THE EFFECT OF ATTENTION HEAD COUNT ON TRANS-FORMER APPROXIMATION

Anonymous authors

000

001

003 004

010 011

012

013

014

016

017

018

019

021

025

026027028

029

031

033

034

037

038

040

041

042

043

044

046

047

048

051

052

Paper under double-blind review

ABSTRACT

Transformer has become the dominant architecture for sequence modeling, yet a detailed understanding of how its structural parameters influence expressive power remains limited. In this work, we study the approximation properties of transformers, with particular emphasis on the role of the number of attention heads. Our analysis begins with the introduction of a generalized D-retrieval task, which we prove to be dense in the space of continuous functions, thereby providing the basis for our theoretical framework. We then establish both upper and lower bounds on the parameter complexity required for ϵ -approximation. Specifically, we show that transformers with sufficiently many heads admit efficient approximation, whereas with too few heads, the number of parameters must scale at least as $O(1/\epsilon^{cT})$, for some constant c and sequence length T. To the best of our knowledge, this constitutes the first rigorous lower bound of this type in a nonlinear and practically relevant setting. We further examine the single-head case and demonstrate that an embedding dimension of order O(T) allows complete memorization of the input, where approximation is entirely achieved by the feed-forward block. Finally, we validate our theoretical findings with experiments on both synthetic data and real-world tasks, illustrating the practical relevance of our results.

1 Introduction

The transformer architecture (Vaswani et al., 2017) has become the foundation of modern sequence modeling, driving progress in natural language processing (Devlin et al., 2019; Brown et al., 2020), computer vision (Dosovitskiy et al., 2020), and multi-modal learning (Radford et al., 2021). Its ability to scale has enabled breakthroughs such as BERT, GPT, and ViT, making it the dominant paradigm across domains. Despite this remarkable empirical success, the theoretical principles underlying transformer expressivity remain incomplete. In particular, while universal approximation results establish that transformers can approximate arbitrary sequence-to-sequence mappings (Yun et al., 2020a; Pérez et al., 2021), much less is known about how their structural hyperparameters influence approximation efficiency.

Among transformer hyperparameters, the number of attention heads plays a central role. In practice, large models often adopt head counts such as 32, 64, or 128 (e.g., Devlin et al. (2019); Dosovitskiy et al. (2020); Touvron et al. (2023); Jiang et al. (2023); Grattafiori et al. (2024) see Table 4 for more), yet this choice is largely heuristic: there is no principled understanding of how many heads are needed for a given task, nor of the costs incurred when the head count is insufficient. Theoretical progress on this question has so far been limited. Most existing results focus on upper bounds, showing that transformers with sufficiently many heads or with extremely large embedding dimension in the single-head case can achieve universal approximation or good approximation rate, but offering little insight into the limitations that arise when the head count is insufficient. Moreover, many analyses rely on strong simplifications—such as restricting to linear embeddings, isolating the attention block, or linearizing the architecture. While these assumptions make the problem more tractable, they severely restrict the model's expressive power and prevent the derivation of rigorous lower bounds in realistic nonlinear settings.

In this work, we address this gap by analyzing single-layer transformers on sequence-to-vector tasks. To this end, we introduce a new function class, the *generalized D-retrieval tasks*, which we design as a structured but expressive family motivated by retrieval problems. Each coordinate is defined

by $\bar{z}_i(X_T) = \min_{t \in S_i} f_i(x(t)), i = 1, \dots, D$ for subsets $S_i \subseteq [T]$, and the overall target takes the form $H(X_T) = F_0(\bar{z}_1(X_T), \dots, \bar{z}_D(X_T))$. By construction, this class extends retrieval-style problems while being dense in the space of continuous sequence-to-vector mappings, ensuring that results obtained in this setting reflect general approximation behavior.

The central challenge arises when the number of heads h is smaller than the intrinsic dimension D of the target. In this case, multiple coordinates $z_i(X_T)$ must be represented by the same head, creating an information bottleneck: the attention layer maps distinct sequences to nearly indistinguishable representations, forcing the feed-forward network to perform the separation. We show that overcoming this bottleneck requires parameter growth exponential in the sequence length T, namely $O(1/\epsilon^{cT})$ parameters for ϵ -accuracy, thus establishing the first rigorous lower bounds for transformers in nonlinear settings. In contrast, when $h \geq D$, heads can specialize to distinct coordinates z_i , eliminating the bottleneck and enabling efficient approximation.

Our results advance the theoretical understanding of attention by showing, that insufficient head count provably limits expressivity in realistic regimes. Experiments on both synthetic tasks and real-world retrieval data confirm that the predicted scaling laws persist in practice.

Contributions. Our main contributions are as follows:

First, we establish the first rigorous lower bounds for transformers in nonlinear settings, showing that when h < D, parameter complexity grows exponentially with sequence length.

Second, we provide constructive upper bounds, proving that $h \ge D$ enables efficient approximation with parameter growth independent of sequence length T.

Third, in the memorization regime, single-head transformers with embedding dimension $n \geq Td$ approximate by memorizing sequences, with the complexity residing in the feed-forward block.

2 Related Work

Several works have studied the approximation and expressivity properties of transformers. The universal approximation property was first established in Yun et al. (2020a), and later extended to transformers with sparse attention matrices in Yun et al. (2020b). The approximation rate of single-layer transformers with one head was analyzed in Jiang & Li (2024). Amsel et al. (2024) investigated how the rank of the attention matrix influences expressivity for a specific nearest-neighbor target can be constructed. They showed that when the rank is insufficient, the number of heads required for approximation grows exponentially, independent of sequence length. In a related direction, Bhojanapalli et al. (2020) argued that setting the rank of the attention matrix equal to the sequence length enhances expressivity. Beyond finite-dimensional settings, Takakura & Suzuki (2023) considered sequences of infinite dimension, characterizing approximation rates in terms of target function smoothness. Similarly, Wang & E (2024) studied special classes of target functions and demonstrated that approximation error scales polynomially with the number of heads. In addition to these approximation-theoretic results, several works have investigated broader notions of expressivity. Dehghani et al. (2019); Pérez et al. (2021) established the Turing completeness of transformers, and Giannou et al. (2023) showed that transformers can represent arbitrary computer programs in a looped setting. Finally, Mahdavi et al. (2024) examined memorization capacity, proving that the number of samples that can be stored scales linearly with the number of heads.

3 Preliminaries

Input and Output We consider the input space

$$\mathcal{X}_T = \{ x(s) \in [0, 1]^d : s \in [T] \}, \tag{1}$$

where $[T] = \{1, ..., T\}$. We call T the length of the input sequence. The output is a single vector $y \in \mathbb{R}^l$, where l is independent of T and specified by the task.

For example, in a text retrieval task one may take d to be the max number of tokens per candidate, T the number of candidates, and l the size of the output representation.

Input Representation. Each token is mapped to an *E*-dimensional vector by a trainable encoder

$$P_{\phi}: [0,1]^d \times [T] \to \mathbb{R}^E, \qquad (\boldsymbol{x},s) \mapsto P_{\phi}(\boldsymbol{x},s),$$

which jointly incorporates the content x and its position s. Given $X_T = \{x(s)\}_{s=1}^T \in \mathcal{X}_T$, the embedded sequence is

$$\hat{X}_T = \{ \hat{x}(s) = P_{\phi}(x(s), s) \in \mathbb{R}^E : s \in [T] \}.$$
(2)

This formulation subsumes common designs where P_{ϕ} combines a content embedding with either learned or deterministic positional encoding.

For example, if $\operatorname{Emb}(x)$ is a content embedding map and p(t) a positional code, then common schemes correspond to

$$P_{\phi}(x(t),t) = \text{Emb}(x(t)) + p(t)$$
 (additive PE),

or

$$P_{\phi}(x(t),t) = (\operatorname{Emb}(x(t)), p(t))$$
 (concatenated PE).

Following common practice, we append a trainable classification token $\hat{c}_0 \in \mathbb{R}^E$ to the sequence. The final input to the transformer is

$$\hat{X}[T] = {\hat{x}(1), \dots, \hat{x}(T), \hat{c}_0} \in \mathbb{R}^{E \times (T+1)},$$
 (3)

and the output \hat{y} is taken from the (T+1)-th position corresponding to \hat{c}_0 .

Transformer Hypothesis Class With the input space and embedding defined, we then formulate the transformer hypothesis space.

We consider a single-layer transformer based on the standard architecture (Vaswani et al., 2017), with two modifications introduced for analytical simplicity. Firstly, we omit layer normalization, noting that its removal does not harm the approximation capacity of the model. Secondly, we exclude residual connections outside the feed-forward network. In the single-layer sequence-to-vector setting, where the output is read from a designated classification token, the residual branch can be merged into the feed-forward transformation by reparameterization, thus these likewise do not alter the expressive power of the architecture.

For an h-head, single-layer transformer, let n denote the embedding dimension $per\ head$ and E=nh the total embedding dimension. The output is

$$\hat{y} = \hat{H}(\hat{X}[T])$$

$$= \hat{F}\Big(\hat{c}_0 + W_O \operatorname{Concat}_{i=1}^h \Big(\sum_{t=1}^T \sigma \big[(W_{Q,i}\hat{c}_0)^\top W_{K,i}\hat{x}(t) \big] W_{V,i}\hat{x}(t) \Big) \Big), \tag{4}$$

where for each head $i, W_{Q,i}, W_{K,i} \in \mathbb{R}^{n \times E}$ are the query/key projection matrices, $W_{V,i} \in \mathbb{R}^{n \times E}$ is the value projection, $W_O \in \mathbb{R}^{E \times E}$ is the output projection applied to the concatenated heads, and $\hat{F} : \mathbb{R}^E \to \mathbb{R}^l$ is a feed-forward network which we call it the *feed-forward block*. The softmax with scaling factor β is defined by

$$\sigma[\rho](t) = \frac{\exp(\beta \,\rho(t))}{\sum_{t'=1}^{T} \exp(\beta \,\rho(t'))}, \qquad \beta > 0.$$
 (5)

and $\beta>0$ may be chosen arbitrarily large in order to make the softmax attention mechanism approximate a hardmax.

We denote this family by

$$\mathcal{H}(h, n, d, T, k), \tag{6}$$

the class of single-layer transformers with h heads, per-head embedding dimension n, input dimension d, sequence length T, and parameter count k. Each $H \in \mathcal{H}(h, n, d, T, k)$ is a mapping

$$H: \mathbb{R}^{d \times T} \to \mathbb{R}^l$$
.

implemented by the encoder $P_{\phi}: [0,1]^d \times [T] \to \mathbb{R}^{nh}$, concatenation of the classification token \hat{c}_0 , a multi-head attention layer with projections $\{W_{Q,i},W_{K,i},W_{V,i}\}_{i=1}^h,W_O$, and a feed-forward network $\hat{F}: \mathbb{R}^{nh} \to \mathbb{R}^l$. Thus H has the form equation 4, with parameter count k referring to the weights and biases in FFNs (P_{ϕ},\hat{F}) .

