O(n) Connections are Expressive Enough: Universal Approximability of Sparse Transformers

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Abstract

Transformer networks use pairwise attention to compute contextual embeddings of inputs, and have redefined the state of the art in many NLP tasks. However, these models suffer from quadratic computational cost in the input sequence length \( n \) to compute attention in each layer. This has prompted recent research into faster attention models, with a predominant approach involving sparsifying the connections in the attention layers. While empirically promising for long sequences, fundamental questions remain unanswered: Can sparse transformers approximate any arbitrary sequence-to-sequence function, similar to their dense counterparts? How does the sparsity pattern and the sparsity level affect their performance? In this paper, we address these questions and provide a unifying framework that captures existing sparse attention models. Our analysis proposes sufficient conditions under which we prove that a sparse attention model can universally approximate any sequence-to-sequence function. Surprisingly, our results show the existence of models with only \( O(n) \) connections per attention layer that can approximate the same function class as the dense model with \( n^2 \) connections. Lastly, we present experiments comparing different patterns/levels of sparsity on standard NLP tasks.

1 Introduction

Transformer networks [24] and their variants [26] have played a key role in the recent advancement of the state of the art in many natural language processing tasks, such as machine translation [24], language modeling [20, 21], and question answering [10, 16, 26]. The key component of these networks is the self-attention layer, which updates the embeddings of the input tokens based on their context. Clark et al. [6], Coenen et al. [7] use probing tasks and show that self-attention layers in trained Transformer models compute embeddings that have substantial linguistic knowledge, and excel at several semantic and syntactic tasks. Naturally, the self-attention layer also plays the key role in the analysis of Transformers [2, 3, 12, 17, 28]; for example, Yun et al. [28] show that Transformers can approximate any continuous sequence-to-sequence functions (i.e., universal approximation), by proving that self-attention layers can compute contextual mappings of the input embeddings.

On the other hand, the self-attention layer is also the main bottleneck in scaling these models. It involves computation of pairwise inner products between input tokens, which results in quadratic computational complexity \( O(n^2) \) in the length of the input sequence \( n \). To mitigate this issue, researchers have developed methods to sparsify the pairwise interactions/connections in self-attention layers to reduce the computational complexity and/or improve model interpretability, and have shown successful empirical results on tasks with long sequence lengths [1, 5, 8, 9, 11, 15, 19, 22, 23, 27, 29]. For example, Child et al. [5] propose sparse Transformers for sequence generation. One of the sparsity patterns considered in [5] is the STRIDED pattern, where the sparse
attention layers alternate between two patterns: each token attends to only i) \( w \) local neighbors, and then ii) one after every \( w \) tokens in a strided manner. By choosing \( w = O(\sqrt{n}) \), they propose sparse attention layers with \( O(n^{3/2}) \) connections and show improvements on both speed and performance over the dense Transformer.

In the existing results, the rule of thumb while designing sparsity patterns (e.g., Strided) is connectivity; the intuition is that if each token can attend to the other tokens in multiple “hops,” then the resulting sparse Transformers do not lose much expressive power. However, there has been no formal justification for this intuition. How does sparsifying the interaction in the self-attention layers affect the model’s expressive power and ability to learn? What are the sparsity levels at which the model still retains its rich expressive power, and how is it affected by the sparsity pattern? Such fundamental questions about sparse attention models still remain unanswered.

1.1 Summary of contributions

In this paper, we take the first step towards a theoretical understanding of sparse Transformers.

- We propose a unified framework to analyze sparse Transformers, which generalizes the existing approaches that sparsify attention layers (§3.1).
- We propose a set of intuitive conditions on the sparsity pattern (Assumption 1) and the probability map (Assumption 2). Then, in Theorem 1, we show that Sparse Transformers, of fixed width and arbitrary depth, satisfying these conditions are universal approximators of any continuous sequence-to-sequence functions (§3.2 and §3.3).
- We next show some examples of existing sparse Transformers \([1, 5, 8, 9, 11, 29]\) that satisfy these conditions, and hence have universal approximability (§3.4). Surprisingly, we show that there are sparse Transformers with only \( O(n) \) connections per self-attention layer (instead of \( n^2 \)) that have enough expressive power to approximate arbitrary continuous functions (Corollary 2).
- We report experimental results on standard NLP tasks using sparse Transformers, comparing different sparsity patterns/levels (§5).

2 Preliminaries and related works

In this section, we summarize the notation we will use throughout the paper, give a brief overview of Transformers, and then discuss existing efforts to sparsify the self-attention mechanism.

2.1 Notation

For a positive integer \( a \), we denote \([a] = \{1, 2, \ldots, a\}\). For any vector \( v \in \mathbb{R}^d \), let \( v_j \) denote its \( j \)-th coordinate. For any matrix \( A \in \mathbb{R}^{d \times n} \), let \( A_j \) denote its \( j \)-th column, and \( A_S \) denote the submatrix consisting of columns of \( A \) in an index set \( S \subseteq [n] \). We use \( \|A\|_p \) to denote the entry-wise \( \ell^p \) norm of \( A \). Let \( c_S(\cdot) \) be the softmax operator, which takes a matrix as input and applies softmax operation to each column of the matrix, which results in a column stochastic matrix.

2.2 Transformers and their universal approximation power

A Transformer network, consisting of multiple layers of Transformer blocks, implements a sequence-to-sequence function that maps \( \mathbb{R}^{d \times n} \) to \( \mathbb{R}^{d \times n} \). A Transformer Block (TB) consists of two layers: a self-attention layer and a token-wise feed-forward layer, and both layers have an identity skip connection. More concretely, for an input \( X \in \mathbb{R}^{d \times n} \) consisting of \( d \)-dimensional embeddings of \( n \)
tokens, a Transformer block consists of the following two layers:

\[
\text{Attn}(X) = X + W_O \begin{bmatrix} \text{Head}^1(X) \\ \vdots \\ \text{Head}^h(X) \end{bmatrix}; \quad \text{Head}^i(X) = W^i_V X \cdot \sigma_S[(W^i_K X)^T W^i_Q X]
\]  

(1a)

\[
\text{TB}(X) = \text{Attn}(X) + W_2 \cdot \text{ReLU}(W_1 \cdot \text{Attn}(X)),
\]  

(1b)

where \( W_O \in \mathbb{R}^{d \times m_h}, W_V^i, W_K^i, W_Q^i \in \mathbb{R}^{m \times d}, W_2 \in \mathbb{R}^{d \times r}, \) and \( W_1 \in \mathbb{R}^{r \times d} \). Although our analysis and experiments rely on bias vectors, we omit those in (1) for simplicity.

To endow the network with information about the position of input tokens, it is common to add a positional embedding \( E \in \mathbb{R}^{d \times n} \) to the input \( X \) before feeding it to the network. The positional embedding \( E \) can be fixed [24] or trainable [10]; we consider the latter. Using a trainable \( E \), \( \mathcal{T}^{h,m,r} \) is defined to be a class of functions of the form \( X \mapsto t(X + E) \), where \( t \) is a composition of an any number of Transformer blocks with \( h \) attention heads of head size \( m \), and hidden layers of width \( r \). Thus, \( \mathcal{T}^{h,m,r} \) is a class of Transformers with a fixed width while the depth can be arbitrary.

Further, let \( \mathcal{F} \) be the class of continuous functions \( f : \mathbb{D} \rightarrow \mathbb{R}^{d \times n} \) defined on any compact domain \( \mathbb{D} \subset \mathbb{R}^{d \times n} \), where continuity is defined with respect to the entry-wise \( \ell_p \) norm (\( 1 \leq p < \infty \)). Yun et al. [28, Theorem 3] show that \( \mathcal{T}^{2,1,4} \) can universally approximate \( \mathcal{F} \). More precisely, for any \( f \in \mathcal{F} \), \( \epsilon > 0 \) and \( 1 \leq p < \infty \), there exists a function \( g \in \mathcal{T}^{2,1,4} \) such that \( d_p(f, g) := (\int_\mathbb{D} \|f(X) - g(X)\|_p^p dX)^{1/p} \leq \epsilon \).

### 2.3 Sparse Transformers

As seen in Eq. (1a), the self-attention layer involves computing the inner product between each pair of tokens, which we will refer to as the **attention score matrix** \( A^i := (W^i_K X)^T W^i_Q X \in \mathbb{R}^{n \times n} \). This leads to quadratic computational complexity in \( n \), which makes it expensive to apply Transformers to tasks with long sequence lengths. To mitigate this problem, one of the predominant approaches is to **sparsify** the interactions in the self-attention layers, which can be sub-classified into three categories.

The first category reduces computation by making \( A^i \) sparse in a **pre-determined** manner. Each token in the sequence only attends to a fixed smaller set of other tokens instead of the whole sequence [1, 5, 19]. In some papers, auxiliary tokens are added to improve connectivity between existing tokens while maintaining sparsity [11, 27]. One drawback of these approaches is that the sparsity pattern is independent of input, so it cannot adapt to the data. To remedy this issue, [23] proposes to learn local attention span from data.

The second category studies making \( A^i \) sparse after the full \( A^i \) has been computed [8, 9, 29]. Here, the focus is not on the computational gain via sparsity, because the full score matrix \( A^i \) has to be computed first; rather, the goal here is to make attention layers more interpretable, as well as to improve performance. This line of works modifies \( \sigma_S \) in (1a) to other probability maps, by using top-\( k \) elements or adopting sparser variants such as sparselin-gen or \( \alpha \)-entmax [14, 18]. Compared to the first category, this approach has an advantage that sparsity patterns are adaptive to data.

The last category attempts to get the best of both worlds. This line of works tries to learn sparsity patterns from data using extra components predicting the connection between tokens, e.g., \( k \)-means clustering [22], LSTM [15], or locality-sensitive hashing [13]. This way, one can adaptively determine the sparsity patterns before computing the score matrix. However, the drawback of this approach is that one needs extra computation to train/run these additional components, which may be expensive.
3 Universal approximation theorem for sparse Transformers

In this section, we derive a unifying framework to study sparse Transformers. We then propose a set of conditions on the sparse self-attention layers, and prove that the sparse Transformers satisfying these conditions are universal approximators of any continuous sequence-to-sequence functions. Finally, we show some examples of existing sparse Transformers that satisfy these conditions.

3.1 A unifying framework for sparse Transformers

We modify the Transformer block in (1) to the following sparse Transformer block (STB):

\[
\text{SAttn}^l(X) = X + W_O \begin{bmatrix} S\text{Head}^{1,l}(X) \\ \vdots \\ S\text{Head}^{h,l}(X) \end{bmatrix}, \quad \text{SHead}^{i,l}(X)_k = W^i_k X_{A^i_k} \cdot \rho \left[ (W^i_k X_{A^i_k})^T W^i_Q X_k \right]
\]

\[
\text{STB}^l(X) = \text{SAttn}^l(X) + W_2 \cdot \text{ReLU}(W_1 \cdot \text{SAttn}^l(X)),
\]

where the sets \(A^i_k \subseteq [n]\), for \(k \in [n]\) and \(l \in [p]\), define the \(p\) sparsity patterns (formally defined below), which are indexed by \(l \in [p]\). Moreover, the parameter dimensions stay the same as in (1).

Note that there are three main modifications from the dense Transformer.

- (Cycling blocks) There are superscripts \(l \in [p]\) added to the symbols such as SAttn. Unlike dense Transformers, some sparse Transformers cycle through \(p\) different patterns. For example, the STRIDED pattern [5] described in § 1 alternates between two different patterns, which corresponds to \(p = 2\). We add the superscript \(l\) to include such cases in our formulation. We assume that the layers in a sparse Transformer cycle through STB\(^1, \ldots, \text{STB}^p\).

- (Sparsity patterns) Note that SHead\(^{i,l}(X)_k\) denotes the \(k\)-th column of the \(i\)-th sparse attention head. Unlike dense Transformers, the inner product of the \(k\)-th query vector \(W^i_Q X_k\) is taken only with \(W^i_k X_{A^i_k}\), the key vectors of tokens in the set \(A^i_k \subseteq [n]\). Hence, instead of all \(n\) tokens, the \(k\)-th token computes attention scores with only tokens in \(A^i_k\). For \(l \in [p]\), we refer to the collection of the index sets \(\{A^i_k\}_{k \in [n]}\), or simply \(\{A^i_k\}\), as a sparsity pattern. As a result, SHead\(^{i,l}(X)_k\) is a linear combination of columns in \(W^i_k X_{A^i_k}\), rather than the whole sequence.

- (Probability map) After computing the attention score matrix, the dense Transformer (1) uses the softmax operator \(\sigma_\rho\) to get a column stochastic matrix. In the sparse Transformers, we generalize \(\sigma_\rho\) to \(\rho\). The probability map \(\rho\) is any map that takes a matrix as input and outputs a column stochastic matrix.

As a sanity check, by choosing \(p = 1\), \(A^i_k = [n]\) for all \(k \in [n]\), and \(\rho = \sigma_\rho\), we recover the dense Transformer. Note also that the sparse Transformer formulation covers the first and second categories of existing results discussed in § 2.3. The first category corresponds to choosing a predetermined sparsity pattern(s) \(\{A^i_k\}\), while setting \(\rho = \sigma_\rho\). The second category corresponds to opting for a probability map \(\rho\) other than softmax \(\sigma_\rho\), while maintaining \(A^i_k = [n]\) for all \(k \in [n]\).

In this paper, we assume for simplicity that all sparse attention heads SHead\(^{1,l}, \ldots, \text{SHead}^{h,l}\) in a single layer have identical sparsity patterns \(\{A^i_k\}\). However, since our result only requires two sparse attention heads per layer (as we will see in Theorem 1), our result can be easily extended to the case that allows multiple sparsity patterns in a single layer.

Similar to \(T^{h,m,j}\) in § 2.2, we define the class of functions represented by sparse Transformers. We hide the dependence of this class on the sparsity patterns and probability map to simplify the
notation.

\[ ST^{h,m,r} := \{ X \mapsto t(X + E) \mid t \text{ is a composition of cycling sparse Transformer blocks } STB^i, \]
\[ \text{each with } h \text{ heads of head size } m \text{ and hidden layer size } r, \]
\[ \text{and positional embedding } E \in \mathbb{R}^{d \times u} \text{ is trainable} \}. \quad (3) \]

### 3.2 Conditions on sparsity patterns and probability map

In this section, we define a set of conditions on the sparsity patterns \( \{A_k^l\} \) and the probability map \( \rho \) that ensures that the sparse Transformer universally approximate the function class \( \mathcal{F} \) (cf. § 2.2).

