research. If you obtained IRB approval, you should clearly state this in the paper.
- We recognize that the procedures for this may vary significantly between institutions and locations, and we expect authors to adhere to the NeurIPS Code of Ethics and the guidelines for their institution.
- For initial submissions, do not include any information that would break anonymity (if applicable), such as the institution conducting the review.

16. Declaration of LLM usage

Question: Does the paper describe the usage of LLMs if it is an important, original, or non-standard component of the core methods in this research? Note that if the LLM is used only for writing, editing, or formatting purposes and does not impact the core methodology, scientific rigorousness, or originality of the research, declaration is not required.

Answer: [NA]

Justification: No LLMs are used in the method, only in standard writing support tools.

Guidelines:

- The answer NA means that the core method development in this research does not involve LLMs as any important, original, or non-standard components.
- Please refer to our LLM policy (<https://neurips.cc/Conferences/2025/LLM>) for what should or should not be described.