Approximation Problem With the hypothesis class specified, we now formalize the approximation problem, which provides the framework for analyzing the expressive power of transformers.

Definition 1 (ϵ -approximation). Let $\mathcal{X}_T \subset \mathbb{R}^{d \times T}$ be a compact domain, and let $F: \mathcal{X}_T \to \mathbb{R}^l$ be a target function. We say that the hypothesis class $\mathcal{H}(h,n,d,T,k)$ ϵ -approximates F on \mathcal{X}_T if there exists $\hat{H} \in \mathcal{H}(h, n, d, T, k)$ such that

$$\sup_{X_T \in \mathcal{X}_T} \|\hat{H}(X_T) - F(X_T)\|_{\infty} < \epsilon.$$

Remark. When the target is a function class \mathcal{F} , we say that $\mathcal{H}(h, n, d, T, k)$ ϵ -approximates \mathcal{F} if it ϵ -approximates every $F \in \mathcal{F}$ on \mathcal{X}_T .

GENERALIZED D-RETRIEVAL TASKS

Target functions. To motivate our construction, consider a simple one-dimensional example:

$$\mathcal{X}_T = \{ X_T = (x(1), \dots, x(T)) : x(t) \in [0, 1] \},$$

with target

162

163

164

165

166

167

168 169 170

171 172 173

174 175

176

177 178

179

181

182

183

184

185

186 187

188

189

190 191

192

193

194

195 196

197

199

200

201

202

203 204

205

206

207

208

209

210

211

212

213

215

$$H(X_T) = \max_{1 \le t \le T} x(t) + \min_{1 \le t \le T} x(t).$$
 (7)

This task requires the model to extract two distinct features from the sequence—the maximum and the minimum—before combining them. It can thus be viewed as a retrieval problem with intrinsic dimension D=2, corresponding to the two independent features being aggregated.

This example illustrates the broader idea behind our target class: retrieval-style problems where multiple salient features must be identified and combined. We now formalize this intuition by defining the family of generalized D-retrieval tasks.

Mathematical Formulation Formally, for each i = 1, ..., D, let $f_i : [0, 1]^d \to [0, 1]$ be C^2 and define

$$\bar{z}_i(X_T) = \min_{t \in S_i} f_i(x(t)), \qquad S_i \subseteq [T], \ |S_i| \ge \frac{1}{4}T, \tag{8}$$

so that $\bar{z}(X_T) = (\bar{z}_1(X_T), \dots, \bar{z}_D(X_T)) \in [0, 1]^D$. The target is then

$$H(X_T) = F_0(\bar{z}(X_T)), \tag{9}$$

where $F_0:[0,1]^D\to\mathbb{R}$ is C^1 . For vector-valued targets $F:[0,1]^{d\times T}\to\mathbb{R}^l$, the extension is coordinate-wise, since each coordinate function can be approximated separately. Therefore, it suffices to consider the scalar-valued case. We denote by $\mathcal{F}_D^{1,T}$ the class of all such functions H, and we call D the *intrinsic dimension* of this target.

Assumptions on the target class For the theoretical analysis to be tractable we impose the following conditions:

Assumption 1 (Model constraints). The model constraints are as follows:

(1.1) The embedding P_{ϕ} satisfies

$$||P_{\phi}(x(s),s)||_2 \le 1, \quad \forall s \in [T], X_T \in \mathcal{X}_T,$$

ensuring embedded inputs remain uniformly bounded.

- (1.2) The post-attention mapping \hat{F} is a two-layer feed-forward network with 1-Lipschitz activation, hence a universal approximator on compact domains.
- (1.3) All weights in \hat{F} and entries of the attention matrices $\{W_{Q,i}, W_{K,i}, W_{V,i}\}, W_{Q}$ are bounded in magnitude by 1, ensuring stability of the model.

Assumption 2 (Target class constraint). The target functions defined in equation 9 satisfy the following:

- (2.1) Each $f_i: [0,1]^d \to [0,1]$ attains its unique global minimum z_i at a point $x^{(i)} \in [0,1]^d$.
- (2.2) The minimizers $\{x^{(i)}\}_{i=1}^{D}$ are pairwise distinct. 214
 - (2.3) The Hessian $\nabla_x^2 f_i(x^{(i)})$ is positive definite for all $i = 1, \dots, D$.
 - (2.4) The gradient $\nabla_z F_0(z_1,\ldots,z_D)$ has all coordinates strictly nonzero.

Having introduced the generalized *D*-retrieval tasks, it remains to ask whether this family is sufficiently expressive. To address this, we now establish the *universality of the target class*: the family is dense in the space of continuous sequence-to-vector mappings.

Theorem 1 (Density of the target class). For fixed d, T, the family $\{\mathcal{F}_D\}_{D=1}^{\infty}$ is dense in $C(\mathcal{X}_T)$. That is, for every $F \in C(\mathcal{X}_T)$ and every $\epsilon > 0$, there exists D and $f \in \mathcal{F}_D$ such that

$$\max_{X \in \mathcal{X}_T} |F(X) - f(X)| \le \epsilon.$$

The proof is deferred to Appendix A.1. This density property highlights that our specially designed target family is not overly restrictive; rather, it forms a sufficiently general class to capture arbitrary continuous sequence-to-vector mappings.

5 Approximation rate of Generalized D-Retrieval Tasks

Theorem 1 establishes that the generalized *D*-retrieval tasks form a dense family in the space of continuous sequence-to-vector functions. The next step is to analyze the efficiency with which transformers approximate these functions. To this end, we begin by stating two standard approximation assumptions regarding how well the fundamental building blocks of the target can be approximated.

Assumption 3 (Approximation of components). We assume the following approximation properties hold.

(A1) There exist constants $C_1 > 0$ and $\gamma > 0$ such that for every $\delta > 0$, the function $F_0 : [0,1]^D \to \mathbb{R}$ can be δ -approximated by a two-layer feed-forward network Φ_{δ} of width at most C_1/δ^{γ} , i.e.,

$$\sup_{x \in [0,1]^D} |F_0(x) - \Phi_{\delta}(x)| \le \delta.$$

(A2) There exist constants $C_2>0$ and $\gamma>0$ (possibly different from (A1)) such that for each $i=1,\ldots,D$ and every $\delta>0$, the function $f_i:[0,1]^d\to[0,1]$ can be δ -approximated by a two-layer feed-forward network $\Psi_{i,\delta}$ of width at most C_2/δ^{γ} , i.e.,

$$\sup_{x \in [0,1]^d} |f_i(x) - \Psi_{i,\delta}(x)| \le \delta.$$

These assumptions are reasonable: by the classical result of (Cybenko, 1989), two-layer networks can approximate continuous functions on compact domains. In particular, if the Barron norm is finite, one may take $\gamma=2$ (Barron, 1993); even in the worst case, setting $\gamma=\max(d,D)$ yields approximation rates comparable to uniform grid discretizations, which still suffices for our analysis.

We now present our main theoretical result. It establishes upper and lower bounds on the approximation rates of transformers within the generalized D-retrieval framework. In particular, the lower bound in part (2) provides the first rigorous evidence that insufficient head count h < D leads to exponential parameter complexity, revealing a fundamental expressivity bottleneck.

Theorem 2 (Approximation rates of transformers). Fix d, T. Under Assumption 3, the following hold for the target class $\mathcal{F}_D^{d,T}$:

- (1) Sufficient expressivity with D heads. For h=D and embedding dimension n=2 per head, there exists a constant $C_{d,D,T}>0$ such that $\forall M>\frac{C_{d,D,T}}{\epsilon^{\gamma}}$. the hypothesis class $\mathcal{H}(h,n,d,T,M)$ ϵ -approximates $\mathcal{F}_D^{d,T}$.
- (2) Lower bound with s < D heads. For h = s < D, define

$$k = \frac{(\frac{1}{4}T - s - D + 1)}{(n+1)s+1} - 1,$$

then

$$\min\{M: \mathcal{H}(h, n, d, T, M) \in \text{approximates } \mathcal{F}_D^{d,T}\} = \Omega(\frac{1}{\epsilon^k}).$$

(3) Single-head large embedding dimension. For h=1 and per-head embedding dimension $n \geq Td$, if the feed-forward block is a 5-layer ReLU neural network, then there exists a constant $C_{d,D,T} > 0$ such that for all $M > \frac{C_{d,D,T}}{\epsilon^{1+\gamma}}$, the hypothesis class $\mathcal{H}(h,n,d,T,M)$ can ϵ -approximate $\mathcal{F}_D^{d,T}$.

The proof is deferred to Appendix A.2.

Remark. The lower bound in Theorem 2 (2) remains essentially tight under several relaxations of the feed-forward block \hat{F} . If \hat{F} uses Heaviside activations instead of 1-Lipschitz activations, matching upper bounds can be constructed, but this case is impractical since Heaviside activations are rarely used in practice. If parameter norms are permitted to scale as $O(T^{1/\epsilon})$, the parameter count can be reduced to $O(1/\epsilon^{\gamma+1})$, though this scenario is likewise unrealistic in practical settings. Finally, if \hat{F} is allowed up to five layers, the lower bound changes to $\Omega(1/\epsilon^{k/4})$, which does not alter the qualitative conclusion.

Theorem 2 highlights how approximation efficiency depends on head count: enough heads allow specialization, too few force inefficient compression, and a single large head can rely on memorization. To illustrate these cases concretely, we now revisit the toy example from equation 7 and discuss how each part of the theorem works in that setting.

Case (1): $h \geq D$ heads. Theorem 2 (1) shows that when the number of heads matches the intrinsic dimension D of the target, the transformer can allocate one head per component feature, allowing each head to specialize and leaving the feed-forward block to aggregate their outputs. This yields efficient approximation with $O(M^{-1/\gamma})$ error for parameter count M, independent of sequence length T.

In the toy example with D=2, one head naturally tracks the maximum and the other the minimum, so the task is solved directly without incurring inefficiency. This illustrates how having "enough heads" removes the unfavorable scaling in T and explains the practical advantage of multiple heads beyond universal approximation results (e.g., Kajitsuka & Sato (2023)).

Case (2): h < D heads. Theorem 2 (2) establishes that when the number of heads is smaller than the intrinsic dimension D, the parameter count required to achieve a given accuracy can grow exponentially in the sequence length T. This lower bound highlights why insufficient heads lead to severe inefficiency. Intuitively, each head can be viewed as specializing in one coordinate of the minima structure in equation 9. When h < D, a single head must encode multiple roles simultaneously.

In the toy example with D=2, one head is forced to capture both the maximum and the minimum across all T positions. Since softmax attention only produces weighted averages, the head must effectively encode information from multiple sequence elements simultaneously. As T increases, the number of relevant elements to distinguish grows linearly with T, yet they are compressed into an n-dimensional vector whose size does not scale with T. The feed-forward block must then disentangle these increasingly entangled representations, which requires parameters exponential in T. This explains why the parameter requirement scales as $\Omega(1/\epsilon^{cT})$ and why the scaling improves dramatically once $h \geq D$.