For \( k \in [n] \) and the index sets \( \{A_k^l\}_{l \in [p]} \), we define a sequence of sets \( \{S_k^l\}_{l \geq 1} \) in a recursive way:

\[ S_k^1 := A_k^1, \quad S_k^l := \bigcup_{j \in A_k^{l-1}} S_{j}^{l-1}. \]

The set \( S_k^l \) is the set of all tokens that the \( k \)-th token can directly/indirectly attend to, after \( t \) sparse attention layers with sparsity patterns cycling through \( \{A_k^1\}, \{A_k^2\}, \ldots, \{A_k^p\} \). We now state our conditions on sparsity patterns.

**Assumption 1.** The sparsity patterns \( \{A_k^l\} \) satisfy the following:

1. For all \( k \in [n] \) and \( l \in [p] \), we have \( k \in A_k^l \).
2. There exists a permutation \( \gamma : [n] \to [n] \) such that, for all \( i \in [n-1] \), \( \gamma(i) \in \bigcup_{t=1}^{p} A_{\gamma(i+1)}^l \).
3. There exists a finite \( s \in \mathbb{N} \) such that \( s = \min \{ u \mid S_k^u = [n] \text{ for all } k \in [n] \} \).

Assumption 1.1 requires the existence of a chain of \( \gamma \) that covers all \( n \) nodes in \( \mathbb{N} \); note that the set \( \bigcup_{t=1}^{p} A_{\gamma(i+1)}^l \) is the set of all tokens that the \( \gamma(i+1) \)-th token directly attends to. To elaborate more about the chain, consider a directed graph with \( n \) vertices corresponding to the \( n \) tokens. For any \( j \in \bigcup_{t=1}^{p} A_{\gamma(i+1)}^l \), we add a directed edge \( j \to k \). Given a graph constructed this way, Assumption 1.2 requires that the graph has a Hamiltonian path \( \gamma(1) \to \gamma(2) \to \cdots \to \gamma(n) \). Assumption 1.3 requires that after \( s \) sparse attention layers, every token can attend to all the other tokens, either directly or indirectly.

We now state the assumption on the probability map \( \rho[\cdot] \). For this, we define \( \sigma_{\mathbf{H}}[\cdot] \) to be the hardmax operator, which outputs the one-hot representation of the arg-max entry for each column of the input matrix. Since both \( \rho \) and \( \sigma_{\mathbf{H}} \) are column-wise operators that output column-stochastic matrices, we state the assumption for the operation of \( \rho \) on a single column.

**Assumption 2.** For any \( \zeta > 0 \) and \( \eta \in (0,1) \), \( \exists t > 0 \) such that, for any column input \( v \) satisfying \( v_j - \max_{j \neq j^*} v_j \geq \zeta \) (where \( j^* = \arg \max_j v_j \)), we have \( \rho[\mathbf{v}]_j \geq 1 - \eta \) and \( \sum_{j \neq j^*} \rho[\mathbf{v}]_j \leq \eta \).

Assumption 2 requires that, for inputs that have some margin between the unique maximum entry and the other entries, \( \rho[\cdot] \) can closely approximate the behavior of the hardmax operator by scaling its input by a positive factor \( t \). This assumption is satisfied by softmax \( \sigma_5 \) and other sparse variants such as sparselin-gen and \( a \)-entmax, as we show in § B of the supplementary material.

It is straightforward to check that the dense Transformer, which corresponds to \( p = 1 \), \( A_k^1 = [n] \), and \( \rho[\cdot] = \sigma_5[\cdot] \) in our framework, satisfies both Assumptions 1 and 2.
3.3 Sparse Transformers are universal approximators

We now state our main theorem, which shows that if the sparsity patterns \( \{A^1_k\} \) and the probability map \( \rho \) satisfy Assumptions 1 and 2, sparse Transformers with \( h = 2 \) attention heads of size \( m = 1 \), and hidden layer width \( r = 4 \) are universal approximators of continuous sequence-to-sequence functions on any compact domain (recall that \( \mathcal{F} \) denotes the class of such continuous functions).

**Theorem 1.** Consider any \( f \in \mathcal{F} \), and the class of sparse Transformers \( ST^{2,1,4} \) (cf. (3)) with the underlying sparse attention layers satisfying Assumptions 1 and 2. Then, for any \( \epsilon > 0 \) and \( 1 \leq p < \infty \), there exists a function \( g \in ST^{2,1,4} \) such that

\[
d_p(f, g) := \left( \int_{\mathcal{D}} \|f(X) - g(X)\|_p^p dX \right)^{1/p} \leq \epsilon.
\]

As discussed earlier, dense Transformers do satisfy Assumptions 1 and 2. Thus, Theorem 1 subsumes the existing result [28] for dense Transformers. Also, we note that the required width parameters \( h, m, \) and \( r \) in Theorem 1 are completely independent of \( d, n, \) or the sparsity patterns.

The key justifying intuition for adopting sparse attention layers is that, if each token can attend to the other tokens in multiple hops\(^1\), then these models do not lose too much expressive power. However, there has been no formal justification for this intuition. Our theorem provides the first formal evidence that well-designed sparse attention layers do not limit Transformer’s universal approximation power. In §3.4, we show a surprising result that there exist sparse self-attention layers with only \( O(n) \) connections (as opposed to \( n^2 \) connections in regular self-attention layers) that retain enough expressive power to approximate \( \mathcal{F} \). This advantage of sparse Transformers over their dense counterpart becomes even stronger with increasing sequence length \( n \), providing a theoretical support for the adoption of sparsity for the tasks with long sequence lengths.

We provide a high-level proof sketch of Theorem 1 in §4.1. Although the outline of the proof is similar to [28], the sparsity in attention mechanism and the choice of general probability map \( \rho \) pose nontrivial challenges in extending the existing result to our setting. We detail these challenges and briefly describe how we overcome them in §4.2.

3.4 Analysis of existing sparse Transformers

By Theorem 1, any sparse Transformer that satisfies our Assumptions 1 and 2 has universal approximation ability. In this section, we give some examples of such sparse Transformers.

Child et al. [5] propose two kinds of 2-step sparsity patterns (i.e., \( p = 2 \)) for sequence generation tasks, namely **strided** and **fixed** patterns. We consider the extension of their autoregressive patterns (i.e., attending only to past tokens) to the whole sequence. In the **strided** pattern, a token first attends to its \( w \) neighbors and then attends to one token after every \( w \) tokens in a strided manner. The sparsity pattern for the \( k \)-th token reads

\[
A^1_k = [n] \cap \{ k - \lfloor w/2 \rfloor, \ldots, k - 1, k, k + 1, \ldots, k + \lfloor w/2 \rfloor \},
\]

\[
A^2_k = [n] \cap \{ \ldots, k - 2w, k - w, k + w, k + 2w, \ldots \}.
\]

In the **fixed** pattern, we divide the token into segments of length \( w \). A token in a segment has access to other tokens in the same segment, and then the last tokens of the other segments:

\[
A^1_k = [n] \cap \{ [k/w] \cdot w - w + 1, \ldots, [k/w] \cdot w \}, \quad A^2_k = [n] \cap (\{ k \} \cup \{ w, 2w, 3w, \ldots \}).
\]

The **strided** and **fixed** patterns satisfy both Assumption 1 and 2 for all values of \( w \). Specifically, Assumption 1.3 holds with \( s = 2 \), because any token can directly/indirectly access all the tokens

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\(^1\)Note that this corresponds to our Assumption 1.3.
in two hops. As for Assumption 1.2, the identity permutation \( \gamma(i) = i \) suffices to satisfy the assumption for both patterns. By choosing \( w = O(\sqrt{n}) \), sparse Transformers with the Strided and Fixed patterns achieve universal approximation power with \( O(n^{3/2}) \) connections per attention layer.

Guo et al. [11] consider the Star sparsity pattern where they add an auxiliary relay token that attends to all the tokens, and the other tokens attend only to \( 2w \) neighboring tokens and the relay token. There is only one sparsity pattern, so \( p = 1 \). The Star sparsity pattern can be written as

\[ A_k^1 = \{ n \} \cup \{ (i - 1) \mod (n - 1) + 1 \mid i \in \{ k - w, \ldots, k + w \} \} \quad \text{for} \quad k \in \{ n - 1 \}, \ A_n^1 = [n], \]

where \( w \geq 1 \). For any fixed \( w \), this sparse Transformer has \( O(n) \) connections per attention layer, and it satisfies both assumptions. Specifically, Assumption 1.2 is satisfied with the identity permutation, i.e., \( \gamma(i) = (i) \) for \( i \in [n] \). Since any token can access other tokens within two hops, Assumption 1.3 is satisfied with \( s = 2 \). This demonstrates that \( O(n) \) connections per layer suffice for sparse attention layers to have universal approximation power. One can similarly check that the sliding window sparsity patterns with/without global attention, proposed in Longformer [1], also satisfy the assumptions with \( O(n) \) connections. We state this interesting observation as a corollary below.

**Corollary 2.** There exist sparse Transformers with \( O(n) \) connections per self-attention layer that are universal approximators in the sense of Theorem 1.

Recall that another line of results that replaces softmax \( \sigma_S \) with sparse variants \( \rho \) [8, 9, 29] also fits into our formulation, with \( p = 1 \) and \( A_k^1 = [n] \). As we show in § B, these alternative \( \rho \)'s satisfy Assumption 2. Thus, by Theorem 1, these models also have the universal approximation property.

4 Proof sketch and discussion

4.1 Sketch of proof of Theorem 1

Now, we sketch the proof of Theorem 1, which consists of three steps. Throughout the proof, we assume without loss of generality that \( D \subset [0, 1)^{d \times n} \).

**Step 1.** In the first step, we approximate \( f \in \mathcal{F} \) with a piecewise constant function. Towards this, consider a class of piecewise constant functions \( \mathcal{F}(\delta) \) that map \( D \) to \( \mathbb{R}^{d \times n} \), where \( \delta > 0 \) and \( \delta^{-1} \) is an integer. Any function in \( \mathcal{F}(\delta) \) maps cubes of the form \( G + [0, \delta)^{d \times n} \) to matrices \( A_G \in \mathbb{R}^{d \times n} \), where \( G \in \{0, \delta, \ldots, 1 - \delta\}^{d \times n} \). We approximate \( f \) with a function \( \overline{f} \in \mathcal{F}(\delta) \) such that \( d_p(f, \overline{f}) \leq \epsilon / 2 \), by choosing small enough \( \delta \). We defer the statement and the proof to § C of the supplementary material.

**Step 2.** We then approximate \( \overline{f} \in \mathcal{F}(\delta) \) with a sparse Transformer network with a slightly different architecture. In this architecture, we replace ReLU in the feed-forward layer with any piecewise linear activation \( \phi \in \Phi \), where \( \Phi \) denotes the class of piecewise linear functions with three pieces. We also replace \( \rho \) in the sparse attention layer with the hardmax \( \sigma_H \) operator. We refer to the function class represented by the modified sparse Transformer as \( \mathcal{T}^{h,m,r} \). The next key result shows that any \( \overline{f} \in \mathcal{F}(\delta) \) can be *exactly* represented by the modified Transformer. See § D and § E in the supplementary material for the proof.

**Lemma 3.** For any \( \overline{f} \in \mathcal{F}(\delta) \), there exists \( \overline{\sigma} \in \mathcal{T}^{2,1,1} \) such that \( \overline{f}(X) = \overline{\sigma}(X) \) for all \( X \in D \).

**Step 3.** The final step is to approximate the function \( \overline{\sigma} \in \mathcal{T}^{2,1,1} \) with a sparse Transformer \( \sigma \in \mathcal{T}^{2,1,4} \). This is done by approximating \( \phi \) and \( \sigma_H \) with ReLU and \( \rho \), respectively, while carefully bounding the accumulation of errors introduced by the approximation. See § F in the supplementary material for the details.
Lemma 4. For $\overline{g} \in \overline{ST}^{2,1,1}$ in Lemma 3, there exists $g \in ST^{2,1,4}$ such that $d_p(\overline{g}, g) \leq \epsilon / 2$.

Combining these three steps, we establish that $d_p(f, g) \leq d_p(f, \overline{f}) + d_p(\overline{f}, \overline{g}) + d_p(\overline{g}, g) \leq \epsilon$. □

4.2 Key challenges in the proof
While the high level outline of the proof is similar to the one for dense Transformers [28], the proof in [28] crucially relies on having all connections for computing attention in each layer, which we do not have in sparse Transformers. Instead, we rely on the sparsity conditions (cf. Assumptions 1 and 2) to establish Theorem 1. We highlight the key differences below.

Establishing the Step 2 of the dense result [28] relies on constructing a contextual mapping using attention layers. A contextual mapping is a function that maps tokens in different sequences to unique values, thereby allowing Transformers to distinguish the same token appearing in different contexts. A crucial ingredient in the construction of such a mapping is a shift operation implemented with two attention heads in an attention layer. This shift operation involves each token taking the maximum and minimum over the entire sequence, which obviously cannot be done with sparse Transformers as it would require each token to attend to every other token in the sequence. We circumvent this issue by carefully choosing the positional embedding $E$ dependent on $\gamma$ (cf. Assumption 1.2), and ensuring that a similar shift operation is applied in a desired order even under sparsity.

As the final phase of the contextual mapping in [28], a single attention layer shifts the entire sequence by the maximum over the sequence. Again, this cannot be directly implemented due to sparsity. Using Assumption 1.3, we instead prove that by stacking $s$ sparse layers, one can successfully implement a similar operation that shifts the entire sequence by the maximum over the whole sequence, up to some controlled errors. This way, we overcome the difficulties posed by the sparsity and construct a new version of contextual mappings. The details can be found in § E.2 of the supplementary material.

Moreover, the proof of Step 3 in [28] uses the simple fact that softmax can approximate hardmax arbitrarily closely. Since we do not restrict ourselves to softmax and generalize the probability map, a more careful argument is required. Since there are many layers in the network $\overline{g}$, it turns out that approximating it with an original sparse Transformer in $ST^{2,1,4}$ requires carefully controlling the approximation errors accumulated over layers. The proof of Lemma 4 in § F of the supplementary material shows that this is indeed possible by utilizing Assumption 2.

5 Experiments
We now present our experimental study comparing different design and implementation choices, including sparsity patterns and levels, on three tasks: i) a synthetic copying task, ii) language modeling, and iii) translation. Our goal is to understand the effect of such choices while employing sparse Transformers to the tasks with small sequence lengths, complementing the existing results for sparse Transformers on long sequence tasks [5].