Case (3): single head with large embedding. Theorem 2 (3) shows that when the embedding dimension scales with the sequence length, $E=n \geq T$, the model can encode the entire sequence into the classification token \hat{c}_0 . Concretely, each input can be embedded as $x(t)e_t$, where e_t is the t-th standard basis vector, so that trivial attention aggregates to

$$\frac{1}{T}(x(1),\ldots,x(T)) \in [0,1]^T$$
,

which preserves the full sequence. The feed-forward block \hat{F} can then recover the target relation efficiently. Unlike memorization of training data (Mahdavi et al., 2024), this mechanism can generalize since it captures the relation itself. Moreover, approximating extrema functions such as max and min with a shallow ReLU network is straightforward (see Lemma 9), requiring width $O(T/\epsilon)$ for ϵ accuracy. However, this regime is impractical, as it demands embedding dimensions that grow linearly with T.

6 EXPERIMENTS

Theorem 2 provides theoretical insights into how the approximation ability of transformers depends on the number of heads. In this section, we illustrate these insights empirically. We begin with syn-

thetic tasks that mirror the structure of the generalized *D*-retrieval tasks, and then turn to real datasets (MS MARCO and CIFAR-10) to examine whether similar scaling behaviors arise in practice.

6.1 Numerical verification of Theorem 2 with synthetic dataset

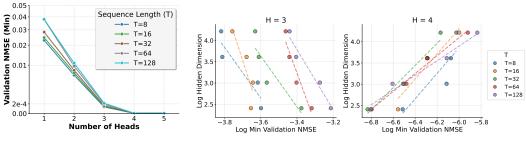
We design a synthetic task aligned with the target class analyzed in Theorem 2. Given a sequence $X = \{x(1), \dots, x(T)\}$ of length T with $x(t) \in \mathbb{R}^4$, the output is

$$y = \sum_{i=1}^{4} \max_{1 \le t \le T} a_i^{\top} x(t),$$

where $a_1, \ldots, a_4 \in \mathbb{R}^4$ are fixed. Inputs are sampled i.i.d. from $x(t) \sim \mathcal{N}(0, I_4)$. For $T \in \{8, 16, 32, 64, 128\}$ we generate 8000 training and 2000 validation examples.

On this task, we evaluate single-layer transformers with head numbers $h \in \{1, 2, 3, 4, 5\}$ and fixed per-head embedding dimension. Each x(t) is embedded via a two-layer ReLU MLP and concatenated with a trainable classification token c_0 , after which a single-layer multi-head attention block (without residuals or normalization) processes the sequence. A two-layer GeLU MLP then outputs the scalar prediction. Both MLPs have the same hidden dimension N.

Then for each (h,T), models are trained under multiple random seeds. We report the *minimal normalized mean squared error (NMSE)* across seeds to reduce optimization noise and highlight expressivity. NMSE, equivalent to $1-R^2$, corrects for the variance shrinkage of maxima as T grows, thus enabling fair comparison across lengths. Further training details are given in Appendix B.1.1.



(a) NMSE vs. Number of Heads h.

(b) Log N vs. Log Accuracy (NMSE)

Figure 1: Results on the synthetic example. (a) NMSE vs. number of heads h for sequence lengths $T \in \{8, 16, 32, 64, 128\}$, hidden dimension fixed at N=32. Note that there is a transition at H=4. (A table of mean and variance values corresponding to these curves is provided in Table 1.) (b) Log Hidden Dimension N vs. Log Accuracy for different sequence lengths T. The parameter count k for the MLPs change linearly with N. (Plots for H=1 and H=2 is in Figure 4.)

Figure 1a shows minimal validation NMSE versus head number h across sequence lengths T. Performance improves monotonically with h and exhibits a clear transition near the intrinsic dimension D=4. For h< D, NMSE grows with T, as limited heads must encode multiple extrema and the FFN becomes inefficient. Once $h\geq D$, curves flatten across T, indicating that heads specialize to different coordinates and the FFN aggregates them very effectively. Normalization by NMSE ensures comparability across T, despite the increasing concentration of the max-of-Gaussians target.

Figure 1b highlights a phase transition between h=3 and h=4, with h=D=4 equal to the intrinsic dimension of the target. When $h\leq 3$, the negative log NMSE scales approximately linearly with the log parameter count (proportional to the MLP hidden dimension N), in agreement with Theorem 2 (2). Moreover, for a fixed parameter count, larger T yields higher NMSE (worse approximation). Equivalently, as indicated by the fitted scaling lines, achieving the same error requires larger parameter counts when T increases, in line with Theorem 2 (2).

In contrast, for h=4 these trends change qualitatively. Validation error reaches the order of 10^{-6} , indicating near-perfect generalization, yet the slope with respect to parameter count reverses: larger MLPs yield slightly higher validation NMSE, a signature of tiny overfitting. The dependence on T also changes in this regime; see Remark 6.1 for details.

Remark. When $h \geq D = 4$, we also observe that the validation NMSE first decreases rapidly and then increases slowly as T grows. For shorter sequences, the model with enough heads can either capture the pattern through attention (Theorem 2 (1)) or rely on a memorization-based strategy with the feed-forward network (Theorem 2 (3)). Both approaches generalize reasonably well, but the memorization-based one does so less effectively. For longer sequences, memorization becomes infeasible and the model relies on attention, which generalizes better; however, longer sequences may also be more sensitive to parameterization, and the observed curve likely reflects a tradeoff between these effects. See Figure 3 in Appendix.

6.2 EXPERIMENTS ON REAL DATASETS

We conduct two additional experiments on real datasets to assess the practical relevance of our theoretical findings. The first is a text retrieval task based on MS MARCO, and the second is an image classification task based on CIFAR-10. We focus on training accuracy as a proxy for approximation error, as it directly reflects model capacity. The experiments examine whether the phase transition around the intrinsic dimension D, predicted by Theorem 2, also manifests in practice.

MS MARCO (text retrieval). We construct retrieval-style datasets from the MS MARCO passage ranking collection (Bajaj et al., 2018), where each query is paired with one positive passage and T-1 mined hard negatives ($T \in \{8, 16, 32, 64\}$). We train a two-layer transformer encoder with per-head embedding dimension fixed at 32, varying the number of heads across $\{1, 2, 4, 6, 8, 10, 12, 14, 16\}$. Input text is tokenized using the BERT tokenizer, and word, positional, and segment embeddings from pretrained BERT (Devlin et al., 2019) are kept frozen. These 768-dimensional embeddings are linearly projected to the embedding size $E = \text{heads} \times 32$, after which only the projection and transformer layers are trained. Full dataset construction and training details are given in Appendix B.2.

CIFAR-10 (image classification). We further evaluate on the CIFAR-10 dataset (Krizhevsky, 2009) using a four-layer Vision transformer (ViT) (Dosovitskiy et al., 2020). Each image of size 32×32 is divided into non-overlapping 8×8 patches (patch size = 8), which are linearly embedded. The transformer encoder has per-head embedding dimension fixed at 16, and we vary the number of heads across $h \in \{1, 2, 4, 8, 10, 11, 12, 13, 14, 16, 20, 24\}$. To vary the sequence length, we extend the border with interpolation around each image to enlarge its side length, after which the sequence length is given by $\left(\frac{\text{image side length}}{\text{patch size}}\right)^2 + 1$, including the classification token. Figure 6 shows some of the examples. Full dataset preprocessing and training details are provided in Appendix B.3.

Result analysis. Both experiments exhibit the same qualitative trend as in the synthetic setting. Figure 2a shows that in the text retrieval experiment, when h < 12, accuracy declines as the sequence length T increases, consistent with Theorem 2 (2). Once h > 12, this dependence on T disappears, and performance remains stable. Taking $Err(h,T) = 1 - \mathrm{Accuracy}(h,T)$ as error, by using $cT^{\beta} \exp(\alpha h/T^{\delta})$ to approximate (Err(h,T)) in log scale under MAE and drop-outs (h=1,12,14,16) are dropped out as outliers, $\delta=0.25>0$, $\alpha=-1.40<0$), figure 2b illustrates that when h < 12, $-\log(Err(h,T)) \propto h/T^{\delta}$, highly consistent with the order in Theorem 2 (2) under fixed parameter count M. The flattening of curves after h > 12 is also consistent with theory.

Figure 2c shows similar trend in image classification, with intrinsic dimension at h=10. Figures 2d and 2e illustrates weighted reversal score, calculated by $R(h)=\frac{1}{w_h}\sum_{T_1< T_2}\max((err(T_1)-err(T_2)),0)$ with normalization factor $w_h=\max_T err(T)-\min_T err(T)$, detects the existence of longer T yielding smaller error for this head number h. Such phenomenon leads to positive R(h), and it also indicates phase transition as explained in remark 6.1. Figure 2e further verified this.

7 Conclusion

In this work we investigated the approximation properties of single-layer transformers. We first introduced a structured target family, the generalized *D*-retrieval task, that is broad enough to capture general sequence-to-vector mappings (Theorem 1). Within this setting, we analyzed how the approximation efficiency of transformers depends on architectural choices, especially the number of head. Our results indicate that having a sufficient number of heads leads to efficient approximation,

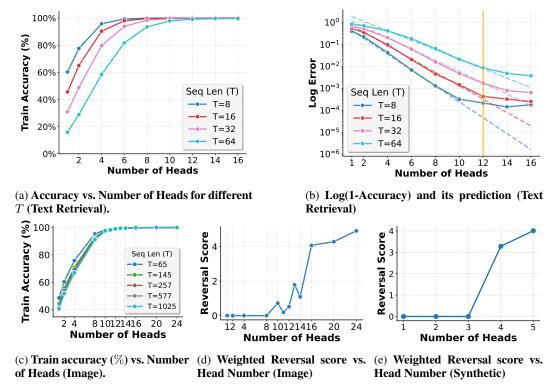


Figure 2: **Experiments on real datasets.** Training performance with different numbers of heads h across different sequence lengths T. (a) Accuracy vs. number of heads for different T in text retrieval; phase transition near h=12. Mean and standard deviation see Table 2. MRR shows a similar trend, see Fig. 5 in the appendix. (b) Phase transition for text retrieval. (c) Accuracy vs. number of heads for different T in image classification; phase transition near h=10. Mean and standard deviation see Table 3. (d) Weighted Reversal Score for Image Classification, err=1-Accuracy. The plot becomes positive when $h\geq 10$, indicating phase transition. (e) Weighted Reversal Score for Synthetic Experiment, it becomes positive at h=4, exactly the intrinsic dimension of the task.

while an insufficient number of heads forces the parameter count to grow exponentially with sequence length T. We also examined the single-head case, where large embedding dimension allows sequence memorization but shifts the complexity to the feed-forward block (Theorem 2). These findings clarify the roles played by head count in transformer expressivity.

Our experiments on both synthetic and real datasets reveal a non-trivial phase transition around the intrinsic dimension D, consistent with theoretical analysis. When the number of heads is below D, models exhibit higher error for the same parameter count as sequence length T increases. Once the head count reaches or exceeds D, approximation rate becomes independent of sequence lengths T. This transition is also observed in real-world datasets with deeper architectures, indicating that the notion of intrinsic dimension is not only theoretical but also practically relevant. In particular, evaluating performance with varying T may serve as a practical probe of the task's intrinsic dimension, which could in turn inform head-count selection and the number of heads to retain under pruning.

Limitations. We conclude by noting several limitations of this study. Firstly, although the analyzed target class is dense, the phenomena of interest are most naturally manifested in retrieval-style tasks aligned with our setting. Secondly, our analysis is restricted to single-layer transformers; while experiments on real datasets suggest similar behaviors in deeper architectures, a rigorous multi-layer theory remains open. Finally, the tradeoff between sequence memorization and pattern learning—observed for shorter sequences (cf. Remark 6.1)—has not yet been established rigorously and merits further investigation.

REFERENCES

- Noah Amsel, Gilad Yehudai, and Joan Bruna. Quality over Quantity in Attention Layers: When Adding More Heads Hurts. In *The Thirteenth International Conference on Learning Representations*, October 2024.
- Payal Bajaj, Daniel Campos, Nick Craswell, Li Deng, Jianfeng Gao, Xiaodong Liu, Rangan Majumder, Andrew McNamara, Bhaskar Mitra, Tri Nguyen, Mir Rosenberg, Xia Song, Alina Stoica, Saurabh Tiwary, and Tong Wang. MS MARCO: A Human Generated MAchine Reading Comprehension Dataset, October 2018.
- A.R. Barron. Universal approximation bounds for superpositions of a sigmoidal function. *IEEE Transactions on Information Theory*, 39(3):930–945, May 1993. ISSN 1557-9654. doi: 10.1109/18.256500.
- Srinadh Bhojanapalli, Chulhee Yun, Ankit Singh Rawat, Sashank J. Reddi, and Sanjiv Kumar. Low-Rank Bottleneck in Multi-head Attention Models, February 2020.
- Tom B. Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, Sandhini Agarwal, Ariel Herbert-Voss, Gretchen Krueger, Tom Henighan, Rewon Child, Aditya Ramesh, Daniel M. Ziegler, Jeffrey Wu, Clemens Winter, Christopher Hesse, Mark Chen, Eric Sigler, Mateusz Litwin, Scott Gray, Benjamin Chess, Jack Clark, Christopher Berner, Sam McCandlish, Alec Radford, Ilya Sutskever, and Dario Amodei. Language Models are Few-Shot Learners, July 2020.
- G. Cybenko. Approximation by superpositions of a sigmoidal function. *Mathematics of Control, Signals and Systems*, 2(4):303–314, December 1989. ISSN 1435-568X. doi: 10.1007/BF02551274.
- Mostafa Dehghani, Stephan Gouws, Oriol Vinyals, Jakob Uszkoreit, and Łukasz Kaiser. Universal Transformers. In *arXiv:1807.03819 [Cs, Stat]*, March 2019.
- Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: Pre-training of Deep Bidirectional Transformers for Language Understanding. *arXiv:1810.04805 [cs]*, May 2019.
- Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, and Neil Houlsby. An Image is Worth 16x16 Words: Transformers for Image Recognition at Scale. In *International Conference on Learning Representations*, September 2020.
- Angeliki Giannou, Shashank Rajput, Jy-Yong Sohn, Kangwook Lee, Jason D. Lee, and Dimitris Papailiopoulos. Looped Transformers as Programmable Computers. In *Proceedings of the 40th International Conference on Machine Learning*, pp. 11398–11442. PMLR, July 2023.
- Aaron Grattafiori, Abhimanyu Dubey, Abhinav Jauhri, Abhinav Pandey, Abhishek Kadian, and Al-Dahle. The Llama 3 Herd of Models, November 2024.
- Albert Q. Jiang, Alexandre Sablayrolles, Arthur Mensch, Chris Bamford, Devendra Singh Chaplot, Diego de las Casas, Florian Bressand, Gianna Lengyel, Guillaume Lample, Lucile Saulnier, Lélio Renard Lavaud, Marie-Anne Lachaux, Pierre Stock, Teven Le Scao, Thibaut Lavril, Thomas Wang, Timothée Lacroix, and William El Sayed. Mistral 7B, October 2023.
- Haotian Jiang and Qianxiao Li. Approximation Rate of the Transformer Architecture for Sequence Modeling. In *The Thirty-eighth Annual Conference on Neural Information Processing Systems*, November 2024.
- Jeff Johnson, Matthijs Douze, and Hervé Jégou. Billion-scale similarity search with GPUs, February 2017.
- Tokio Kajitsuka and Issei Sato. Are Transformers with One Layer Self-Attention Using Low-Rank Weight Matrices Universal Approximators?, July 2023.
 - A. Krizhevsky. Learning Multiple Layers of Features from Tiny Images. In *Technical Report 0*, 2009.

- Sadegh Mahdavi, Renjie Liao, and Christos Thrampoulidis. Memorization Capacity of Multi-Head Attention in Transformers, March 2024.
- Jorge Pérez, Pablo Barceló, and Javier Marinkovic. Attention is Turing-Complete. *Journal of Machine Learning Research*, 22(75):1–35, 2021. ISSN 1533-7928.
 - Alec Radford, Jong Wook Kim, Chris Hallacy, Aditya Ramesh, Gabriel Goh, Sandhini Agarwal, Girish Sastry, Amanda Askell, Pamela Mishkin, Jack Clark, Gretchen Krueger, and Ilya Sutskever. Learning Transferable Visual Models From Natural Language Supervision, February 2021.
 - Stephen Robertson and Hugo Zaragoza. The Probabilistic Relevance Framework: BM25 and Beyond. *Found. Trends Inf. Retr.*, 3(4):333–389, April 2009. ISSN 1554-0669. doi: 10.1561/1500000019.
 - Shokichi Takakura and Taiji Suzuki. Approximation and Estimation Ability of Transformers for Sequence-to-Sequence Functions with Infinite Dimensional Input, May 2023.
 - Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, Aurelien Rodriguez, Armand Joulin, Edouard Grave, and Guillaume Lample. LLaMA: Open and Efficient Foundation Language Models, February 2023.
 - Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N Gomez, Ł ukasz Kaiser, and Illia Polosukhin. Attention is All you Need. In *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017.
 - Mingze Wang and Weinan E. Understanding the Expressive Power and Mechanisms of Transformer for Sequence Modeling, February 2024.
 - Chulhee Yun, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank J. Reddi, and Sanjiv Kumar. Are Transformers universal approximators of sequence-to-sequence functions? In *arXiv:1912.10077* [Cs, Stat], February 2020a.
 - Chulhee Yun, Yin-Wen Chang, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank Reddi, and San-jiv Kumar. O(n) Connections are Expressive Enough: Universal Approximability of Sparse Transformers. In *Advances in Neural Information Processing Systems*, volume 33, pp. 13783–13794. Curran Associates, Inc., 2020b.

A PROOFS OF MAIN THEOREMS

A.1 PROOF OF THEOREM 1

Proof Sketch. The proof proceeds in three steps. First, by Lemma 1, we approximate a broader function class that relaxes the smoothness requirements and the assumptions in Assumption 2. Second, Lemmas 2 and 3 show that by constructing appropriate S_i , we can faithfully recover all information from the original input sequence with simple f_i . Finally, the outer function F_0 can be applied to approximate an arbitrary sequence-to-vector target within this class. Together, these steps establish the result.

Proof of Theorem 1. To prove Theorem 1, we first establish a few auxiliary lemmas.

Lemma 1 (Relaxed target class and closure equivalence). Let $\widetilde{\mathcal{F}}_D^{d,T}$ be defined as in 9 but with only $f_i \in C([0,1]^d,[0,1])$, i.e., we drop "unique minimizer", "pairwise distinct" and "PD Hessian". Set $\mathcal{F}^{d,T}:=\bigcup_{D\geq 1}\mathcal{F}_D^{d,T}$ and $\widetilde{\mathcal{F}}^{d,T}:=\bigcup_{D\geq 1}\widetilde{\mathcal{F}}_D^{d,T}$. Then

$$\overline{\mathcal{F}^{d,T}}^{\|\cdot\|_{\infty}} = \overline{\widetilde{\mathcal{F}}^{d,T}}^{\|\cdot\|_{\infty}} \quad on \ \mathcal{X}_T.$$

Proof. Fix $\widetilde{H}(X_T) = \widetilde{F}_0(\widetilde{z}_1(X_T), \dots, \widetilde{z}_D(X_T)) \in \widetilde{\mathcal{F}}_D^{d,T}$ with $\widetilde{z}_i(X_T) = \min_{t \in S_i} \widetilde{f}_i(x(t))$ and $\widetilde{f}_i \in C([0,1]^d,[0,1])$. Let $\varepsilon > 0$. We will construct $H \in \mathcal{F}^{d,T}$ with $\|H - \widetilde{H}\|_{\infty} \leq \varepsilon$. Firstly, by Stone–Weierstrass, choose $p_i \in C^{\infty}([0,1]^d)$ so that $\|p_i - \widetilde{f}_i\|_{\infty} \leq \eta$, where $\eta > 0$ will be fixed later. Because the uniform approximation can slightly leave [0,1], compose with a smooth strictly increasing squashing $s: [-c,1+c] \to [0,1]$ with s(u) = u on [0,1] and $\|s \circ p_i - p_i\|_{\infty} \leq \eta$ (for small enough c > 0), and replace p_i by $s \circ p_i$. We still write p_i and retain $\|p_i - \widetilde{f}_i\|_{\infty} \leq 2\eta$.

Secondly, let $\xi_i \in \arg\min_{x \in [0,1]^d} p_i(x)$ (nonempty by compactness). Pick $r \in (0,\frac{1}{4})$ small and a C^{∞} bump ϕ_i supported in $B(\xi_i,2r) \cap [0,1]^d$, with $\phi_i(\xi_i)=1$, $\nabla \phi_i(\xi_i)=0$, and with $\nabla^2 \phi_i(\xi_i)$ negative definite. Define, for parameters $\delta_{i,1},\delta_{i,2}>0$ to be fixed,

$$g_i(x) := p_i(x) - \delta_{i,1} \phi_i(x) + \delta_{i,2} \phi_i(x) \|x - \xi_i\|^2.$$

(i) Since $g_i(\xi_i) = p_i(\xi_i) - \delta_{i,1}$ while $g_i(x) \ge p_i(x)$ whenever $\phi_i(x) = 0$ and $g_i(x) > p_i(x)$ for $x \in B(\xi_i, 2r) \setminus \{\xi_i\}$, we get that ξ_i is the unique global minimizer of g_i .