5.1 Experiment Settings
We consider four sparsity patterns: STRIDED (4), FIXED (5), STAR (6) and RANDOM. The first three patterns are proposed in [5] and [11]; we test them for different values of $w$. In case of the RANDOM pattern, given a sparsity level, we make connections uniformly at random. Following [5], STRIDED and FIXED patterns are tested for three different head configurations: i) SEQUENTIAL, where the sparse attention layers alternate between $\{A_k^1\}$ and $\{A_k^2\}$, as described in the previous sections; ii) UNION, where all sparse attention layers use the sparsity pattern $\{A_k^1 \cup A_k^2\}$; and iii) MULTITHEAD, where half of the attention heads in every attention layer use $\{A_k^1\}$ and the other half use $\{A_k^2\}$. 

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Table 1. Accuracy on the synthetic copying task. Percentages in parentheses mark the sparsity levels.

| Depth | Strided | Fixed |
|-------|---------|-------|
|       |union |multhead |sequential |union |multhead |sequential |
| 1-layer | 0.79% | 0.78% | 0.78% | 7.02% | 7.04% | 0.81% | 0.77% | 33.13% |
| 2-layer | 12.40% | 8.26% | 1.57% | 73.43% | 13.24% | 92.10% | 12.32% | 67.30% |
| 3-layer | 94.50% | 65.58% | 60.88% | 99.87% | 70.82% | 99.84% | 14.03% | 89.50% |
| 4-layer | 100% | 100% | 98.40% | 99.97% | 99.16% | 99.97% | 31.19% | 95.88% |

Figure 1. Comparison of sparsity patterns and different head configurations on the One Billion Benchmark (a language modeling task) and WMT en-cs (a translation task). Note that the number of connections in the attention layers goes down as we increase the sparsity level.

Note that, given the same sequence length, **Union** is less sparse than the other two configurations. Thus, to ensure fair comparisons, we compare different configurations based on their sparsity levels.

We use maximum sequence length 256 in all our experiments. For the copying task, we experiment with only one sparse Transformer block (cf. Eq (2)), with varying numbers of attention layers, where each attention layer has 4 attention heads. For the language modeling and the translation, we use the Tensor2Tensor [25] framework and employ 12-block and 6-block (respectively) Transformers with 8 attention heads per block. For more details of the setup, see § G of the supplementary material.

5.2 Results

**Copying task.** We consider a synthetic copying task proposed in [13], where the input sequence has the format 0s8s, where s is a 127 length sequence of symbols in [0, 127]. The models have to predict (copy) the second part, given the first half of the input. This task tests the ability of sparse Transformers to communicate the information. Table 1 presents the results for this task. Except for the **Star** and **Random** patterns, we can see that the networks learn to copy the sequences with four sparse attention layers. One possible explanation for the bad performance of **Star** is that, except for the relay token, it only attends to local neighbors while the task requires to copy distant tokens.

**Language modeling.** We conduct the language modeling experiments on the One Billion Word Benchmark [4] which has almost one billion tokens and a vocabulary of more than 800K unique tokens. In Figure 1a, we plot the perplexity against the sparsity level. We observe that the **Strided** pattern and the **Star** achieve the best performance across all sparsity levels. For both the **Strided** and **Fixed** patterns, the **Union** configuration shows the best performance.
Translation. For the translation task, we train the model on WMT18 English-Czech (en-cs) dataset and test it on the Newstest 2015 dataset. We plot the BLEU score against the sparsity level in Figure 1b. We apply the same sparsity pattern to both the encoder and the decoder. The Strided and Fixed patterns with UNION configuration show the best scores, which are similar to the dense attention. The UNION configuration is also the least sensitive to the sparsity levels.

Discussion. In both language modeling and translation, the RANDOM pattern performs significantly worse than the deterministic patterns, demonstrating the need for a careful design of sparsity patterns. Overall, our experiments suggest that the design of the optimal sparsity patterns is dependent on specific tasks. For example, the STAR pattern shows the best performance on the language modeling task, while having trouble with copying and translation. Among the three head configurations tested for STRIDED and FIXED, the UNION performs the best in all tasks and is also insensitive to sparsity levels, possibly because it suffers less from the “unbalance” between $|A^{1}_k| = O(w)$ and $|A^{2}_k| = O(n/w)$ (cf. Eqs (4) and (5)).

6 Conclusion
Recently, sparse Transformers have received a lot of attention as they enable more efficient/faster attention mechanisms for the tasks with very long sequence lengths. We take an initial step to provide a theoretical understanding of these models. We provide a unifying framework that captures existing sparse attention models, and prove a universal approximation theorem for sparse Transformers which holds under intuitive conditions on sparsity patterns and probability maps. We also carry out experiments comparing different sparsity patterns and levels on standard NLP tasks. We hope that this work will shed light on the understanding of sparsity in attention layers, and provide guidance for the design of sparse attention models.

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A Outline and notation

The supplementary material is organized as follows. First, § B proves that the softmax operator as well as its sparse versions indeed satisfy Assumption 2. Next, § C provides formal statements of Step 1 in the proof sketch (§ 4.1). The outline of proof of Lemma 3 (Step 2 in the proof sketch) is presented in § D, followed by a separate section (§ E) proving the three key sublemmas in the proof. The proof of Step 3, Lemma 4, is given in § F. Lastly, § G presents the detailed setup of our experiments.

We next review some of the notation and also introduce additional notation used throughout the supplementary material. For a positive integer \( a \), let \( [a] := \{1, \ldots, a\} \). For \( a, b, c \in \mathbb{R} \) where \( b - a > 0 \) is an integer multiple of \( c > 0 \), we write \( [a : c : b] := \{a, a + c, a + 2c, \ldots, b - c, b\} \). For any matrix \( A \in \mathbb{R}^{d \times n} \), let \( A_j \) denote its \( j \)-th column, and \( A_S \) denote the submatrix consisting of columns of \( A \) in the index set \( S \subseteq [n] \). We also use \( A_{ij} \) to denote its \((i,j)\)-th entry. Let \( I \{ \cdot \} \) be the 0-1 indicator for an event. Let \( 1_n \in \mathbb{R}^n \) be a vector whose components are all 1.

B Sparse probability maps satisfy Assumption 2

In this section, we show that the softmax operator \( \sigma_S \) as well as the probability maps \( \rho \) used to replace softmax in the existing approaches, namely softmax with only top-\( k \) inputs [29], sparselngen [9], and \( \alpha \)-entmax [8], all satisfy Assumption 2. We restate the assumption for reader’s convenience:

Assumption 2. For any \( \zeta > 0 \) and \( \eta \in (0, 1] \), \( \exists \ t > 0 \) such that, for any column input \( v \) satisfying \( v_j - \max_{j \neq j^*} v_j \geq \zeta \) (where \( j^* = \arg\max_j v_j \)), we have \( \rho[tv]_j \geq 1 - \eta \) and \( \sum_{j \neq j^*} \rho[tv]_j \leq \eta \).

As in the assumption, we only consider the operation of these probability maps on a single vector, as they are applied column-wise. For each of the probability maps, we will show that for any \( \zeta > 0 \) and \( \eta \in (0, 1] \), we can choose \( t > 0 \) that satisfies the conditions of Assumption 2.

B.1 Softmax & softmax with top-\( k \) inputs

Given an input vector \( v \in \mathbb{R}^n \), the \( j \)-th coordinate of the output of softmax \( \sigma_S[v] \) is defined as

\[
\sigma_S[v]_j := \frac{\exp(v_j)}{\sum_{i=1}^{n} \exp(v_i)}.
\]

We assume without loss of generality that the entry of \( v \) is in decreasing order, where the first two entries satisfy \( v_1 - v_2 \geq \zeta \). For any such \( \zeta > 0 \) and any \( 0 < \eta \leq 1 \), our aim is to show the existence of \( t > 0 \) such that \( \sigma_S[1tv]_1 = \frac{\exp(tv_1)}{\sum_{i=1}^{n} \exp(tv_i)} \geq 1 - \eta \). Then, \( \sum_{j=2}^{n} \sigma_S[1tv]_j \leq \eta \) follows.

Now, since \( v_i \leq v_1 - \zeta \) for \( i \in [2 : n] \), note that

\[
\sigma_S[1tv]_1 = \frac{\exp(tv_1)}{\sum_{i=1}^{n} \exp(tv_i)} \geq \frac{\exp(tv_1)}{\exp(tv_1) + (n - 1) \exp(tv_1 - t\zeta)} = \frac{1}{1 + (n - 1) \exp(-t\zeta)}.
\]

Since \( \frac{1}{1 + (n - 1) \exp(-t\zeta)} \) is an increasing function in \( t > 0 \), one can increase \( t \) sufficiently large to make it greater than \( 1 - \eta \).

The same argument holds for the softmax with top-\( k \) inputs, used in [29]. By the assumption on \( v \), entries \( v_1, \ldots, v_k \) are the top \( k \) components. Thus,

\[
\rho[1tv]_1 \geq \frac{1}{1 + (k - 1) \exp(-t\zeta)} \geq 1 - \eta
\]

can be satisfied by choosing large enough \( t > 0 \).
B.2 Sparselin-gen

We now consider the case where $\rho$ is sparselin-gen [14], which was used to sparsify the attention score matrices in [9]. Given a regularization parameter $\lambda \in [0,1)$, the sparselin-gen used in [9] is defined as

$$
\rho[v] := \arg\min_{p \in \Delta^{n-1}} \|p - v\|^2 - \lambda \|p\|^2,
$$

where $\Delta^{n-1} := \{ p \in \mathbb{R}^n \mid p \geq 0, \sum_{i=1}^n p_i = 1 \}$ is the probability simplex. Then, the solution for optimization problem above can be written as

$$
\rho[v]_j = \max \left\{ 0, \frac{v_j - \tau(v)}{1 - \lambda} \right\}, \text{ for } j \in [n],
$$

where $\tau : \mathbb{R}^n \to \mathbb{R}$ is a threshold function that chooses the threshold $\tau(v)$ such that $\sum_{j=1}^n \rho[v]_j = 1$.

Now, assume without loss of generality that the entry of $v$ is in decreasing order, where the first two entries satisfy $v_1 - v_2 > \zeta$. For any such $\zeta > 0$ and any $0 < \eta < 1$, our aim is to show the existence of $t > 0$ such that $\rho[tv]_1 \geq 1 - \eta$. This is done by choosing $t = \frac{1-\eta}{\zeta}$. To see this, notice that if $v_j$’s are in decreasing order, then $\rho[v]_j$ are also in decreasing order. Now consider

$$
\rho[tv]_1 = \max \left\{ 0, \frac{tv_1 - \tau(tv)}{1 - \lambda} \right\}, \quad \rho[tv]_2 = \max \left\{ 0, \frac{tv_2 - \tau(tv)}{1 - \lambda} \right\}.
$$

If $\rho[tv]_2 = 0$, then $\rho[tv]_j = 0$ for all $j = 3, \ldots, n$, and $\rho[tv]_1 = 1 \geq 1 - \eta$. If $\rho[tv]_2 > 0$, then

$$
\rho[tv]_1 - \rho[tv]_2 = \frac{tv_1 - \tau(tv)}{1 - \lambda} - \frac{tv_2 - \tau(tv)}{1 - \lambda} = t(v_1 - v_2) - t(v_1 - v_2) \geq t\zeta = 1 - \eta.
$$

B.3 $\alpha$-entmax

Next, we consider the case where $\rho$ is $\alpha$-entmax [18], which was used to sparsify the attention score matrices in [8]. Given a parameter $\alpha \geq 1$, the $\alpha$-entmax is defined as

$$
\rho[v] := \arg\max_{p \in \Delta^{n-1}} p^T v + H_\alpha(v),
$$

where $\Delta^{n-1}$ is the probability simplex and $H_\alpha$ is the Tsallis continuous family of entropies

$$
H_\alpha(v) := \begin{cases}
\frac{1}{\alpha(a-1)} \sum_j v_j - \frac{\alpha}{a} v^a & \alpha > 1, \\
- \sum_j v_j \log v_j & \alpha = 1.
\end{cases}
$$

As shown in [8], the solution of $\alpha$-entmax is equal to softmax if $\alpha = 1$, and otherwise ($\alpha > 1$) it is given in the form

$$
\rho[v]_j = \left( \max\{0, (\alpha - 1)v_j - \tau(v)\} \right)^{1/\alpha}, \text{ for } j \in [n],
$$

where $\tau : \mathbb{R}^n \to \mathbb{R}$ is a threshold function that chooses the threshold $\tau(v)$ such that $\sum_{j=1}^n \rho[v]_j = 1$. Since softmax ($\alpha = 1$) is already covered above, we focus on $\alpha > 1$.

Again, assume without loss of generality that the entry of $v$ is in decreasing order, where the first two entries satisfy $v_1 - v_2 \geq \zeta$. For any such $\zeta > 0$ and any $0 < \eta < 1$, our aim is to show the existence of $t > 0$ such that $\rho[tv]_1 \geq 1 - \eta$. This is done by choosing $t = \frac{1-\eta}{\zeta(a-1)}$.

Note that $(\alpha - 1)t(v_1 - v_2) \geq 1$ due to our choice of $t$. Then, we will show that with such a $t$, $\rho[tv]_1 = 1$ must hold. For the sake of contradiction, suppose not: $\rho[tv]_1 < 1$. Then, by monotonicity of $\rho[tv]_j$, we have $\rho[tv]_2 > 0$. This means

$$
\rho[tv]_2 = \left( (\alpha - 1)tv_2 - \tau(tv) \right)^{1/\alpha} > 0,
$$

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in particular, we have \((\alpha - 1)t v_2 - \tau(tv) > 0\). However, recall that \((\alpha - 1)t(v_1 - v_2) \geq 1\), which implies \((\alpha - 1)t v_1 - \tau(tv) > 1\). This results in

\[
\rho[tv]_1 = \left[ (\alpha - 1)t v_1 - \tau(tv) \right]^{\frac{1}{\alpha - 1}} > 1,
\]

thus contradicting \(\rho[tv]_1 < 1\). Therefore, \(\rho[tv]_1 = 1\) must hold.

## C Details of the Step 1 in the proof sketch (§ 4.1)

We start by formally defining the function class \(\mathcal{F}(\delta)\).

\[
\mathcal{F}(\delta) := \left\{ Z \mapsto \sum_{G \in G_{\delta}} A_G 1 \{ Z \in G + [0, \delta)^{d \times n} \} \mid Z \in \mathcal{D}, A_G \in \mathbb{R}^{d \times n} \right\},
\]

where \(G_{\delta} := \{0, \delta, \ldots, 1 - \delta\}^{d \times n}\). We now state and prove the lemma.