(ii) At ξ_i , because $\nabla \phi_i(\xi_i) = 0$,

$$\nabla^2 g_i(\xi_i) = \nabla^2 p_i(\xi_i) - \delta_{i,1} \nabla^2 \phi_i(\xi_i) + 2\delta_{i,2} I.$$

Here $-\nabla^2 \phi_i(\xi_i) \succ 0$, so choosing $(\delta_{i,1}, \delta_{i,2})$ suitably makes $\nabla^2 g_i(\xi_i) \succ 0$ (PD). Because $\|\phi_i\|_{\infty} \le 1$ and $\|\|x - \xi_i\|^2\|_{\infty} \le d$ on $[0, 1]^d$,

$$||g_i - p_i||_{\infty} \le \delta_{i,1} + \delta_{i,2} (2r)^2.$$

Hence, by taking r small and then $\delta_{i,1}, \delta_{i,2}$ small (using the r^{-2} scaling in $\nabla^2 \phi_i(\xi_i)$ to keep the Hessian PD), we can ensure both PD at ξ_i and $\|g_i - p_i\|_{\infty} \leq \eta$.

Thirdly, we use tiny translation to remove distinctiveness. It may happen that $\xi_i = \xi_{i'}$ for some $i \neq i'$. Choose pairwise distinct small vectors $v_i \in \mathbb{R}^d$ and fix a smooth cutoff $\chi \in C^{\infty}([0,1]^d,[0,1])$ that equals 1 on $[r,1-r]^d$ and vanishes near the boundary. Define a C^{∞} diffeomorphism of the cube,

$$\Phi_i(x) := x - \varepsilon_i \chi(x) v_i, \quad \text{with } \varepsilon_i > 0 \text{ small.}$$

Then Φ_i is arbitrarily close to the identity in C^1 for small ε_i , maps $[0,1]^d$ to itself, and $h_i := g_i \circ \Phi_i$ has a (unique) minimizer at $x^{(i)} := \Phi_i^{-1}(\xi_i)$. For different i, these points are distinct if the v_i 's are distinct and ε_i 's are small but nonzero. Moreover, because $\nabla g_i(\xi_i) = 0$, the Hessian at $x^{(i)}$ satisfies

$$\nabla^2 h_i(x^{(i)}) = D\Phi_i(x^{(i)})^\top \nabla^2 g_i(\xi_i) D\Phi_i(x^{(i)}) \succ 0,$$

¹For instance take $\overline{\phi_i(x)} = \psi(\|x - \xi_i\|^2/r^2)$ with $\psi(0) = 1$, $\psi' < 0$ near 0, $\psi \equiv 0$ on $[1, \infty)$; then $\nabla^2 \phi_i(\xi_i) \prec 0$ and its norm scales like r^{-2} .

so PD is preserved. Since g_i is Lipschitz on the compact cube, $||h_i - g_i||_{\infty} \le L_i \varepsilon_i$ for some L_i , hence by taking ε_i small we get $||h_i - g_i||_{\infty} \le \eta$.

Finally, if needed, compose with the same strictly increasing squashing s as in Step 1 and set

$$f_i := s \circ h_i \in C^2([0,1]^d,[0,1]).$$

Because s is strictly increasing, it preserves the minimizer location and, at the minimizer $x^{(i)}$, $\nabla^2(s \circ h_i)(x^{(i)}) = s'(h_i(x^{(i)})) \nabla^2 h_i(x^{(i)}) \succ 0$. Also $||f_i - h_i||_{\infty} \le \eta$ by construction.

Collecting the bounds from previous deduction:

$$||f_i - \widetilde{f_i}||_{\infty} \leq \underbrace{||p_i - \widetilde{f_i}||_{\infty}}_{\leq 2\eta} + \underbrace{||g_i - p_i||_{\infty}}_{\leq \eta} + \underbrace{||h_i - g_i||_{\infty}}_{\leq \eta} + \underbrace{||f_i - h_i||_{\infty}}_{\leq \eta} \leq 5\eta.$$

For each i, the map $u \mapsto \min_{t \in S_i} u_t$ is 1-Lipschitz in $\|\cdot\|_{\infty}$. Hence the corresponding features $\bar{z}_i(X_T) := \min_{t \in S_i} f_i(x(t))$ and $\tilde{z}_i(X_T) := \min_{t \in S_i} \widetilde{f}_i(x(t))$ satisfy $\|\bar{z}_i - \widetilde{z}_i\|_{\infty} \leq 5\eta$. Let $\omega_{\widetilde{F}_0}$ be a modulus of continuity of \widetilde{F}_0 on $[0,1]^D$. Choose η so small that $\omega_{\widetilde{F}_0}(5\eta) \leq \varepsilon/2$. Then

$$\|\widetilde{F}_0(\bar{z}(X_T)) - \widetilde{F}_0(\widetilde{z}(X_T))\|_{\infty} \le \varepsilon/2.$$

Finally, approximate \widetilde{F}_0 uniformly on $[0,1]^D$ by some $F_0 \in C^1([0,1]^D)$ within $\varepsilon/2$ (Stone–Weierstrass). Setting

$$H(X_T) := F_0(\bar{z}_1(X_T), \dots, \bar{z}_D(X_T)) \in \mathcal{F}^{d,T},$$

we obtain

$$||H - \widetilde{H}||_{\infty} \leq \underbrace{||F_0(\overline{z}) - \widetilde{F}_0(\overline{z})||_{\infty}}_{\leq \varepsilon/2} + \underbrace{||\widetilde{F}_0(z) - \widetilde{F}_0(\widetilde{z})||_{\infty}}_{\leq \varepsilon/2} \leq \varepsilon.$$

This shows $\widetilde{\mathcal{F}}^{d,T} \subset \overline{\mathcal{F}^{d,T}}^{\|\cdot\|_{\infty}}$. The reverse inclusion is simple, hence we have the lemma.

Remark. Thus, we now focus on the relaxed class $\widetilde{\mathcal{F}}^{d,T}$ and Lemma 1 lifts the result to the original class $\mathcal{F}^{d,T}$.

Lemma 2 (Order-statistic in the relaxed class). Without loss of generation, suppose 4|T. Let $m = \frac{T}{4}$. For each $j \in [d]$ and $X_T = \{x(1), \dots, x(T)\}$, define

$$U_j(X_T) := \max_{\substack{B \subseteq [T] \\ |B| = m}} \min_{u \in B} x(u)_j,$$

and for each fixed $t \in [T]$,

$$Y_{t,j}(X_T) := \max_{\substack{A \subseteq [T] \ |A| = m, \ t \in A}} \min_{u \in A} x(u)_j, \qquad Z_{t,j}(X_T) := \max_{\substack{A \subseteq [T] \ |A| = m, \ t \in A}} \min_{u \in A} (1 - x(u)_j).$$

Let $v_{1,j} \geq \cdots \geq v_{T,j}$ be the sorted values of $\{x(1)_j,\ldots,x(T)_j\}$ and set $U_j = v_{m,j}$. For the multi-set $\{x(u)_j: u \in [T]\}$, let $v_{1,j} \geq \cdots \geq v_{T,j}$ (nonincreasing) and $w_{1,j} \leq \cdots \leq w_{T,j}$ (nondecreasing). Then we have

$$Y_{t,j} = \min\{x(t)_j, v_{m,j}\}, \qquad 1 - Z_{t,j} = \max\{x(t)_j, w_{m,j}\}.$$

In particular:

$$x(t)_{i} \leq v_{m,i} \Rightarrow Y_{t,i} = x(t)_{i}, \qquad x(t)_{i} \geq w_{m,i} \Rightarrow 1 - Z_{t,i} = x(t)_{i}.$$

Proof. Among all m-subsets B, the maximum of $\min_{u \in B} x(u)_j$ is attained by picking the m largest coordinates, so $U_j = v_{m,j}$. Forcing $t \in A$, the choice of the other m-1 indices to maximize the minimum is the m-1 largest among $\{x(u)_j: u \neq t\}$, hence $Y_{t,j} = \min\{x(t)_j, v_{m,j}\}$. For $Z_{t,j}$, note that $\min_{u \in A} (1-x(u)_j) = 1 - \max_{u \in A} x(u)_j$, so maximizing it over A is the same as minimizing $\max_{u \in A} x(u)_j$, which picks t plus the (m-1) smallest leading to $1-Z_{t,j}$. The particular statements follow immediately.

Lemma 3 (Smooth selector). For q > 0 define

$$\widehat{x}_q(t)_j := \frac{e^{q(1-Z_{t,j}-w_{m,j})^2} (1-Z_{t,j}) + e^{q(Y_{t,j}-v_{m,j})^2} Y_{t,j}}{e^{q(1-Z_{t,j}-w_{m,j})^2} + e^{q(Y_{t,j}-v_{m,j})^2}}.$$

Then $\widehat{x}_q(t)_j \to x(t)_j$ uniformly on \mathcal{X}_T as $q \to \infty$.

Proof. From Lemma 2, if $x(t)_j \geq U_j$, we have $Y_{t,j} = v_{m,j}$ and $(Y_{t,j} - v_{m,j})^2 = 0$ while $1 - Z_{t,j} = x(t)_j$ and $(1 - Z_{t,j} - w_{m,j})^2 > 0$. Thus, as $q \to \infty$, the weight concentrates on $(1 - Z_{t,j}) = x(t)_j$. If $x(t)_j \leq U_j$ and $w_{m,j} \geq x(t)_j$, we have $(1 - Z_{t,j} - w_{m,j})^2 = 0$ while $Y_{t,j} = x(t)_j$ and $(Y_{t,j} - v_{m,j})^2 > 0$ concentrating on $Y_{t,j} = x(t)_j$. If $w_{m,j} \leq x(t)_j \leq U_j$, we have $1 - Z_{t,j} = Y_{t,j} = x(t)_j$, so either of three settings leads to $x(t)_j$. The compactness of \mathcal{X}_T gives us the uniform property.

Now, we begin our formal proof for Theorem 1.

By Lemma 1, for any $F \in C(\mathcal{X}_T)$ and $\varepsilon > 0$, it suffices to construct an $\widetilde{H} \in \widetilde{\mathcal{F}}^{d,T}$ with $\|F - \widetilde{H}\|_{\infty} \le \varepsilon/2$, since the lemma 1 could lift it to $\mathcal{F}^{d,T}$ with another $\varepsilon/2$.

Fix $m = \frac{T}{4}$. For each coordinate j and each $S \subseteq [T]$ with |S| = m, include the relaxed primitives

$$z^{(j,S)}(X_T) := \min_{t \in S} x(t)_j, \qquad \bar{z}^{(j,S)}(X_T) := \min_{t \in S} (1 - x(t)_j).$$

To form the thresholds $v_{m,j}$ and $w_{m,j}$ needed in Lemma 2, additionally include:

$$\min_{t \in S} x(t)_j \quad \text{for all } S \subseteq [T] \setminus \{t\} \text{ with } |S| = m,$$

and

$$\min_{t \in S} (1-x(t)_j) \quad \text{for all } S \subseteq [T] \setminus \{t\} \text{ with } |S| = T-m,$$

Using smooth log-sum-exp (softmax) in the outer function \widetilde{F}_0 , we can recover the subset-wise maximum required to compute U_j , $Y_{t,j}$, $Z_{t,j}$, $v_{m,j}$ and $w_{m,j}$ from these primitives.

By Lemma 3, for any $\delta > 0$ there exists q such that

$$\max_{X_T \in \mathcal{X}_T} \max_{t \in [T], j \in [d]} |\widehat{x}_q(t)_j - x(t)_j| \leq \delta.$$

By uniform continuity of F on the compact \mathcal{X}_T , choose δ so that this implies $|F(X_T) - F(\widehat{X}_q(T))| \leq \varepsilon/4$ for all X_T , where $\widehat{X}_q(T)$ stacks the coordinates $\widehat{x}_q(t)_j$. We approximate the continuous map $u \mapsto F(u)$ on $[0,1]^{dT}$ uniformly by a polynomial P within $\varepsilon/4$ (Stone–Weierstrass). Define

$$\widetilde{H}(X_T) := (P \circ \operatorname{vec})(\widehat{X}_q(T)),$$

which is a C^1 function of the inner features. Hence $\widetilde{H} \in \widetilde{\mathcal{F}}^{d,T}$ and

$$\|F - \widetilde{H}\|_{\infty} \leq \underbrace{\|F - F \circ \widehat{X}_q\|_{\infty}}_{\leq \varepsilon/4} + \underbrace{\|F \circ \widehat{X}_q - P \circ \widehat{X}_q\|_{\infty}}_{\leq \varepsilon/4} \leq \varepsilon/2.$$

Apply Lemma 1 to replace each relaxed primitives by admissible C^2 functions with unique minimizers and to replace \widetilde{F}_0 by function F_0 so that the final error increases by at most $\varepsilon/2$. This leads to $f \in \mathcal{F}_D^{d,T}$ with $\|F - f\|_{\infty} \leq \varepsilon$.

A.2 PROOF OF THEOREM 2

A.2.1 PROOF OF THEOREM 2 (1)

Here we prove Theorem 2 (1)

Proof Sketch. The idea is straightforward. Each attention head is assigned to approximate one term $\min_{t \in S_i} f_i(x(t))$. Once these components are extracted, the outer function F_0 can be approximated by a suitable \hat{F} , completing the construction.

Proof of Theorem 2 (1): Sufficient expressivity with D heads. Fix d, T and $\alpha \in (0, 1)$, and let $\varepsilon > 0$ be given. Throughout the proof, constants depending only on (d, D, T) are absorbed into $C_{d,D,T} > 0$ which may change from line to line.

In the display equation 4, each head produces an n-dimensional vector and $\operatorname{Concat}_{i=1}^h$ gives a vector in \mathbb{R}^{nh} before \hat{F} . For the construction, we realize the usual *block-by-head* parameterization, which means that the encoder outputs a block-decomposed embedding

$$\hat{x}(t) = (\hat{x}^{(1)}(t), \dots, \hat{x}^{(D)}(t)) \in \mathbb{R}^{2D}, \qquad \hat{x}^{(i)}(t) \in \mathbb{R}^{2}$$

and the *i*-th head only reads the *i*-th block via block-diagonal $W_{Q,i}, W_{V,i}$ (entries bounded by 1). This keeps the parameter counts within the same order. We therefore set the *per-head embedding dimension* to n=2.

Firstly, from Assumption (A2), for any $\delta > 0$ there exist two-layer FFNs $\Psi_{i,\delta} : [0,1]^d \to [0,1]$ such that

$$\max_{x \in [0,1]^d} |f_i(x) - \Psi_{i,\delta}(x)| \le \delta, \quad \text{width}(\Psi_{i,\delta}) \le \frac{C_2}{\delta^{\gamma_f}}, \tag{10}$$

where $\gamma_f > 0$ is the exponent from (A2). Define for each head i, the position gate

$$r_i(s) := \begin{cases} 0, & s \in S_i, \\ -1, & s \notin S_i, \end{cases} \quad s \in [T].$$

(Recall $S_i \subset [T]$ with $|S_i| \geq \alpha T$ by equation 8.) We implement the encoder P_ϕ so that its i-th block is

$$\hat{x}^{(i)}(t) = (\Psi_{i,\delta}(x(t)), r_i(t)) \in [0,1] \times \{-1,0\} \subset [-1,1]^2.$$
(11)

This choice follows $\|\hat{x}(t)\|_2 \leq \sqrt{2D}$. After a fixed rescaling (absorbed into β), this meets the norm constraint.

Secondly, we would like to use head-wise attention to isolate the minimum on S_i . For each head i, we take a single attention logit $(m_h = 1)$ by choosing

$$W_{O,i} = I,$$
 $W_{K,i} = [-1 \quad 1],$ $W_{Q,i}\hat{c}_0 = 1,$ $W_{V,i} = I_2.$

All entries are within the allowed bound 1. With the block equation 11, the (pre-softmax) score of token t in head i is

$$\rho_i(t) = (W_{K,i}\hat{x}^{(i)}(t))^{\top}(W_{Q,i}\hat{c}_0) = -\Psi_{i,\delta}(x(t)) + r_i(t).$$
(12)

Let $\sigma[\rho_i]$ be the softmax equation 5 with $\beta > 0$. Define the head-i value readout (first coordinate of the head output)

$$\tilde{z}_i(X_T) := \sum_{t=1}^T \sigma[\rho_i](t) \, \Psi_{i,\delta}(x(t)). \tag{13}$$

Here, the second coordinate is unused. \hat{F} could ignore it via a fixed linear projection, counted in the constant $C_{d,D,T}$.

Now, we give a uniform bound on S_i . Take $a_t := \Psi_{i,\delta}(x(t)) \in [0,1]$ and split the sum into S_i and S_i^c . From $r_i(t) = 0$ on S_i and $r_i(t) = -1$ on S_i^c , we have

$$\sigma[\rho_i](t) = \frac{e^{\beta(-a_t + r_i(t))}}{\sum_{u \in S_i} e^{-\beta a_u} + \sum_{u \in S_i^c} e^{-\beta(a_u + 1)}} \le \begin{cases} \frac{e^{-\beta a_t}}{\sum_{u \in S_i} e^{-\beta a_u}}, & t \in S_i, \\ e^{-\beta a_t} & e^{-\beta a_t} & t \in S_i^c. \end{cases}$$

Hence, we have

$$\tilde{z}_i = \sum_{t \in S_i} \sigma[\rho_i](t) a_t + \sum_{t \in S_i^c} \sigma[\rho_i](t) a_t \le \underbrace{\frac{\sum_{t \in S_i} a_t e^{-\beta a_t}}{\sum_{u \in S_i} e^{-\beta a_u}}}_{\text{Gibbs mean on } S_i} + e^{-\beta} \underbrace{\frac{\sum_{t \in S_i^c} a_t e^{-\beta a_t}}{\sum_{u \in S_i} e^{-\beta a_u}}}_{\text{Current}}.$$
 (14)

To simplify, we denote $a_* := \min_{t \in S_i} a_t$ and $b_t := a_t - a_* \in [0, 1]$ for $t \in S_i$. Then, we have

$$\frac{\sum_{t \in S_i} a_t e^{-\beta a_t}}{\sum_{u \in S_i} e^{-\beta a_u}} = a_* + \frac{\sum_{t \in S_i} b_t e^{-\beta b_t}}{\sum_{u \in S_i} e^{-\beta b_u}} \ \le \ a_* + \sum_{t \in S_i} b_t e^{-\beta b_t} \ \le \ a_* + \frac{|S_i| - 1}{e\beta},$$

The inequality comes from $\sup_{b\in[0,1]}be^{-\beta b}=e^{-1}/\beta$ for $\beta\geq 1$ and one of the b_t is 0, so the denominator in the middle fraction is ≥ 1 . For the S_i^c term in 14, we use $a_t\leq 1$ and $\sum_{u\in S_i}e^{-\beta a_u}\geq 1$ to get

$$e^{-\beta} \frac{\sum_{t \in S_i^c} a_t e^{-\beta a_t}}{\sum_{u \in S_i} e^{-\beta a_u}} \le e^{-\beta} |S_i^c| \le e^{-\beta} T.$$

Combining the two bounds, we have the uniform estimate:

$$\min_{t \in S_i} \Psi_{i,\delta} \big(x(t) \big) \leq \tilde{z}_i(X_T) \leq \min_{t \in S_i} \Psi_{i,\delta} \big(x(t) \big) + \frac{|S_i| - 1}{e\beta} + Te^{-\beta} \qquad (\beta \ge 1). \tag{15}$$

In particular, since $|S_i| \leq T$, there is a constant C_T with

$$0 \le \tilde{z}_i(X_T) - \min_{t \in S_i} \Psi_{i,\delta}(x(t)) \le C_T \left(\frac{1}{\beta} + e^{-\beta}\right), \qquad C_T := \max\{T/e, T\}. \tag{16}$$

Thirdly, we need to lift bounds from \tilde{z}_i to z_i . From equation 10 and the definition of z_i ,

$$\left| \min_{t \in S_i} f_i(x(t)) - \min_{t \in S_i} \Psi_{i,\delta}(x(t)) \right| \leq \delta.$$

Together with equation 16,

$$\left|\tilde{z}_i(X_T) - \bar{z}_i(X_T)\right| \le \delta + C_T \left(\frac{1}{\beta} + e^{-\beta}\right) \quad \text{for all } X_T \in \mathcal{X}_T, \ i = 1, \dots, D.$$
 (17)

Let $L_0 := \sup_{z \in [0,1]^D} \|\nabla F_0(z)\|_1 < \infty$ (compactness and C^1). Choose

$$\delta := \frac{\varepsilon}{4L_0D}, \qquad \beta \ge \beta_\varepsilon := \max \left\{ 1, \ \frac{4C_TL_0D}{\varepsilon}, \ \log \left(\frac{4C_TL_0D}{\varepsilon} \right) \right\}.$$

Then by equation 17,

$$\|\tilde{z}(X_T) - z(X_T)\|_{\infty} \le \frac{\varepsilon}{2L_0 D}$$
 for all $X_T \in \mathcal{X}_T$. (18)

Finally, we construct the approximation for F_0 and count the number of parameter. By Assumption (A1), there exists a two-layer FFN $\Phi_{\delta_0}: [0,1]^D \to \mathbb{R}$ with width $\leq C_1/\delta_0^{\gamma_0}$ (for some $\gamma_0 > 0$) such that

$$\max_{z \in [0,1]^D} |F_0(z) - \Phi_{\delta_0}(z)| \le \delta_0.$$

Set $\delta_0 := \varepsilon/2$. Define the model's final feed-forward \hat{F} to project $\mathbb{R}^{2D} \to \mathbb{R}^D$ by keeping the first coordinate of each head (a fixed linear map with entries in $\{0,1\}$) and apply Φ_{δ_0} .

Then for all X_T , we have

$$\begin{aligned} \left| \hat{F}(\operatorname{Concat}_{i}(\cdot)) - F_{0}(z(X_{T})) \right| &\leq \left| \Phi_{\delta_{0}}(\tilde{z}(X_{T})) - \Phi_{\delta_{0}}(z(X_{T})) \right| + \left| \Phi_{\delta_{0}}(z(X_{T})) - F_{0}(z(X_{T})) \right| \\ &\leq L_{0} \|\tilde{z}(X_{T}) - z(X_{T})\|_{1} + \delta_{0} \\ &\leq L_{0} D \|\tilde{z}(X_{T}) - z(X_{T})\|_{\infty} + \varepsilon/2 \\ &\leq \varepsilon/2 + \varepsilon/2 = \varepsilon, \end{aligned}$$

where we used equation 18 in the last inequality.