**Lemma 5.** For any \(f \in \mathcal{F}\) and \(\epsilon > 0\), there exists a small enough \(\delta > 0\) such that there exists \(\bar{f} \in \mathcal{F}(\delta)\) such that \(d_p(f, \bar{f}) \leq \epsilon / 2\).

**Proof** Since \(f : \mathcal{D} \rightarrow \mathbb{R}^{d \times n}\) is a continuous function on a compact domain, it is uniformly continuous. Also, continuity is defined with respect to entry-wise \(\ell_p\) norm which is equivalent to entry-wise \(\ell_\infty\) norm, uniform continuity leads to

\[
\forall \epsilon > 0, \exists \delta > 0 \text{ such that } \forall X, Y, \|X - Y\|_\infty < \delta \implies \|f(X) - f(Y)\|_p < \epsilon / 2.
\]

Then, suppose we create a set of cube grid points \(G_{\delta} := \{0, \delta, \ldots, 1 - \delta\}^{d \times n}\), and define a piece-wise constant approximation

\[
\bar{f}(X) = \sum_{G \in G_{\delta}} f(G) 1 \{ X \in G + [0, \delta)^{d \times n} \}.
\]

Note that for any \(X \in G + [0, \delta)^{d \times n}\) we have \(\|X - G\|_\infty < \delta\), so we have

\[
\|f(X) - \bar{f}(X)\|_p = \|f(X) - f(G)\|_p < \epsilon / 2.
\]

This implies that

\[
d_p(f, \bar{f}) = \left( \int_{\mathcal{D}} \|f(X) - \bar{f}(X)\|_p^p \right)^{1/p} \leq \epsilon / 2,
\]

finishing the proof of the lemma.

## D Proof of Lemma 3 (Step 2 in § 4.1)

In this section, we describe in further details how modified sparse Transformers (the class \(ST^{2,1,1}\)) are able to exactly express arbitrary piecewise constant functions in \(\mathcal{F}(\delta)\). We show that we can compute a contextual mapping of the entire input sequences without relying on dense self-attention layers. The token-wise feed-forward layers then transform these contextual mappings to the desired output sequence.
To give a high level summary of the proof, we want to show that given a piece-wise constant function \( \mathcal{F} \in \mathcal{F}(\delta) \), there exists a modified Transformer network \( \mathcal{G} \in \mathcal{SF}^{2,1,1} \) that exactly represents \( \mathcal{F} \). Recall first that the function class \( \mathcal{SF}^{2,1,1} \) has an additive positional embedding matrix \( E \in \mathbb{R}^{d \times n} \) that is added to input before the input is fed to the network. We start by choosing the positional embedding \( E \) and construct a Transformer network that implements quantization of the input, contextual mapping of the quantized input, and value mapping of the context ids.

1. Choose the positional embedding \( E \) according to \( \gamma \) in Assumption 1.2. After addition, each column of the input \( X_k + E_k \) are in disjoint intervals.
2. Given the input \( X + E \), a series of modified feed-forward layers quantizes it so that each entry of the quantized input has a value in \( \{0, \delta, \ldots, n - \delta\} \) (Lemma 6).
3. Next, a series of modified sparse self-attention layers takes the quantized input \( H \) and implement a contextual mapping \( \eta \) such that, for different quantized input sequences \( H \) and \( H' \), all the elements in \( \eta(H) \) and \( \eta(H') \) are distinct (Lemma 7).
4. Finally, a series of modified feed-forward layers maps each element in the context id \( \eta(H) \) to the desired output value of \( f \in \mathcal{F} \) at the input \( X \) (Lemma 8).

We defer the proofs of Lemmas 6, 7, and 8 to a separate section: see §E.

Before discussing the details of each step, we note that although a Transformer network stacks self-attention and feed-forward layers in an alternate manner, we can use a series of arbitrary number of the same layers, thanks to skip connections. The outline of the proof is similar to [28], but key component in their proof called selective shift operation relies on the fact that each token can attend to the entire sequence; this is not true in sparse Transformers, which poses a nontrivial challenge. We overcome this issue by a more careful construction of the positional embedding \( E \) and sparse self-attention layers.

### D.1 Choosing the positional embedding

Recall from Assumption 1.2 that there exists a permutation \( \gamma : [n] \to [n] \) such that for all \( i \in [n - 1] \), \( \gamma(i) \) is one of the tokens that the \( \gamma(i + 1) \)-th token directly attends to. Using this permutation \( \gamma \), we choose the columns of positional embedding \( E \) in the following way:

\[
E_{\gamma(1)} = (n - 1)1_n, \text{ and } E_{\gamma(i)} = (i - 2)1_n, \text{ for } i \in [2 : n]
\]

As a result, the \( \gamma(1) \)-th column of \( X + E \) will be in the range \( [n - 1, n)^d \), and similarly \( X_{\gamma(i)} + E_{\gamma(i)} \in [i - 2, i - 1)^d \) for \( i \in [2 : n] \). This means that the entries corresponding to different tokens lie be in disjoint intervals of the form \( [j, j + 1) \), where \( j \in [0 : n - 1] \).

### D.2 Quantization by feed-forward layers

Note from the previous step that each entry of \( X + E \) must be in \( [0, n) \). Next, we quantize this interval \( [0, n) \) of input using to a set of \( \delta \)-grid points \( \{0, \delta, \ldots, n - \delta\} \). This allows us to deal with finite set of values, which proves useful in the later stages of the proof. The next lemma shows that the quantization can be carried out using a series of the modified feed-forward layers.

**Lemma 6.** Consider a entry-wise quantization map \( \delta_q^{\text{ent}} : \mathbb{R} \to \mathbb{R} \):

\[
\delta_q^{\text{ent}}(t) = \begin{cases} 
k\delta & \text{if } k\delta \leq t < (k + 1)\delta, \; k \in [0 : n/\delta - 1], \\
\frac{t}{\delta} & \text{otherwise.}
\end{cases}
\]

There exists a function \( g_q : \mathbb{R}^{d \times n} \to \mathbb{R}^{d \times n} \) composed of \( \frac{d_2}{\delta} \) token-wise feed-forward layers with \( r = 1 \) and an activation \( \phi \in \Phi \), which implements the entry-wise quantization \( \delta_q^{\text{ent}} \) to each entry of its input.
D.3 Contextual mapping by sparse self-attention layers

After the input $X + E$ is quantized, the output of $g_q$ must be in the following set $H_\delta \subset \mathbb{R}^{d \times n}$:

$$H_\delta := \{ G + E \in \mathbb{R}^{d \times n} \mid G \in G_\delta \},$$

where $G_\delta := \{0, \delta, \ldots, 1 - \delta\}^{d \times n}$ was defined to be the $\delta$-cubic grid points of $[0,1)^{d \times n}$. Using this finite set of sequences, we construct a contextual mapping that maps each sequence in $H_\delta$ to unique numbers. Recall that the sparse attention layer has $p$ sparsity patterns that rotate in cycles, and Assumption 1.3 assumes that one token directly/indirectly access all the other tokens after $s$ such sparse attention layers. We now state the lemma.

**Lemma 7.** Assume that $n \geq 2$, and $\delta^{-1}$ is an integer satisfying $\delta^{-1} \geq 2$. Suppose that the sparse self-attention layers ($h = 2, m = 1$) satisfy Assumption 1 and employ the hardmax $\sigma_H$ operator, and that the positional embedding $E$ was chosen as described in § D.1. Then, there exist a function $g_c : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ composed of $\frac{p(n-1)}{d} + s$ sparse self-attention layers, and a vector $u \in \mathbb{R}^d$, such that $q(H) := u^T g_c(H)$ satisfies the following properties:

1. For any $H \in H_\delta$, the entries of $q(H)$ are all distinct.
2. For any $H, H' \in H_\delta$ such that $H \neq H'$, all entries of $q(H), q(H')$ are distinct.

This contextual mapping maps each unique sequence/context into different context ids, enabling the network to distinguish the same token appearing in different sequences.

D.4 Value mapping by feed-forward layers

After the contextual mapping, we use the token-wise feed-forward layers to map each different context ids to the desired output value of the target function $\tilde{f}$. More specifically, recall the function $g_c$ from Lemma 7. For any $H \in H_\delta$, we need to map the output $g_c(H)$ of Lemma 7 to the desired function value $\tilde{f}(H - E)$ (recall that $H$ is the quantized input after adding $E$ to $X$, so we need to subtract $E$). This is done by implementing a token-wise value mapping using the feed-forward layers.

**Lemma 8.** There exists a function $g_v : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ composed of $n(\frac{1}{2})^{dn}$ token-wise feed-forward layers ($r = 1$) with an activation $\phi' \in \Phi$ such that $g_v$ is defined by a token-wise function $g_v^{kn} : \mathbb{R}^{d} \rightarrow \mathbb{R}^{d}$ on each column,

$$g_v(Z) = \left[ g_v^{kn}(Z_1) \cdots g_v^{kn}(Z_n) \right],$$

where for all $H \in H_\delta$ and $k \in \{1, \ldots, n\}$,

$$g_v^{kn}(g_c(H)_k) = \tilde{f}(H - E)_k.$$

D.5 Finishing the proof

Given Lemmas 6, 7, and 8, one can easily check that for any $G \in G_\delta := \{0, \delta, \ldots, 1 - \delta\}^{d \times n}$ and any input value $X \in G + [0, \delta)^{d \times n}$, we have

$$g_v \circ g_c \circ g_q(X + E) = g_v \circ g_c(G + E)$$

$$= \begin{pmatrix} g_v^{kn}(g_c(G + E)_1) & g_v^{kn}(g_c(G + E)_2) & \cdots & g_v^{kn}(g_c(G + E)_n) \end{pmatrix}$$

$$= \begin{bmatrix} \tilde{f}(G)_1 & \tilde{f}(G)_2 & \cdots & \tilde{f}(G)_n \end{bmatrix} = \tilde{f}(G) = \tilde{f}(X).$$

Therefore, we have constructed a modified sparse Transformer network $\tilde{g}(X) := g_v \circ g_c \circ g_q(X + E)$ that satisfies $\tilde{g}(X) = \tilde{f}(X)$ for all $X \in \mathbb{D}$, hence proving Lemma 3.
E Proof of Lemmas 6, 7, and 8

E.1 Proof of Lemma 6

The proof goes as follows. Using \( \frac{d}{2} \) token-wise feed-forward layers, we implement the quantization function \( \delta_{q}^{\text{int}} \) that quantizes the first row of the input. Then we stack another \( \frac{d}{2} \) layers to quantize the second row, and so on.

For the first row, we add \( n/\delta \) layers of the following form, for \( k \in [0 : n/\delta - 1] \).

\[
Z \mapsto Z + e^{(1)} \phi((e^{(1)})^T Z - k\delta 1_n^T), \quad \phi(t) = \begin{cases} 0 & t < 0 \text{ or } t \geq \delta, \\ -t & 0 \leq t < \delta, \end{cases}
\]

where \( e^{(1)} \in \mathbb{R}^{d} \) is the first canonical basis vector \( e^{(1)} = (1, 0, \ldots, 0) \). Each layer quantizes \( Z_1 \) in \([k\delta, k\delta + \delta) \) to \( k\delta \), without modifying other intervals or other rows of \( Z \). Note that the activation \( \phi \) is a piecewise linear function with three pieces; hence, \( \phi \in \Phi \). Therefore, the layers satisfy the definition of modified feed-forward layers. We can now repeat the same construction for the \( d-1 \) remaining rows.

E.2 Proof of Lemma 7

In order to construct a network \( g_c \), that implements the contextual mapping, we first introduce two operations referred to as the sparse selective shift operation and all-max-shift operation, implemented by at most two (modified) sparse attention heads of head size \( 1 \). Then, we proceed to stack layers implementing the selective shift operations and all-max-shift operations, and prove that these layers map input \( H \in \mathbb{H}_k \) to unique context ids.

E.2.1 Preliminaries

Sparse selective shift operation. Given any vector \( u \in \mathbb{R}^{d} \), first consider the following function implementable with a sparse attention head with head size \( 1 \) and sparsity pattern \( \{A_k^j\}_{k \in [n]} \): For \( k \in [n] \), the function \( \psi^j : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{1 \times n} \) computes each of its output column in the following way:

\[
\psi^j(Z; b_Q) := u^T Z_{A_k^j} \phi_H[(u^T Z_{A_k^j})^T (u^T Z_k - b_Q)] = \begin{cases} \max_{j \in A_k^j} u^T Z_j & \text{if } u^T Z_k > b_Q, \\ \min_{j \in A_k^j} u^T Z_j & \text{if } u^T Z_k < b_Q. \end{cases}
\]

One can consider a sparse self-attention layer that consists of two such heads, with \( b_Q < b_Q' \):

\[
\Psi^l(Z; c, b_Q, b_Q') := Z + [ce^{(1)} \quad -ce^{(1)}] \begin{bmatrix} \psi^l(Z; b_Q) \\ \psi^l(Z; b_Q') \end{bmatrix}.
\]

The \((1, k)\)-th entry of \( \Psi^l(Z; c, b_Q, b_Q') \) reads

\[
\Psi^l(Z; c, b_Q, b_Q')_{1,k} = Z_{1,k} + c(\Psi^l(Z; b_Q)_{k} - \psi^l(Z; b_Q)_{k}) = \begin{cases} Z_{1,k} + c(\max_{j \in A_k^j} u^T Z_j - \min_{j \in A_k^j} u^T Z_j) & \text{if } b_Q < u^T Z_k < b_Q', \\ Z_{1,k} & \text{if } u^T Z_k \notin [b_Q, b_Q'). \end{cases}
\]

This means that for input columns \( Z_k \) satisfying \( u^T Z_k \in (b_Q, b_Q') \) only, \( \Psi^l \) shifts up the first entry of \( Z_k \) by the difference of maximum and minimum values of \( u^T Z_j \) over the sparsity pattern \( j \in A_k^j \), while leaving other columns intact. By choosing \( b_Q \) and \( b_Q' \) properly, we can selectively modify
certain columns without touching other columns; we refer to this operation \( \Psi^l \) as the \textit{sparse selective shift operation}, and we will see later that this is indeed the key ingredient of our proof.

In fact, this operation is a sparse version of the selective shift operation used in \cite{28}. Since \( A_k^l \) is usually only a small subset of \([n]\), one cannot calculate the maximum and minimum of \( u^T Z_j \) over the whole sequence, as done in \cite{28}. Instead, we use Assumption 1.2 and a more careful choice of \( E \) to get around the restriction posed by sparsity.

**All-max-shift operation.** Suppose the input \( Z \in \mathbb{R}^{d \times n} \) satisfies \( u^T Z > 0 \) entry-wise, for a vector \( u \in \mathbb{R}^d \). Then, the \textit{all-max-shift operation} \( \gamma_l^k : \mathbb{R}^{d \times n} \to \mathbb{R}^{d \times n} \) is a sparse self-attention layer that consists of one attention head:

\[
\gamma_l^k(Z; c) = Z + c e^{(1)} \psi_l^k(Z; 0).
\]

The \((1, k)\)-th entry of \( \gamma_l^k(Z; c) \) reads

\[
\gamma_l^k(Z; c)_{1,k} = Z_{1,k} + c \psi_l^k(Z; 0)_k = Z_{1,k} + c \max_{j \in A_k^l} u^T Z_j.
\]

So, for each column \( k \), the all-max-shift operation shifts up the first entry of \( Z_k \) by the maximum value of \( u^T Z_j \) over the sparsity pattern \( j \in A_k^l \). Unlike the selective shift operation, the all-max-shift operation is applied to all the columns.

**Column ids.** Recall that the any input to this step is in

\[
H_\delta := \{ G + E \in \mathbb{R}^{d \times n} \mid G \in G_\delta := [0 : \delta : 1 - \delta]^{d \times n} \}.
\]

Because of the way \( E \) is chosen according to the permutation \( \gamma \) in Assumption 1.2, for any \( H \in H_\delta \) we have

\[
H_{\gamma(1)} \in [n - 1 : \delta : n - \delta]^d,
\]

\[
H_{\gamma(i)} \in [i - 2 : \delta : i - 1 - \delta]^d \text{ for all } i \in [2 : n].
\]

Now consider \( u := (1, \delta^{-1}, \delta^{-2}, \ldots, \delta^{-d+1}) \). It is easy to check that for any \( H \in H_\delta \), the map \( H_k \mapsto u^T H_k \) is one-to-one, and

\[
u^T H_{\gamma(1)} \in \left( (n - 1) \sum_{i=0}^{d-1} \delta^{-i} : (n - 1) \sum_{i=0}^{d-1} \delta^{-i} + \delta^{-d+1} - \delta \right),
\]

\[
u^T H_{\gamma(i)} \in \left( (i - 2) \sum_{i=0}^{d-1} \delta^{-i} : (i - 2) \sum_{i=0}^{d-1} \delta^{-i} + \delta^{-d+1} - \delta \right), \text{ for } i \in [2 : n].
\]

Hence, for each column \( H_k \), the inner product \( u^T H_k \) is in an interval disjoint from the other columns. Thus, \( u^T H_k \) can be thought as a “column id” that identifies the column’s original input value \( G_k \) as well as its position \( k \). Note furthermore that for any \( H \in H_\delta \),

\[
u^T H_{\gamma(2)} < u^T H_{\gamma(3)} < \cdots < u^T H_{\gamma(n)} < u^T H_{\gamma(1)}.
\]

**E.2.2 Construction of layers**

Given these preliminaries, we now describe our construction of \( g_c \). Recall from Assumption 1.2 that the permutation \( \gamma \) satisfies \( \gamma(i - 1) \in \bigcup_{i=1}^n A_{\gamma(i)} \) for \( i \in [2 : n] \). From this, for \( i \in [2 : n] \) we
let $i \in [p]$ be any index such that $\gamma(i) \in A_{\gamma(i)}^l$. For simplicity of notation, let $z_k := u^T H_k$ for $k \in [n]$ and $\Delta = \sum_{j=0}^{d-1} \delta^{-i}$.

Next, starting from $i = 2$, we want to sequentially stack $\delta^{-d}$ sparse selective shift operations
\[ \Psi^l(\cdot; \delta^{-d}, b - \delta/2, b + \delta/2), \]
in increasing order of $b \in [(i-2)\Delta : \delta : (i-2)\Delta + \delta^{-d+1} - \delta]$. That is, we want to add sparse attention layers with sparsity patterns $A^l_{\gamma(i)}$ that apply the selective shift operation to each possible value of $z_{\gamma(i)}$. Recall that the sparsity patterns have to cycle from $A^1_k$ to $A^p_k$, so we have to place other remaining $p-1$ sparsity patterns (whose indices are not $l_i$) in between the $\Psi^l_i$. This can be done by setting all the other sparse attention layers to be the identity. This way, we stack a total of $p\delta^{-d}$ sparse attention layers for $i = 2$, another $p\delta^{-d}$ for $i = 3$, and so on, up to $i = n$.

After these layers, we further stack $s$ all-max-shift operations. For $i = 1, \ldots, s$, we add all-max-shift operations of the form
\[ \Omega^{(i-1) \mod p + 1}(\cdot; 2s\delta^{-nd-1}). \]
Here, the superscript $(i-1) \mod p + 1$ is there to make sure that we cycle through the sparsity patterns from 1 to $p$, until we stack $s$ layers in total. This finishes the construction of our function $g_e$ composed of $\frac{p(n-1)}{\delta d} + s$ sparse self-attention layers.

E.2.3 Selective shift operations

We now explain how these stacked self-attention layers implement a contextual mapping. This subsection will consider the selective shift operations part; all-max-shift operations are described in the next subsection. Suppose that after the input $H \in H_\delta$ is processed through the first $\frac{p(n-1)}{\delta d}$ layers, we get $\tilde{H} \in \mathbb{R}^{d \times n}$ at the output. We will show at the end of this subsection that the map $H \mapsto u^T \tilde{H}_{\gamma(n)}$ is a one-to-one map for column $\gamma(n)$, so the selective shift operations compute a “unique id” for each possible input sequence $H \in H_\delta$.

First selective shift. First consider the first $p\delta^{-d}$ layers. Omitting layers that are identity, they are essentially selective shift operations $\Psi^l(\cdot; \delta^{-d}, b - \delta/2, b + \delta/2)$ for $b \in [0 : \delta : \delta^{-d+1} - \delta]$. Since $[0 : \delta : \delta^{-d+1} - \delta]$ is the set of possible values of $z_{\gamma(2)}$, these layers perform selective shift operation on the $\gamma(2)$-th column without changing the other columns. Each possible value of $H_{\gamma(2)}$ undergoes one and only shift operation (by the corresponding layer with $b = u^T H_{\gamma(2)}$), by which the $(1, \gamma(2))$-th entry of the input is updated.

Recall by Assumption 1.2 that $\gamma(1) \in A^2_{\gamma(2)}$, and that $z_{\gamma(1)}$ and $z_{\gamma(2)}$ are the maximum and minimum over the whole sequence $z_1, \ldots, z_n$ (see (8)). By Assumption 1.1 we also have $\gamma(2) \in A^2_{\gamma(2)}$. Since both $\gamma(1)$ and $\gamma(2)$ are in $A^2_{\gamma(2)}$, the maximum and minimum value of $z_j := u^T H_j$’s over $j \in A^2_{\gamma(2)}$ are $z_{\gamma(1)}$ and $z_{\gamma(2)}$, respectively. Therefore, the $(1, \gamma(2))$-th entry of the input matrix is shifted up as follows:
\[ \tilde{H}_{1,\gamma(2)} := H_{1,\gamma(2)} + \delta^{-d}(z_{\gamma(1)} - z_{\gamma(2)}). \]
Let $\tilde{H}_{\gamma(2)}$ be the $\gamma(2)$-th column after the shift operation has shifted $H_{1,\gamma(2)}$ to $\tilde{H}_{1,\gamma(2)}$. Then, define
\[ \tilde{z}_{\gamma(2)} := u^T \tilde{H}_{\gamma(2)} = z_{\gamma(2)} + \delta^{-d}(z_{\gamma(1)} - z_{\gamma(2)}). \]
Note that \( \bar{z}_{\gamma(2)} > z_{\gamma(1)} \) because
\[
z_{\gamma(2)} + \delta^{-d} (z_{\gamma(1)} - z_{\gamma(2)}) > z_{\gamma(1)} \iff (\delta^{-d} - 1)(z_{\gamma(1)} - z_{\gamma(2)}) > 0,
\]
which is true. Therefore, \( \bar{z}_{\gamma(2)} \) becomes the new maximum among the current values \( \bar{z}_{\gamma(1)}, \bar{z}_{\gamma(2)}, z_{\gamma(3)}, \ldots, z_{\gamma(n)} \), and the new minimum element is \( z_{\gamma(3)} \).

**Second selective shift.** We now consider the next \( p\delta^{-d} \) layers, which are essentially \( \Psi^b(.; \delta^{-d}, b - \delta/2, b + \delta/2) \) for \( b \in [\Delta : \delta : \Delta + \delta^{-d} + 1 - \delta] \). They apply the shift operation to the \( \gamma(3) \)-th column. Since we have \( \gamma(2), \gamma(3) \in \mathcal{A}_{\gamma(3)}^b \), the shift operation similarly yields
\[
\bar{z}_{\gamma(3)} := z_{\gamma(3)} + \delta^{-d}(\bar{z}_{\gamma(2)} - z_{\gamma(3)}) = z_{\gamma(3)} + \delta^{-d}(z_{\gamma(2)} - z_{\gamma(3)}) + \delta^{-2d}(z_{\gamma(1)} - z_{\gamma(2)}).
\]
We can also show \( \bar{z}_{\gamma(3)} > \bar{z}_{\gamma(2)} \), because
\[
z_{\gamma(3)} + \delta^{-d}(\bar{z}_{\gamma(2)} - z_{\gamma(3)}) > \bar{z}_{\gamma(2)} \iff (\delta^{-d} - 1)(\bar{z}_{\gamma(2)} - z_{\gamma(3)}) > 0.
\]
So after this operation \( \bar{z}_{\gamma(3)} \) and \( z_{\gamma(4)} \) are the new maximum and minimum over the updated sequence \( \bar{z}_{\gamma(1)}, \bar{z}_{\gamma(2)}, \bar{z}_{\gamma(3)}, \bar{z}_{\gamma(4)}, \ldots, \bar{z}_{\gamma(n)} \).

**Repeating the process.** The same process continues. The next \( p\delta^{-d} \) layers shifts the \( \gamma(4) \)-th columns and results in \( \bar{z}_{\gamma(4)} \) which is greater than \( \bar{z}_{\gamma(3)} \). After the first \( p(n-1)\delta^{-d} \) layers, all columns except \( \gamma(1) \)-th column have been shifted, resulting in \( \bar{z}_{\gamma(1)}, \bar{z}_{\gamma(2)}, \ldots, \bar{z}_{\gamma(n)} \) satisfying
\[
(n-1)\Delta \leq z_{\gamma(1)} < \bar{z}_{\gamma(2)} < \cdots < \bar{z}_{\gamma(n)}.
\]
Let us denote the output of the \( p(n-1)\delta^{-d} \)-th layer as \( \bar{H} \).

**Selective shifts implement a one-to-one map.** Next, we prove that the map from \( H \in \mathbb{H}_\delta \) to
\[
\bar{z}_{\gamma(n)} := u^T \bar{H}_{\gamma(n)} = z_{\gamma(n)} + \sum_{i=1}^{n-1} \delta^{-id}(z_{\gamma(n-i)} - z_{\gamma(n+1-i)})
\]
is one-to-one. Recall that for each column \( H_k \), the map \( H_k \mapsto u^T H_k := z_k \) is one-to-one. Also, permutation of columns is one-to-one, which implies that it suffices to show that the map \( [z_{\gamma(1)} \ldots z_{\gamma(n)}] \mapsto \bar{z}_{\gamma(n)} \) is one-to-one.

Suppose we have two sequences \( [z_{\gamma(1)} \ldots z_{\gamma(n)}] \) and \( [z'_{\gamma(1)} \ldots z'_{\gamma(n)}] \) that map to the same value of \( \bar{z}_{\gamma(n)} = \bar{z}'_{\gamma(n)} \). Then,
\[
0 = \bar{z}_{\gamma(n)} - \bar{z}'_{\gamma(n)} = z_{\gamma(n)} - z'_{\gamma(n)} + \sum_{i=1}^{n-1} \delta^{-id}(z_{\gamma(n-i)} - z_{\gamma(n+1-i)} - z'_{\gamma(n-i)} + z'_{\gamma(n+1-i)}).
\]
Suppose \( z_{\gamma(n)} \neq z'_{\gamma(n)} \). Since they both lie inside \( [(n-2)\Delta : \delta : (n-2)\Delta + \delta^{-d+1} - \delta] \), we have
\[
-\delta^{-d+1} + \delta \leq z_{\gamma(n)} - z'_{\gamma(n)} \leq \delta^{-d+1} - \delta.
\]
Note that all the terms other than \( z_{\gamma(n)} - z'_{\gamma(n)} \) are of “coarser resolution.” For example, the first term
\[
\delta^{-d}(z_{\gamma(n-1)} - z_{\gamma(n-1)} + z'_{\gamma(n-1)} + z'_{\gamma(n)}).
\]
in the summation can only take values \(0, \delta^{-d+1}, \delta^{-d+1}, 2\delta^{-d+1}, -2\delta^{-d+1}, \ldots\), so it can never cancel the difference \(z_{\gamma(n)} - z'_{\gamma(n)}\) and make the sum \(\bar{z}_{\gamma(n)} - \bar{z}'_{\gamma(n)}\) zero. This implies that \(z_{\gamma(n)} = z'_{\gamma(n)}\) must hold.

Next, suppose \(z_{\gamma(n-1)} \neq z'_{\gamma(n-1)}\). Since we have \(z_{\gamma(n)} = z'_{\gamma(n)}\),
\[
-\delta^{-2d+1} < \delta^{-d}(z_{\gamma(n-1)} - z_{\gamma(n)}) - \delta^{-d}(z'_{\gamma(n-1)} - z'_{\gamma(n)}) = \delta^{-d}(z_{\gamma(n-1)} - z_{\gamma(n)}) < -\delta^{-2d+1}.
\]

But similarly, any other terms in the summation have coarser resolution than \(\delta^{-2d+1}\), so they cannot cancel the difference \(\delta^{-d}(z_{\gamma(n-1)} - z'_{\gamma(n-1)})\). Thus \(z_{\gamma(n-1)} = z'_{\gamma(n-1)}\) must hold. Repeating the same argument up to \(\gamma(1)\) proves that the two sequences must be equal: \([\tilde{z}_{\gamma(1)} \ldots \tilde{z}_{\gamma(n)}] = [z'_{\gamma(1)} \ldots z'_{\gamma(n)}]\). This proves that the map \(H \mapsto \tilde{z}_{\gamma(n)}\) is one-to-one and \(\tilde{z}_{\gamma(n)}\) can be seen as the unique id for the input sequence \(H \in \mathbb{H}_{\delta}\).