Here, the trainable components are composed of three parts:

- the D subnetworks $\Psi_{i,\delta}$ inside the encoder blocks equation 11;
- the fixed-size projections $W_{Q,i}, W_{K,i}, W_{V,i}$ (size O(D) and independent of ε);
- the two-layer FFN Φ_{δ_0} used inside \hat{F} .

Thus

$$M \leq C' D \cdot \frac{1}{\delta^{\gamma_f}} + C'' \cdot \frac{1}{\delta_0^{\gamma_0}} + C'''$$
 for constants $C', C'', C''' = C_{d,D,T}$.

With $\delta = \Theta(\varepsilon)$ and $\delta_0 = \Theta(\varepsilon)$ chosen above,

$$M \; \leq \; \frac{C_{d,D,T}}{\varepsilon^{\gamma}}, \qquad \gamma := \max\{\gamma_f,\gamma_0\},$$

and the construction uses h=D heads with per-head dimension n=2 and achieves ε -approximation on \mathcal{X}_T . This proves Theorem 2 (1).

A.2.2 PROOF OF THEOREM 2 (2)

Proof Sketch. The argument proceeds in two parts. The core idea is to construct two sequences whose representations after the attention layer are indistinguishably close, on the order of $O(\epsilon^{k+1})$, yet whose target outputs differ by at least 3ϵ . Lemma 4 then implies the lower bound on the parameter count required for approximation.

Using Lemmas 5, 6, and 7, we obtain D disjoint neighborhoods around the minima $x^{(i)}$. Since D>s=h, there exists at least one neighborhood not selected by the s heads. Within this region, the pigeonhole principle guarantees the existence of two distinct subsequences. By carefully designing these subsequences, we ensure that their outputs after the attention layer are nearly indistinguishable, while their target values differ by at least 3ϵ . Extending them to full sequences completes the construction.

We now turn to the full proof. To establish Theorem 2 (2), we begin by introducing several auxiliary lemmas that will serve as building blocks for the argument.

Lemma 4. Let $v_1, v_2 \in \mathbb{R}^n$. Suppose

$$||v_1 - v_2||_2 \le A$$
 and $||\hat{F}(v_1) - \hat{F}(v_2)|| \ge B$,

where $\hat{F}: \mathbb{R}^n \to \mathbb{R}^m$ is a two-layer feed-forward network satisfying the constraints stated above. Then \hat{F} must use at least

$$\Omega\left(\frac{B}{A\sqrt{n}}\right)$$

parameters.

Proof of Lemma 4. Let $\Delta x := v_1 - v_2$ and $\Delta F := \hat{F}(v_1) - \hat{F}(v_2)$. Suppose the two-layer network with width p be

$$\hat{F}(x) = V \sigma(Ux + b) + c,$$

where $U \in \mathbb{R}^{p \times n}$, $V \in \mathbb{R}^{m \times p}$, $b \in \mathbb{R}^p$, $c \in \mathbb{R}^m$, σ is 1-Lipschitz acting coordinate-wise and every entry of U, V, b, c has magnitude at most 1.

For the j-th output coordinate, we have

$$\Delta F_j = \sum_{r=1}^{p} V_{jr} \left(\sigma(u_r^{\top} v_1 + b_r) - \sigma(u_r^{\top} v_2 + b_r) \right),$$

where u_r^{\top} is the r-th row of U. Using the 1-Lipschitz property of σ and Cauchy–Schwarz inequality, we have

$$|\Delta F_j| \le \sum_{r=1}^p |V_{jr}| |u_r^\top \Delta x| \le \sum_{r=1}^p |V_{jr}| ||u_r||_2 ||\Delta x||_2.$$

By the entrywise weight bound, $||u_r||_2 \le \sqrt{n}$ and $|V_{jr}| \le 1$. Therefore, for all j, we have

$$|\Delta F_i| \le p\sqrt{n} \, ||\Delta x||_2. \tag{19}$$

Let $\|\cdot\|$ be the norm used in the lemma statement. By norm equivalence in finite dimensions, there exists $c_m \in (0,1]$ depending only on the chosen norm and m such that

$$||y|| \le \frac{1}{c_m} ||y||_{\infty}$$
 for all $y \in \mathbb{R}^m$.

 $\|\Delta F\| \geq B$ implies $\|\Delta F\|_{\infty} \geq c_m B$, so there is some j^* with

$$|\Delta F_{i^*}| \geq c_m B.$$

Combining this with equation 19 and $\|\Delta x\|_2 \leq A$, we have

$$c_m B \le p \sqrt{n} A \implies p \ge \frac{c_m B}{A \sqrt{n}}.$$

Finally, let $p_{\text{eff}} \leq p$ be the number of hidden units that actually affect the output, i.e., those with a nonzero row in U and a nonzero entry in the j^* -th row of V. The above bound holds with p_{eff} in place of p, hence $p_{\text{eff}} \geq c_m B/(A\sqrt{n})$. Each such unit uses at least one nonzero parameter in U and one in V, so the parameter counts k satisfy $k \geq p_{\text{eff}}$. Therefore

$$k \geq \frac{c_m B}{A\sqrt{n}} = \Omega\left(\frac{B}{A\sqrt{n}}\right),$$

which proves the lemma.

Lemma 5. There exists R > 0 such that for every $i \in \{1, ..., D\}$ and every r < R, there exist constants $\delta_i > 0$ and $L_i > 0$ with the following property: there exists a segment $G_i \subset B(x^{(i)}, r)$ of length δ_i such that

$$|f_i(x) - f_i(y)| \ge L_i ||x - y||_2, \quad \forall x, y \in G_i.$$

and moreover

$$f_i(x) > z_i, \quad \forall x \in G_i,$$

Proof of Lemma 5. Fix $i \in \{1, \ldots, D\}$ and denote $x^* := x^{(i)}$, $f := f_i$ and $H_* := \nabla_x^2 f(x^*)$. By positive definiteness, let $\lambda_i := \lambda_{\min}(H_*) > 0$. By continuity of $\nabla^2 f$, there exists $R_i^{\mathrm{H}} > 0$ such that

$$abla^2 f(x) \;\succeq\; rac{\lambda_i}{2} \, I \qquad \text{for all } x \in B(x^\star, R_i^{\mathrm{H}}).$$

Set $\mu_i := \lambda_i/2 > 0$. Because the domain is $[0,1]^d$ and $x^* \in [0,1]^d$, we could choose a unit vector v_i pointing strictly into the cube at x^* (if x^* is interior, take any unit vector). Define

$$\tau_i := \sup\{t > 0 : x^* + sv_i \in [0, 1]^d \text{ for all } s \in [0, t]\} > 0,$$

and set $R_i := \min\{R_i^H, \tau_i\}$. Take $R := \min_{1 \le i \le D} R_i > 0$. Fix any $r \in (0, R)$ and consider the restriction

$$g(t) := f(x^* + tv_i), \qquad t \in [0, r].$$

Then

$$g''(t) = v_i^\top \nabla^2 f(x^* + tv_i) v_i \ge \mu_i$$
 for all $t \in [0, r]$.

Since x^* minimizes f on $[0,1]^d$ and v_i is feasible inward, we have $g(t) \geq g(0)$ for small $t \geq 0$ leading to the one-sided derivative $g'(0+) \geq 0$ (if x^* is interior then $\nabla f(x^*) = 0$ so g'(0) = 0). Because $g'' \geq \mu_i$, the derivative g' is increasing and thus

$$g'(t) \geq g'(0+) + \mu_i t \geq \mu_i t, \quad t \in [0, r].$$

Let a := r/4 and b := r/2 and define the segment

$$G_i := \{ x^* + tv_i : t \in [a, b] \} \subset B(x^*, r),$$

whose length is $\delta_i := b - a = r/4$. For any $x = x^* + tv_i$ and $y = x^* + sv_i$ in G_i with t > s, the mean value theorem gives some $\xi \in (s,t) \subset [a,b]$ such that

$$|f(x) - f(y)| = |g(t) - g(s)| = |g'(\xi)| |t - s| \ge \mu_i a |t - s| = \left(\frac{\lambda_i r}{8}\right) ||x - y||_2.$$

Therefore the choice

$$L_i := \frac{\lambda_i r}{8} > 0$$

works uniformly for all $x, y \in G_i$. The segment G_i does not contain x^* , for all its points are at distance at least a = r/4 > 0 from x^* . By uniqueness of the minimizer, $f(x) > f(x^*) = z_i$ for all $x \in G_i$.

The lemma holds with $\delta_i = r/4$ and $L_i = (\lambda_{\min}(\nabla_x^2 f_i(x^{(i)})) r)/8$.

Lemma 6. Let (z_1, \ldots, z_D) denote the minima defined above. Then there exist constants $r_0 > 0$ and $L_0 > 0$ such that the following holds: for any $i \in \{1, \ldots, D\}$ and any perturbation δ_0 with $|\delta_0| < r_0$,

 $|F_0(z_1,\ldots,z_i+\delta_0,\ldots,z_D)-F_0(z_1,\ldots,z_D)| \geq L_0 |\delta_0|.$

Proof of Lemma 6. Denote e_i for the *i*-th standard basis vector of \mathbb{R}^D . By assumption, $m_i := |\partial_i F_0(z)| > 0$ for each *i*. Since $F_0 \in C^1$, the map $u \mapsto \partial_i F_0(u)$ is continuous at *z*. Hence for each *i*, there exists $r_i^{\text{cont}} > 0$ such that

$$\left| \partial_i F_0(u) \right| \geq \frac{1}{2} m_i$$
 whenever $\|u - z\|_{\infty} < r_i^{\text{cont}}$.

If necessary, shrink r_i^{cont} so that the line segment $\{z + te_i : |t| < r_i^{\text{cont}}\}$ lies in $[0,1]^D$. Define uniform constants

$$L_0 := \frac{1}{2} \min_{1 \le i \le D} m_i > 0, \qquad r_0 := \min_{1 \le i \le D} r_i^{\text{cont}} > 0.$$

Fix i and δ_0 with $|\delta_0| < r_0$. Consider the one-dimensional slice $g_i(t) := F_0(z + te_i)$ for $|t| < r_0$. Then g_i is C^1 and $g_i'(t) = \partial_i F_0(z + te_i)$. By the mean value theorem, there exists $\theta \in (0,1)$ such that

$$F_0(z + \delta_0 e_i) - F_0(z) = g_i'(\theta \delta_0) \, \delta_0 = \partial_i F_0(z + \theta \delta_0 e_i) \, \delta_0.$$

Taking absolute values and using the lower bound on $|\partial_i F_0(\cdot)|$ inside the ℓ_∞ -ball of radius r_0 around z, we have

$$|F_0(z + \delta_0 e_i) - F_0(z)| \ge |L_0|\delta_0|,$$

which is the desired inequality.