### E.2.4 All-max-shift operations

Next, we explain the operation of the \(s\) all-max-shift layers. Recall from Assumption 1.3 that any token can attend to all the other tokens after \(s\) steps, either directly or indirectly. Also recall from the last subsection that the input to the first all-max-shift layer is \(\tilde{H}\), and the maximum entry of \(u^T \tilde{H}\) is \(\tilde{z}_{\gamma(n)}\), the unique id for input \(H\). From the statement of Lemma 7, the output after the \(s\) all-max-shift operations for input \(H\) is denoted as \(g_{c}(H)\). In this subsection, we show that through \(s\) all-max-shift operations, the maximum \(\tilde{z}_{\gamma(n)}\) will propagate to all tokens and be a “dominant” term, which determines the interval that \(u^T g_{c}(H)\) lies in. As a result, we can show Properties 7.1 and 7.2 of \(g_{c}\) at the end.

### Some preliminaries

Note that the unique id \(\tilde{z}_{\gamma(n)}\) has the following upper bound:
\[
\tilde{z}_{\gamma(n)} := z_{\gamma(n)} + \sum_{i=1}^{n-2} \delta^{-id}(z_{\gamma(n-i)} - z_{\gamma(n+1-i)}) + \delta^{-(n-1)d}(z_{\gamma(1)} - z_{\gamma(2)})
\]
\[
\leq z_{\gamma(n)} + \delta^{-d} \sum_{i=1}^{n-2} (z_{\gamma(n-i)} - z_{\gamma(n+1-i)}) + \delta^{-(n-1)d}(z_{\gamma(1)} - z_{\gamma(2)})
\]
\[
= z_{\gamma(n)} + \delta^{-d}(z_{\gamma(2)} - z_{\gamma(n)}) + \delta^{-(n-1)d}(z_{\gamma(1)} - z_{\gamma(2)})
\]
\[
= \delta^{-(n-1)d}z_{\gamma(1)} + (\delta^{-(n-1)d} - \delta^{d})z_{\gamma(2)} - (\delta^{d} - 1)z_{\gamma(n)}
\]
\[
\leq \delta^{-(n-1)d}z_{\gamma(1)} + (n - 1)\Delta + \delta^{-2d+1} - \delta
\]
\[
\leq \delta^{-(n-1)d}(n - 1 + \delta)(\delta^{d} - 1) \leq \delta^{-nd} - \delta
\]
(10)

where we used \(\Delta := \sum_{i=0}^{d-1} \delta^{-i} = \frac{\delta^{d-1}}{\delta - 1} \leq \delta^{d} - 1\). A similar bound
\[
\tilde{z}_{\gamma(n)} \leq n\delta^{-id} - \delta
\]
(11)
also holds from a similar derivation. Next, recall from Assumption 1.3 the definitions
\[
S^1_k := A^1_k, \quad S^s_k := \bigcup_{j \in A^{(l-1) \mod p + 1}} S^{l-1}_j,
\]
and that there exists \(s \geq 1\) such that, for all \(k \in [n], S^s_k = [n]\). Finally, the following inequality will be useful throughout: for any integer \(s \geq 1\),
\[
\left(\frac{2s + 1}{2s}\right)^s \leq \left(\frac{2s + 1}{2s}\right)^2 \leq \cdots \leq \left(\frac{2s + 1}{2s}\right)^s \leq 2.
\]
(12)
Let us now describe the operation that the all-max-shift layers $\Omega_{(i-1) \mod p+1}^{(\cdot;2s)}$, $i = 1, \ldots, s$, carry out.

**First all-max-shift.** The input to the first all-max-shift layer is $\tilde{H}$. Let the output of the layer be $M^1$. Recall that $u^T \tilde{H}$ consists of values $z_{\gamma(1)}, z_{\gamma(2)}, \ldots, z_{\gamma(n)}$, which are all strictly greater than 0 and strictly less than $n \delta^{-nd}$ (by (10)). So, for each column $k \in [n]$, the layer update reads

$$
M_{1,k}^1 := \tilde{H}_{1,k} + 2sn\delta^{-nd-1} \max_{j \in A_k^1} u_j^T \tilde{H}_j = \tilde{H}_{1,k} + 2sn\delta^{-nd-1} u_j^T \tilde{H}_j,
$$

where $j_k^1 := \arg \max_{j \in A_k^1} u_j^T \tilde{H}_j$. After the update, $u^T M_k^1$ is “dominated” by $2sn\delta^{-nd-1} u_j^T \tilde{H}_j$, meaning that for any $k, k' \in [n]$,

$$
u_k^T \tilde{H}^1_{k'} < u_k^T \tilde{H}^1_k \implies u_k^T M_{k'} < u_k^T M_k.
$$

This is because the minimum gap between different values of $u_k^T \tilde{H}_{k'}$ is at least $\delta$, and we have

$$
u_k^T \tilde{H}_k < n\delta^{-nd} < 2sn\delta^{-nd-1} \cdot \delta,
$$

so if $u_k^T \tilde{H}_{k'} < u_k^T \tilde{H}_k$, that solely determines the order $u_k^T M_{k'} < u_k^T M_k$ because $u_k^T \tilde{H}_k$ cannot reverse it. Also, by the definition of $j_k^1$, for any index set $\mathcal{B} \subset [n]$ we have

$$
\max_{i \in \mathcal{B}} u_i^T \tilde{H}_{k}^1 = \max_{j \in \{j \mid i \in \mathcal{B}, j \in A^1_{k} \}} u_j^T \tilde{H}_{j}.
$$

(13)

If $s \geq 2$, we move on to the second layer.

**Second all-max-shift.** At the second all-max-shift, we have sparsity patterns $A_{k}^{1 \mod p+1}$. Let us the output of this layer as $M^2$. For each column $k \in [n]$, the layer update reads

$$
M_{1,k}^2 := M_{1,k}^1 + 2sn\delta^{-nd-1} \max_{j \in A_{k}^{1 \mod p+1}} u_j^T M_{j}^1 = M_{1,k}^1 + 2sn\delta^{-nd-1} u_j^T M_{j}^1,
$$

where $j_k^2 := \arg \max_{j \in A_{k}^{1 \mod p+1}} u_j^T M_j^1$. If we look at the update more closely, we can apply (13) and get

$$
u_k^T \tilde{H}^2_k = u_k^T \tilde{H}_k + 2sn\delta^{-nd-1} u_k^T \tilde{H}_j^2 + 2sn\delta^{-nd-1} (u_k^T \tilde{H}_k^2 + 2sn\delta^{-nd-1} \max_{i \in A_{k}^{1 \mod p+1}} u_i^T \tilde{H}_i^1))
\begin{align*}
&= u_k^T \tilde{H}_k + 2sn\delta^{-nd-1}(u_k^T \tilde{H}_k^2 + u_k^T \tilde{H}_j^2) + (2sn\delta^{-nd-1})^2 \max_{j \in S_k^2} u_j^T \tilde{H}_j.
\end{align*}

Again, the last term dominates the rest of the terms in $u_k^T M_k^2$, because the minimum gap between different values of $u_j^T \tilde{H}_j$ is at least $\delta$, and

$$
u_k^T M_k^2 - (2sn\delta^{-nd-1})^2 \max_{j \in S_k^2} u_j^T \tilde{H}_j = u_k^T \tilde{H}_k + 2sn\delta^{-nd-1}(u_k^T \tilde{H}_k^2 + u_k^T \tilde{H}_j^2)
\begin{align*}
&< (1 + 4sn\delta^{-nd-1})n\delta^{-nd} \leq (1 + 4s)n^2\delta^{-2nd-1} \leq (2sn\delta^{-nd-1})^2 \cdot \delta = 4s^2n^2\delta^{-2nd-1}.
\end{align*}

The last inequality holds due to inequality (12), because

$$
\left(\frac{2s+1}{2s}\right)^2 \leq 2 \iff 1 + 4s \leq 4s^2
$$

is true for $s \geq 2$.  

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Remaining all-max-shifts. If \( s \geq 3 \), we move on to the third layer, which outputs \( M^3 \). Similarly, we can show that \( u^T M^3_k \) is dominated by \((2sn\delta^{-nd-1})^3 \max_{j \in S_k^3} u^T H_j \) because the rest of the terms in \( u^T M^3_k \) is strictly upper-bounded

\[
u^T M^3_k - (2sn\delta^{-nd-1})^3 \max_{j \in S_k^3} u^T H_j < (1 + 3 \cdot 2sn\delta^{-nd-1} + 3 \cdot (2sn\delta^{-nd-1})^2)n\delta^{-nd-1},\]

which can then be shown to be smaller than \((2sn\delta^{-nd-1})^3 \cdot \delta\):

\[
(1 + 3 \cdot 2sn\delta^{-nd-1} + 3 \cdot (2sn\delta^{-nd-1})^2)n\delta^{-nd} \leq (1 + 6s + 12s^2)n^3\delta^{-3nd-2} \leq 8s^3n^3\delta^{-3nd-3} \cdot \delta.
\]

The last inequality is due to the fact that \( 1 + 6s + 12s^2 \leq 8s^3 \) for \( s \geq 3 \), which can derived from (12). Repeating this process, after all \( s \) layers we get \( M^s \), and \( u^T M^s_k \) is dominated by

\[
(2sn\delta^{-nd-1})^s \max_{j \in S_k^s} u^T H_j = (2sn\delta^{-nd-1})^s n\delta^{-nd},
\]

This is because the remaining terms in \( u^T M^s_k \) can be strictly upper-bounded

\[
u^T M^s_k - (2sn\delta^{-nd-1})^s n\delta^{-nd} \leq (\sum_{i=0}^{s-1} \binom{s}{i} (2sn\delta^{-nd-1})^i)n\delta^{-nd} \leq (1 + 2s)^s - (2s)^s \leq (2s)^s \delta \cdot (2sn\delta^{-nd-1})^s \delta \leq (2sn\delta^{-nd-1})^s \delta.
\]

The last inequality used \( (1 + 2s)^s - (2s)^s \leq (2s)^s \), derived from (12).

E.2.5 Verifying Properties 7.1 and 7.2

After these all-max-shift operations, we define the output \( M' \) of the last all-max-shift layer to be the output of the function \( g_c \) for input \( H \), i.e., \( g_c(H) := M' \).

Property 7.1 requires that for any \( H \in \mathbb{H}_c \), all the components \( u^T g_c(H) \) need to be distinct. This is true, because for each column of \( u^T g_c(H) \), we have

\[
u^T g_c(H)_k \mod 2sn\delta^{-nd} = u^T H_k.
\]

This is because anything added by the all-max-shift operations is an integer multiple of \( 2sn\delta^{-nd} \), and \( u^T H_k < n\delta^{-nd} < 2n\delta^{-nd} \) for all \( k \). Recall that \( H \) is the input matrix for the first max-shift operation, and that the components of \( u^T H \) are \( z_{\gamma(1)}, z_{\gamma(2)}, \ldots, z_{\gamma(n)} \), which were shown to be distinct by (9). Since \( u^T g_c(H)_k \) produce distinct outputs for a mod operation, they themselves have to be distinct. This proves Property 7.1.

Also, by the “domination” argument in the previous subsection, the output \( g_c(H) \) has the property that for any column, \( u^T g_c(H)_k \) lies inside an interval determined by \( z_{\gamma(n)} \), the unique id for the input \( H \):

\[
u^T g_c(H)_k \in \left[ (2sn\delta^{-nd-1})^s z_{\gamma(n)} + (2sn\delta^{-nd-1})^s (z_{\gamma(n)} + \delta) \right],
\]

and these intervals do not overlap because any different values of \( z_{\gamma(n)} \) must differ by at least \( \delta \). This means that for any input \( H, H' \in \mathbb{H}_c \), the components in \( u^T g_c(H) \) and \( u^T g_c(H') \) lie in disjoint intervals. Together with Property 7.1, this proves Property 7.2.
E.3 Proof of Lemma 8

To prove this lemma, we implement a token-wise function that maps

\[ g_v^{\text{kn}}(g_c(H)_k) = \bar{f}(H - E)_k, \]

for all \( H \in H_\delta \) and \( k \in [n] \). From the construction of Lemma 7, there are \( n|H_\delta| = \frac{n}{\delta^2} \) distinct values of \( u^Tg_c(H)_k \), and different values of \( u^Tg_c(H)_k \) differ by at least \( \delta \). The implementation of \( g_v^{\text{kn}} \) can be done by stacking feed-forward layers so that each layer maps one unique number to the corresponding output column.

More precisely, choose any \( H \in H_\delta \). For each of the \( n \) values of \( u^Tg_c(H)_k \), we add one feed-forward layer of the form

\[ Z \mapsto Z + (\bar{f}(H - E)_k - g_c(H)_k)\phi'(u^TZ - u^Tg_c(H)_k1^T_n), \quad \phi'(t) = \begin{cases} 0 & t < -\delta/2 \text{ or } t \geq \delta/2, \\ -\delta/2 & -\delta/2 \leq t < \delta/2. \end{cases} \]

This layer updates any column \( j \) of its input \( Z \) that satisfies \( u^Tg_c(H)_k - \delta/2 \leq u^TZ_j < u^Tg_c(H)_k + \delta/2 \), without modifying any other columns that are out of this range.

We stack these layers for all possible values of \( H \in H_\delta \). After \( \frac{n}{\delta^2} \) such layers, we get the desired function \( g_v \) that satisfies

\[ g_v(Z) = [g_v^{\text{kn}}(Z_1) \ldots g_v^{\text{kn}}(Z_n)], \]

where for all \( H \in H_\delta \) and \( k \in [n] \),

\[ g_v^{\text{kn}}(g_c(H)_k) = \bar{f}(H - E)_k. \]

F Proof of Lemma 4 (Step 3 in § 4.1)

In this section, we describe how the modified sparse Transformer network \( \tilde{g} \in ST^{2,1,1} \) constructed in Lemma 3 can be approximated with an original sparse Transformer network \( g \in ST^{2,1,4} \). Recall that \( \tilde{g} \) is a “modified” sparse Transformer network, which employ the hardmax \( \sigma_H \) operators in place of \( \rho \) operators in sparse self-attention layers and piecewise linear activations \( \phi \in \Phi \) instead of ReLUs in feed-forward layers. The goal of this lemma is to approximate the function \( \tilde{g} = g_v \circ g_c \circ \bar{g}_q \in ST^{2,1,1} \) with a standard sparse Transformer \( g = \tilde{g}_v \circ \tilde{g}_c \circ \tilde{g}_q \in ST^{2,1,4} \) with accuracy \( d_p(\tilde{g}, g) \leq \epsilon/2 \). As the construction of \( \tilde{g} \) consists of three steps, we will approximate each of them step by step. The whole intuition behind the proof is that as long as we are considering \( L_p \) approximation, we can approximate \( \sigma_H \) and \( \phi \in \Phi \) as closely as we want with \( \rho \) and ReLUs, respectively. However, as the proof will show, controlling the aggregated error over layers is not a trivial job.

F.1 Approximating the quantization function \( g_q \) (Lemma 6)

We first consider approximating \( g_q \) from Lemma 6 with a standard feed-forward layer counterpart, \( \tilde{g}_q \). Recall from § E.1 that the modified feed-forward layers used in \( g_q \) are of the form

\[ Z \mapsto Z + e^{(i)} \phi((e^{(i)})^T Z - k\delta1^T_n), \quad \phi(t) = \begin{cases} 0 & t < 0 \text{ or } t \geq \delta, \\ -t & 0 \leq t < \delta, \end{cases} \]

(14)
for \( i \in [d] \) and \( k \in [0 : n / \delta - 1] \). Note that the activation \( \phi \in \Phi \) can be closely approximated by three ReLUs:

\[
\tilde{\phi}_a(t) := -\text{ReLU}(t) + \frac{1}{\alpha} \text{ReLU}(t - (1 - \alpha)\delta) - \frac{1 - \alpha}{\alpha} \text{ReLU}(t - \delta)
\]

\[
= \begin{cases} 
0 & t \leq 0 \text{ or } t \geq \delta, \\
-t & 0 \leq t \leq (1 - \alpha)\delta, \\
\frac{1 - \alpha}{\alpha} (t - \delta) & (1 - \alpha)\delta \leq t \leq \delta,
\end{cases}
\]

where \( 0 < \alpha < 1 \). Note that \( \tilde{\phi}_a(t) = \phi(t) \) except for an interval \(((1 - \alpha)\delta, \delta)\), and by shrinking \( \alpha > 0 \) this interval can be made arbitrarily small. Consider approximating the layers (14) with standard feed-forward layers, by replacing \( \phi \) with its approximation \( \tilde{\phi}_a \). Let the resulting function be \( g_q \in ST^{21,3} \).

Then, it is easy to check that \( g_q(X + E) = \tilde{g}_q(X + E) \) holds if all coordinates of \( X \in [0,1)^{d \times n} \) are in the intervals of the form \([k\delta, (k + 1 - \alpha)\delta]\) for some \( k \in [0 : n / \delta - 1] \); i.e., the intervals in which \( \tilde{\phi}_a \) perfectly approximates \( \phi \). The Lebesgue measure of the set of such inputs \( X \) is

\[
((1 - \alpha)\delta)^{nd} \times \frac{1}{\delta^{nd}} = (1 - \alpha)^{nd},
\]

and this can be made arbitrarily close to 1 by making \( \alpha \) small. As a result, “most” of the input \( X \in D \) satisfies \( g_q(X + E) = \tilde{g}_q(X + E) \in H_\delta \), while a small fraction (of measure at most \( 1 - (1 - \alpha)^{nd} \)) can map to some other values. For most of the remaining of the proof, we will consider the fraction of inputs mapped correctly to \( H_\delta \) and bound their approximation error. We will come back to the \( 1 - (1 - \alpha)^{nd} \) fraction at the end of the proof.

### F.2 Approximating the contextual mapping \( \tilde{g}_c \) (Lemma 7)

Let us now consider approximating the contextual mapping \( \tilde{g}_c \) in Lemma 7, constructed using the hardmax \( \sigma_H \) operators, with the standard sparse self-attention layers employing \( \rho \) operator. We will call the approximation \( \tilde{g}_c \). Recall that \( \rho \) satisfies Assumption 2.

**Assumption 2.** For any \( \zeta > 0 \) and \( \eta \in (0,1) \), \( \exists t > 0 \) such that, for any column input \( v \) satisfying \( v_{j^*} - \max_{j \neq j^*} v_j \geq \zeta \) (where \( j^* = \arg \max_j v_j \)), we have \( \rho[\rho(v)]_{j^*} \geq 1 - \eta \) and \( \sum_{j \neq j^*} \rho[\rho(v)]_j \leq \eta \).

This means that \( \rho \) can closely approximate \( \sigma_H \) in the sense that whenever the input vector \( v \) to the \( \rho \) operator has a maximum element \( v_{j^*} \) by some margin \( \zeta \), then the \( j^* \)-th component of the output \( \rho[\rho(v)] \) is close to 1, while the other components of \( \rho[\rho(v)] \) are close to 0.

Recall that \( \tilde{g}_c \) consists of two parts. The first part is a composition of sparse selective shift operations, and the second is a composition of all-max-shift operations. We will first examine how “errors” are introduced when \( \sigma_H \) is replaced with \( \rho \) in both operations, discuss how the errors accumulate, and show how to choose the right \( \zeta \) and \( \eta \) to control the errors in the approximation \( \tilde{g}_c \).

#### Errors introduced by \( \rho \): Sparse selective shift operation

Recall that the key component in both the selective shift operation and all-max-shift operation is the sparse attention head \( \psi^l(\cdot) \), which computes its \( k \)-th column as the following:

\[
\psi^l(Z; b_Q)_k := u^T Z_{A_k}^l \sigma_H[(u^T Z_{A_k}^l)^T (u^T Z_k - b_Q)] = \begin{cases} 
\max_{j \in A_k^l} u^T Z_j & \text{if } u^T Z_k > b_Q, \\
\min_{j \in A_k^l} u^T Z_j & \text{if } u^T Z_k < b_Q.
\end{cases}
\]
Now suppose we replaced \( \sigma_H \) with \( \rho \) satisfying Assumption 2. Suppose each entry in \( u^T Z \) differs at least by \( \delta \), which is true in the construction of \( \zeta \). We choose \( \zeta = \delta / 2 \) and some \( 0 < \eta < 1 \), and corresponding \( t > 0 \). Then, replace \( \sigma_H[|\cdot|] \) with \( \rho[|\cdot|] \) and define

\[
\Psi^l(Z; b_Q) := u^T Z A_k^l \rho[t(u^T Z A_k^l)^T (u^T Z_k - b_Q)].
\]

If \( u^T Z_k > b_Q \), it is easy to check that \( \Psi^l(Z; b_Q) \) satisfies

\[
(1 - \eta) \max_{j \in A_k^l} u^T Z_j + \eta \min_{j \in A_k^l} u^T Z_j \leq \Psi^l(Z; b_Q) \leq \max_{j \in A_k^l} u^T Z_j.
\]

(15)

Similarly, if \( u^T Z_k < b_Q \), we have

\[
\min_{j \in A_k^l} u^T Z_j \leq \Psi^l(Z; b_Q) \leq (1 - \eta) \min_{j \in A_k^l} u^T Z_j + \eta \max_{j \in A_k^l} u^T Z_j.
\]

Now consider the approximate sparse selective shift operator \( \tilde{\Phi}^l \), implemented with \( \Psi^l \). For \( b_Q < b'_Q \), we define

\[
\tilde{\Phi}^l(Z; c, b_Q, b'_Q) := Z + [c \- \epsilon(1)] \left[ \Psi^l(Z; b_Q) \right].
\]

For any column \( Z_k \) satisfying \( b_Q < u^T Z_k < b'_Q \), we have

\[
(1 - 2\eta) \left( \max_{j \in A_k^l} u^T Z_j - \min_{j \in A_k^l} u^T Z_j \right) \leq \Psi^l(Z; b_Q) - \Psi^l(Z; b'_Q) \leq \max_{j \in A_k^l} u^T Z_j - \min_{j \in A_k^l} u^T Z_j,
\]

and for any column \( Z_k \) satisfying \( u^T Z_k \notin [b_Q, b'_Q] \), we get

\[
|\Psi^l(Z; b_Q) - \Psi^l(Z; b'_Q)| \leq \eta \left( \max_{j \in A_k^l} u^T Z_j - \min_{j \in A_k^l} u^T Z_j \right).
\]

Recall that for the hardmax \( \sigma_H \) version, we had

\[
\Psi^l(Z; b_Q) = \begin{cases} 
\max_{j \in A_k^l} u^T Z_j - \min_{j \in A_k^l} u^T Z_j & \text{if } b_Q < u^T Z_k < b'_Q, \\
0 & \text{if } u^T Z_k \notin [b_Q, b'_Q].
\end{cases}
\]

From this observation, the approximation error \( \tilde{\Phi}^l - \Psi^l \) of the selective shift operator on the \((j, k)\)-th entry of the output can be bounded as follows:

\[
\tilde{\Phi}^l(Z; c, b_Q, b'_Q)_{j, k} = \Psi^l(Z; c, b_Q, b'_Q)_{j, k} \in \begin{cases} 
[-2c\eta D_k^l, 0] & \text{if } j = 1, u^T Z_k \in (b_Q, b'_Q), \\
[-c\eta D_k^l, c\eta D_k^l] & \text{if } j = 1, u^T Z_k \notin [b_Q, b'_Q], \\
\{0\} & \text{if } j \neq 1,
\end{cases}
\]

where we used \( D_k^l := \max_{j \in A_k^l} u^T Z_j - \min_{j \in A_k^l} u^T Z_j \) for simplicity.

**Errors introduced by \( \rho \): All-max-shift operation**. Next, we examine the approximation error of the all-max-shift operation introduced by replacement of \( \sigma_H \) with \( \rho \). Let us define the approximate all-max-shift operation \( \tilde{\Omega}^l \):

\[
\tilde{\Omega}^l(Z; c) = Z + c \epsilon(1) \Psi^l(Z; 0).
\]

From (15), we can check that the approximation error \( \tilde{\Omega}^l - \Omega^l \) of the all-max-shift operation is bounded as

\[
\tilde{\Omega}^l(Z; c)_{j, k} - \Omega^l(Z; c)_{j, k} \in \begin{cases} 
[-c\eta D_k^l, 0] & \text{if } j = 1, \\
\{0\} & \text{if } j \neq 1.
\end{cases}
\]
Errors in selective shift operations. Given these approximation error bounds of single operations, we now analyze the accumulation of errors through multiple layers. We first consider the first $p\delta^{-d}$ self-attention layers in $g_c$. Recall that they consist of selective shift layers $\Psi^2(\cdot; \delta^{-d}, b - \delta/2, b + \delta/2)$ for $b \in [0 : \delta : \delta^{-d} + 1 - \delta]$ and $(p - 1)\delta^{-d}$ identity layers. A natural way to approximate these layers with standard self-attention layers is to use approximate layers $\tilde{\Psi}^2(\cdot; \delta^{-d}, b - \delta/2, b + \delta/2)$, with sufficiently large $t > 0$. As we have seen above, there is no error introduced by $\rho$ except for the first row. Thus, we will analyze the approximation error of $\tilde{\Psi}^2(\cdot; \delta^{-d}, b - \delta/2, b + \delta/2)$ for the first row only.

Let us remind the readers how the first selective shift operation (done by the first $p\delta^{-d}$ layers) originally worked in $g_c$. The input to $g_c$ is $H$, and we define $z_k := u^T H_k$ and $\Delta = \sum_{i=0}^{d-1} \delta^{-i}$. Recall from Eqs. (7) and (8) in § E.2 that

$$0 \leq z_{\gamma(2)} < z_{\gamma(3)} < \cdots < z_{\gamma(n)} < z_{\gamma(1)} \leq (n-1)\Delta + \delta^{-d+1} - \delta < n\delta^{-d}$$

and $z_{\gamma(2)} \in [0 : \delta : \delta^{-d+1} - \delta]$, so $z_{\gamma(2)}$ will undergo the selective shift by one of the self-attention layers, which updates the $(1, \gamma(2))$-th entry of the input. Let $\tilde{H}_{\gamma(2)}$ be the updated value of the column and $\tilde{z}_{\gamma(2)} := u^T \tilde{H}_{\gamma(2)}$. The new sequence satisfies

$$\Delta \leq z_{\gamma(3)} < \cdots < z_{\gamma(n)} < z_{\gamma(1)} < \tilde{z}_{\gamma(2)} < n\delta^{-2d},$$

where the strict upper bound on $\tilde{z}_{\gamma(2)}$ is from Eq. (11).

In case of the approximation $\tilde{\Psi}^2$, we have seen that the error depends on the gap between maximum and minimum of $u^T Z_i$'s, and this gap may grow larger as error accumulates; in the worst case, it may grow exponentially. To see this, suppose $a_0$ and $b_0$ are the maximum and minimum value of $u^T Z_i$'s, and they go through a selective shift operation, but they do not belong to the range of the operation $(b_0, b_0')$. Then, $a_0$ and $b_0$ will be updated to $a_1$ and $b_1$, which are bounded by

$$a_1 \leq a_0 + \delta^{-d}\eta(a_0 - b_0), \quad b_1 \geq b_0 - \delta^{-d}\eta(a_0 - b_0).$$

After the next layer, we get

$$a_2 \leq a_1 + \delta^{-d}\eta(a_1 - b_1) \leq a_0 + \delta^{-d}\eta(a_0 - b_0) + \delta^{-d}\eta(1 + 2\delta^{-d}\eta)(a_0 - b_0),$$

$$b_2 \geq b_1 - \delta^{-d}\eta(a_1 - b_1) \geq b_0 - \delta^{-d}\eta(a_0 - b_0) - \delta^{-d}\eta(1 + 2\delta^{-d}\eta)(a_0 - b_0).$$

Similarly, after $k$ such layers, we get

$$a_k \leq a_0 + (a_0 - b_0)\delta^{-d}\eta \sum_{i=0}^{k-1} (1 + 2\delta^{-d}\eta)^i,$$

$$b_k \geq b_0 - (a_0 - b_0)\delta^{-d}\eta \sum_{i=0}^{k-1} (1 + 2\delta^{-d}\eta)^i,$$

showing that the gap $a_k - b_k$ may grow exponentially in the worst case:

$$a_k - b_k \leq (1 + 2\delta^{-d}\eta)^k (a_0 - b_0).$$

In the error-less case ($\sigma_\delta$), for any input sequence $H$, the maximum possible difference between maximum and minimum of $u^T H$ is bounded above by $n\delta^{-d}$, and after one selective shift operation was done on the $\gamma(2)$-th column, the difference is then bounded by $n\delta^{-2d}$. Therefore, the worst-case possible error introduced by $\rho$ is bounded above by the sum of the worst-case errors calculated.
assuming that we started off with max-min difference \( n\delta^{-2d} \). Using this observation, the error on each first-row entry of the sequence after the first \( p\delta^{-d} \) layers is bounded above by

\[
2n\delta^{-2d} \cdot \delta^{-d} \eta^{\delta^{-d}-1} \sum_{i=0}^{\delta^{-d}-1} (1 + 2\delta^{-d}\eta)^i,
\]

where a factor of 2 is introduced because when the selective shift operation is applied to the \( \gamma(2) \)-th column, it may introduce an error which is twice the magnitude of the error introduced to the other columns. We want to make \( t > 0 \) that satisfies the assumption for

\[
\tilde{\delta} = \frac{\delta}{2}, \quad \text{and} \quad \eta = \frac{1}{2} \delta^{2d} \log \left( 1 + \frac{\delta^{2d}\tilde{\delta}}{8n^2} \right) > 0, \quad \text{where} \quad \tilde{\delta} := \min \left\{ \delta, \frac{2^{1 - 1/p}\varepsilon}{n^{1/p}} \right\}.
\]

Using such \( t \), we can control the total accumulated error by the first \( p\delta^{-d} \) selective shift operations below \( \frac{\tilde{\delta}}{8n} \):

\[
2n\delta^{-2d} \cdot \delta^{-d} \eta^{\delta^{-d}-1} \sum_{i=0}^{\delta^{-d}-1} (1 + 2\delta^{-d}\eta)^i \leq 2n\delta^{-3d} \eta (1 + 2\delta^{-d}\eta)^{\delta^{-d} - 1} - 1
\]

\[
= n\delta^{-2d} \left( 1 + \frac{\log \left( 1 + \frac{\delta^{2d}\tilde{\delta}}{8n^2} \right)}{\delta^{-d}} \right)^{\delta^{-d} - 1} \leq n\delta^{-2d} \left( \exp \log \left( 1 + \frac{\delta^{2d}\tilde{\delta}}{8n^2} \right) - 1 \right)
\]

\[
= n\delta^{-2d} \delta^{2d}\tilde{\delta} = \frac{\tilde{\delta}}{8n}.
\]

Therefore, after the first \( p\delta^{-d} \) selective shift layers, the accumulated error for each entry of the first row is at most \( \tilde{\delta}/8n \).

We can also apply similar arguments to the remaining selective shift layers. For example, for the \( j \)-th set of \( p\delta^{-d} \) selective shift layers where the operation is done on \( \gamma(j + 1) \)-th column of the input, the gap between the maximum and the minimum, including the accumulated error from previous layers, is bounded above by \( n\delta^{-(j + 1)d} \). Therefore, for this set of layers, the maximum accumulated error is bounded by

\[
2n\delta^{-(j + 1)d} \cdot \delta^{-d} \eta^{\delta^{-d}-1} \sum_{i=0}^{\delta^{-d}-1} (1 + 2\delta^{-d}\eta)^i.
\]

So, choosing \( t > 0 \) that satisfies Assumption 2 for \( \eta = \frac{\delta}{2} \) and \( \eta = \frac{1}{2} \delta^{2d} \log(1 + \frac{\delta^{(j+1)d}\tilde{\delta}}{8n^2}) \), we can control the accumulated error introduced by the \( p\delta^{-d} \) layers below \( \frac{\tilde{\delta}}{8n} \):

\[
2n\delta^{-(j + 1)d} \cdot \delta^{-d} \eta^{\delta^{-d}-1} \sum_{i=0}^{\delta^{-d}-1} (1 + 2\delta^{-d}\eta)^i \leq 2n\delta^{-(j + 2)d} \eta (1 + 2\delta^{-d}\eta)^{\delta^{-d} - 1} - 1
\]

\[
\leq n\delta^{-(j + 1)d} \left( 1 + \frac{\log \left( 1 + \frac{\delta^{(j+1)d}\tilde{\delta}}{8n^2} \right)}{\delta^{-d}} \right)^{\delta^{-d} - 1} \leq \frac{\tilde{\delta}}{8n}.
\]

In total, the accumulated error by the first \( p(n - 1)/\delta^d \) layers, which correspond to the selective shift operation part of the construction, is at most \( \frac{2(n - 1)\tilde{\delta}}{8n} \leq \frac{\tilde{\delta}}{8} \).
Errors in all-max-shift operations. For all-max-shift operations, we approximate the hardmax \( a_{\text{H}} \) all-max-shift operations \( \tilde{\Omega}^t(Z; n\delta^{-nd}) \) with its \( \rho \)-counterparts, \( \bar{\Omega}^t(Z; n\delta^{-nd}) \). We can similarly bound the accumulated error in the all-max-shift operations. Recall from § E.2 that during the whole series of all-max-shift operations, the maximum entry in the sequence is upper-bounded by \((2sn\delta^{-nd-1})^s n\delta^{-nd}\) and minimum entry is lower-bounded by \((n - 1)\Delta\). Therefore, the gap between the max and min elements, taking into consideration the errors from selective shift operations, is bounded from above by \((2sn\delta^{-nd-1})^s n\delta^{-nd}\). Then, using a similar argument as the select shift operation layers, the maximum error is bounded above by
\[
(2sn\delta^{-nd-1})^s n\delta^{-nd} \cdot n\delta^{-nd} = \sum_{i=0}^{s-1} (1 + n\delta^{-nd})^i,
\]
and we want to make it smaller than \( \bar{\delta} \). By Assumption 2, we can always choose \( t > 0 \) that satisfies the assumption for
\[
\tilde{\varepsilon} = \frac{\delta}{2}, \quad \text{and} \quad \eta = \frac{sn\delta^{-nd}}{\varepsilon} \log \left( 1 + \frac{\delta^{(nd+1)} n\delta^{-nd}}{2^{s+3s^2n^2+1}} \right) > 0.
\]
Using such \( t \), we can control the total accumulated error by the first \( p\delta^{-d} \) selective shift operations below \( \bar{\delta} \).
\[
(2sn\delta^{-nd-1})^s n\delta^{-nd} \cdot n\delta^{-nd} \eta \sum_{i=0}^{s-1} (1 + n\delta^{-nd})^i 
\leq (2sn\delta^{-nd-1})^s n\delta^{-nd} \cdot n\delta^{-nd} \eta \left( \frac{1 + n\delta^{-nd}}{1 + n\delta^{-nd}} \right)^s - 1
\leq (2sn\delta^{-nd-1})^s n\delta^{-nd} \left( \left( 1 + \frac{\delta^{(nd+1)} n\delta^{-nd}}{2^{s+3s^2n^2+1}} \right)^s - 1 \right)
\leq (2sn\delta^{-nd-1})^s n\delta^{-nd} \left( \frac{2^{s+3s^2n^2+1}}{2^{s+3s^2n^2+1} + \delta} \right) = \frac{\delta}{8}.
\]
So far, we have analyzed the total accumulated error of approximating the contextual mapping function \( \bar{g}_c \) (constructed with hardmax \( a_{\text{H}} \)) and \( \tilde{g}_c \) (constructed with \( \rho \)). We have seen that for any input \( H \in \mathbb{H}_\delta \), the approximation error can be controlled so that the error by the selective shift operation part is at most \( \tilde{\delta}/8 \) and the all-max-shift operation part is at most \( \delta/8 \). Therefore, the total error of the \((j, k)\)-th entry can be bounded as
\[
\bar{g}_c(H)_{jk} - g_c(H)_{jk} \subseteq \begin{cases} \left[ \frac{-\delta}{4}, \frac{\delta}{4} \right] & j = 1, \\ \{0\} & j \neq 1, \end{cases}
\]
for any \( H \in \mathbb{H}_\delta \).

F.3 Approximating the value mapping \( g_v \) (Lemma 8)

We now consider the approximation of the value mapping \( g_v \) with standard feed-forward layers. In \( g_v \), we implemented the function with layers of the form
\[
Z \mapsto Z + (\bar{f}(H - E)k - g_c(H)k)\phi'(u^TZ - u^Tg_c(H)k1_n^T), \quad \phi'(t) = \begin{cases} 0 & t < -\delta/2 \text{ or } t \geq \delta/2, \\ -\delta/2 \leq t < -\delta/2. \end{cases}
\]
Since the output of contextual mapping \( g_c(H) \) and its approximation \( \tilde{g}_c(H) \) differ in only the first row and by \( \delta/4 \leq \delta/4 \), one can approximate each layer in \( g_c \) by replacing \( \phi' \) with an approximation \( \tilde{\phi}' \), implementable with four ReLU’s:

\[
\tilde{\phi}'(t) = \begin{cases} 
0 & t < -\delta/2 \text{ or } t \geq \delta/2, \\
\frac{1}{2}t + 2 & -\delta/2 \leq t < -\delta/4, \\
1 & -\delta/4 \leq t < \delta/4, \\
-\frac{1}{2}t + 2 & \delta/4 \leq t < \delta/2.
\end{cases}
\]

Let \( \tilde{g}_v \) be the approximation of \( g_v \) constructed this way. Because the error on \( \tilde{g}_c \) is bounded by \( \delta/4 \), the error on the final output \( \tilde{g}_v \) is also bounded by \( \delta/4 \). That is, for any \( H \in \mathcal{H}_\delta \),

\[
\tilde{g}_v(\tilde{g}_c(H))_{jk} - g_v(g_c(H))_{jk} \in \left\{ \left[ -\frac{\delta}{4}, \frac{\delta}{4} \right], \{0\} \right\} \quad j \neq 1.
\]

Hence, using \( \tilde{\delta} := \min \left\{ \delta, \frac{2^{1/\alpha}}{n^{1/p}} \right\} \), we have

\[
\|\tilde{g}_v(\tilde{g}_c(H)) - g_v(g_c(H))\|_p^p \leq n (\frac{\tilde{\delta}}{4})^p \leq \frac{1}{2} \left( \frac{\epsilon}{2} \right)^p,
\]

for all \( H \in \mathcal{H}_\delta \).

### F.4 Finishing the proof

Recall from § F.1 that the approximated quantization function \( \tilde{g}_q \) maps most of the input \( X \in \mathcal{D} \) to \( H \in \mathcal{H}_\delta \), and a small fraction of them (of measure at most \( 1 - (1 - \alpha)^{nd} \)) to something else. Note now that the original function \( \tilde{g} = g_v \circ g_c \circ g_q \) and the approximation \( g = \tilde{g}_v \circ \tilde{g}_c \circ \tilde{g}_q \) are both bounded, so there is a global constant \( B \) such that \( \|\tilde{g}(X + E) - g(X + E)\|_p \leq B \) for all \( X \in \mathcal{D} \).

We can divide the integral over \( \mathcal{D} \) to two disjoint sets. The first one \( \mathcal{D}_1 := \{ X \in \mathcal{D} \mid \tilde{g}_q(X + E) \in \mathcal{H}_\delta \} \) is the set of input \( X \) mapped to \( \mathcal{H}_\delta \) by \( \tilde{g}_q \), and the other is its complement \( \mathcal{D}_2 = \mathcal{D} \setminus \mathcal{D}_1 \).

\[
d_p(\tilde{g}, g)^p := \int_{\mathcal{D}} \|\tilde{g}(X + E) - g(X + E)\|_p^p dX
\]

\[
= \int_{\mathcal{D}_1} \|\tilde{g}(X + E) - g(X + E)\|_p^p dX + \int_{\mathcal{D}_2} \|\tilde{g}(X + E) - g(X + E)\|_p^p dX
\]

\[
\leq \frac{1}{2} \left( \frac{\epsilon}{2} \right)^p + (1 - (1 - \alpha)^{nd}) B^p.
\]

One can make \( \alpha \) close enough to 1 so that the second term is less than \( \frac{1}{2} \left( \frac{\epsilon}{2} \right)^p \). This makes \( d_p(\tilde{g}, g) \leq \epsilon/2 \), hence finishing the proof.

### G Experimental setup

#### G.1 Copying task

We generated the synthetic dataset for the copying task. The input sequence to the copying task has the format 080s, where \( s \) is a 127 length sequence of symbols randomly sampled from the range of \([0, 127]\). The training set contains 100K sequences, while the testing set contains 10K sequences.
The maximum sequence length is $n = 256$, and we use embedding dimension $d = 256$. The model has one Transformer block with one to four attention layers with $h = 4$ attention heads of size $m = 64$, and feed-forward hidden layer size $r = 512$. We train the model with the AdamW optimizer with weight decay and no dropout. We train the model using 3,000 warmup steps and a total of 500K training steps. The learning rate is $1e^{-4}$. We use the batch size 1,024 on 8 TPUv3 chips.

For all sparsity patterns other than the RANDOM pattern, we choose the segment length $w$ to be 16 for all patterns. This segment length results in the sparsest level for the STRIDED and FIXED patterns. In Table 1, we include the sparsity level as a reference. For this task, we report the prediction accuracy for all the tokens.

### G.2 Language modeling

For the language modeling task, we train on the One Billion Word Benchmark \cite{4} which contains almost one billion tokens and a vocabulary of more than 800K tokens.

We use the Transformer model in the Tensor2Tensor framework \cite{25}. We use a 12-block (2) Transformer, with embedding dimension $d = 256$, maximum sequence length $n = 256$, number of heads $h = 8$, head size $m = 64$, and feed-forward hidden layer size $r = 1024$. Since language modeling task is autoregressive (attending to only past tokens) in nature, we evaluate the (sparse) attention score matrices and mask them to be an upper-triangular matrix. We train the model with the Adafactor with weight decay. We train the model using 10K warmup steps and a total of 240K steps. We use the batch size 4,096 on 8 TPUv2 chips.

For this task, we report the perplexity.

### G.3 Translation

For the translation task, we train on the WMT18 en-cs datasets (Europarl v7, Common Crawl corpus, News Commentary v13, and CzEng), with a total of 15M pairs of sentences, and test on the newstest2015 en-cs dataset, with 2,656 pairs.

We use the Transformer model in the Tensor2Tensor framework \cite{25} and the same setup as the language modeling task, except for having 6 blocks in the Transformer networks, with head size $m = 32$ and having autoregressive patterns only in decoders.

For this task, we report the cased BLEU score.