Lemma 7. Let $z_i = \min_{x \in [0,1]^d} f_i(x)$ and let $x^{(i)}$ denote the unique minimizer of f_i (as assumed above). Then there exist constants $R_0 > 0$ and $\varepsilon_0 > 0$ such that:

- 1. The open balls $\{B(x^{(i)}, R_0)\}_{i=1}^D$ are pairwise disjoint.
- 2. For each $i \in \{1, ..., D\}$ and every $x \in [0, 1]^d \setminus B(x^{(i)}, R_0)$,

$$f_i(x) > z_i + \varepsilon_0$$
.

Proof of Lemma 7. Since the minimizers $\{x^{(i)}\}_{i=1}^{D}$ are pairwise distinct and finite in number, we have

$$\Delta := \min_{i \neq j} \|x^{(i)} - x^{(j)}\|_2 > 0.$$

Set $R_0 := \frac{1}{2}\Delta$. If $i \neq j$ and $x \in B(x^{(i)}, R_0)$, by the triangle inequality, we have

$$||x - x^{(j)}||_2 \ge ||x^{(i)} - x^{(j)}||_2 - ||x - x^{(i)}||_2 > \Delta - R_0 = R_0,$$

so $x \notin B(x^{(j)}, R_0)$. Hence the balls are pairwise disjoint, proving the first part.

For the second part, fix i and define the compact set $K_i := [0,1]^d \setminus B(x^{(i)}, R_0)$. The continuity of f_i implies that the minimum

$$m_i := \min_{x \in K_i} f_i(x)$$

is attained on K_i . Because $x^{(i)} \notin K_i$ and $x^{(i)}$ is the unique global minimizer on $[0,1]^d$, we have $m_i > z_i$. Let $\varepsilon_i := m_i - z_i > 0$ and set

$$\varepsilon_0 := \frac{1}{2} \min_{1 \le i \le D} \varepsilon_i > 0.$$

Then, for every $x \in K_i$, we have

$$f_i(x) \geq m_i = z_i + \varepsilon_i \geq z_i + 2\varepsilon_0 > z_i + \varepsilon_0$$

Thus, we have proved this lemma.

Proof of Theorem 2 (2). Given the target function under the assumptions. For any given single-layer transformer defined in the main context, our goal is to find two different sequences such that their output in the part

$$\operatorname{Concat}_{i=1}^{h} \left(\sum_{t=1}^{T} \sigma \left[(W_{K,i} \hat{x}(t))^{\top} W_{Q,i} \hat{c}_{0} \right] W_{V,i} \hat{x}(t) \right)$$
(20)

are very close (differs by only $O(\epsilon^{k+1})$), but their output from the target function differs by at least 3ϵ , then according to lemma 4, we have the required parameter count for the FFN \hat{F} to be at least $\Omega(1/\epsilon^k)$.

Notations For each head $i = 1, \dots, s$, define the attention weight function

$$\lambda_i(x,t) = \exp(\gamma (W_{K,i} P_{\phi}(x,t))^{\top} W_{Q,i} \hat{c}_0),$$

and the value mapping

$$v_i(x,t) = W_{V,i}P_{\phi}(x,t) \in \mathbb{R}^n,$$

where $\gamma > 0$ is the softmax scaling factor, $W_{Q,i}, W_{K,i} \in \mathbb{R}^{n \times E}$ are the query and key projections, and $W_{V,i} \in \mathbb{R}^{n \times E}$ is the value projection for head i.

Notation of sets Without loss of generality, we assume $x^{(i)}$ belongs to the interior of $[0,1]^d$, and the other case can be treated with the same method below. From lemma 5, lemma 6 and lemma 7 we have that there exists R>0 and segments $G_i\subset B(x^{(i)},R), i=1,\ldots,D$ and $L,\delta_0,r>0$ satisfying the following:

- $\forall i, \forall x, y \in G_i$, we have $|f_i(x) f_i(y)| > L||x y||_2$.
- $\forall j \neq i \text{ and } \forall x \in B(x^{(j)}, R), y \in B(x^{(i)}, R), \text{ we have } f_i(y) f_i(x) > \delta_0.$
- The length of G_i is $r, \forall i = 1, \dots, D$.
- For any $i \in \{1, \ldots, D\}$ and any perturbation δ_1 with $|\delta_1| < \max_{x \in B(x^{(i)} | B)} (f_i(x) z_i)$,

$$|F_0(z_1,\ldots,z_i+\delta_1,\ldots,z_D)-F_0(z_1,\ldots,z_D)| \geq L |\delta_1|.$$

We denote by $K_i := G_i \cup \{x^{(i)}\}, i = 1, \dots, D$, and $P_0 = \bigcup_{i=1}^D K_i$. Recall that $k = \frac{\frac{1}{4}T - s - D + 1}{(n+1)s+1} - 1$. We assume without loss of generality that k > 0 and $\frac{1}{4}T - s - D + 1 > 0$, otherwise the result would be trivial.

Max weight for each head For j = 1, ..., s, define recursively the pairs (y_j, t_j) as follows:

• For the first head,

$$(y_1, t_1) = \underset{\substack{y \in P_0 \\ t \in S_1}}{\operatorname{arg}} \lambda_1(y, t).$$

• For
$$j>1$$
,
$$(y_j,t_j) \ = \ \arg\max_{\substack{y\in P_0\\t\in S_j\\t\notin\{t_1,\dots,t_{j-1}\}}}\lambda_j(y,t).$$

• If maximum can be obtained at multiple (y, t), then choose one of them.

Let $Y = \{y_1, \dots, y_s\}$. Since the sets K_1, \dots, K_D are pairwise disjoint and s < D, there exists at least one index $i \in \{1, \dots, D\}$ such that

$$K_i \cap Y = \varnothing.$$

Without loss of generality, we assume that i=1. As we have $|S_i| \ge \frac{1}{4}T > s+D-1, i=1,\ldots,D$, we have that there exists a set of (t_2^*,\ldots,t_D^*) such that

- $t_i^* \notin \{t_1, \dots, t_s\}$, for $j = 2, \dots, D$.
- t_i^* are pairwise distinct.

• $t_i^* \in S_j, j = 2, \dots, D$.

Let $T_0 = \frac{1}{4}T - s - D + 1 > 0$ and assume that T_0 is a integer. Then we have $|S_1 - \{t_1, \dots, t_s, t_2^*, \dots, t_D^*\}| \ge T_0 > 0$. Without loss of generality, suppose $\{1, 2, \dots, T_0\} \subset S_1 - \{t_1, \dots, t_s, t_2^*, \dots, t_D^*\}$.

Sequences to be considered As G_1 is a segment of length r, then it is natural to assign coordinate system $\eta:[0,1]\to G_1$ on G_1 , with $q:=f_1\circ\eta$ being a monotonically increasing function on [0,1]. The monotone property is as a result of $|f_1(x)-f_1(y)|\geq L\|x-y\|_2$.

We denote by $M = T_0 \lfloor \frac{rL^2}{3T_0\epsilon} \rfloor$. As $T_0 | M$, Construct the following T_0 sets:

$$U_j = \frac{j-1}{T_0} + \{\frac{1}{M}, \dots, \frac{\binom{T_0}{M}}{M}\}, j = 1, \dots, T_0$$
 (21)

We have $|U_j| = \lfloor \frac{rL^2}{3T_0\epsilon} \rfloor = O(1/\epsilon)$.

Claim 2.1. Existence of two distinct sub-sequence

There exists two subsequences $z_1(1), \ldots, z_1(T_0)$ and $z_2(1), \ldots, z_2(T_0)$ with $z_i(t) \in \eta(U_t)$ satisfying the following conditions.

$$\bullet \left\| \frac{\sum_{t=1}^{T_0} \lambda_i(z_1(t),t) v_i(z_1(t),t)}{\sum_{t=1}^{T_0} \lambda_i(z_1(t),t)} - \frac{\sum_{t=1}^{T_0} \lambda_i(z_2(t),t) v_i(z_2(t),t)}{\sum_{t=1}^{T_0} \lambda_i(z_2(t),t)} \right\|_2 \le \frac{\epsilon^{k+1}}{3T_0}, \text{ for } i = 1,\ldots,s.$$

For each i = 1, ..., s, either of the following holds:

1.
$$\frac{\sum_{t=1}^{T_0} \lambda_i(z_1(t),t)}{\sum_{t=1}^{T_0} \lambda_i(z_2(t),t)} \in \left[1/(1 + \frac{\epsilon^{k+1}}{12T_0^2}), 1 + \frac{\epsilon^{k+1}}{12T_0^2} \right].$$

2.
$$\max_{j=1,2} \sum_{t=1}^{T_0} \lambda_i(z_j(t), t) \le \frac{\epsilon^{k+1}}{4} \sum_{w=1}^s \lambda_i(y_w, t_w)$$
.

Proof. We compare the orders of $1/\epsilon$ appearing on both sides of the conditions.

First, since $|U_t| = O(1/\epsilon)$ for each t, the total number of possible choices of subsequences $(z(1), \ldots, z(T_0))$ is at most $O(1/\epsilon^{T_0})$.

Next, to satisfy condition (1), note that both vectors involved are n-dimensional with norms bounded by 1. Thus, the discretization required to achieve accuracy $\epsilon^{k+1}/(3T_0)$ in the ℓ_2 norm leads to at most $O(1/\epsilon^{(k+1)ns})$ distinct possibilities, since there are s heads.

For condition (2), observe that

$$\sum_{w=1}^{s} \lambda_i(y_w, t_w) \geq \frac{1}{T_0} \max_{j=1,2} \sum_{t=1}^{T_0} \lambda_i(z_j(t), t).$$

Hence, for each i, the relevant interval can be partitioned into at most $O\left(\frac{-\log \epsilon}{\epsilon^{k+1}}\right)$ sub-intervals. Taken across s heads, this contributes at most $O\left((-\log \epsilon)^s/\epsilon^{(k+1)s}\right)$ possibilities.

Combining the two conditions, the total number of distinct admissible cases is bounded above by

$$O\left(\frac{(-\log \epsilon)^s}{\epsilon^{(k+1)ns+(k+1)s}}\right).$$

Since $T_0 \ge (k+1)ns + (k+1)s + 1$, we have

1136
$$O\left(\frac{1}{\epsilon^{T_0}}\right) \gg O\left(\frac{(-\log \epsilon)^s}{\epsilon^{(k+1)ns+(k+1)s}}\right).$$

Therefore, by the pigeonhole principle, there must exist two distinct subsequences $(z_1(1),\ldots,z_1(T_0))$ and $(z_2(1),\ldots,z_2(T_0))$ satisfying all the conditions of Claim 2.1.

Construction of Distinct sequences From Claim 2.1, we have constructed two sub-sequences Z_1, Z_2 satisfying the given conditions. We now consider the construction of two full input sequence W_1, W_2 :

- For $t = 1, ..., T_0$, if $z_1(t) = z_2(t)$, then $w_1(t) = w_2(t) = x^{(D)}$. Otherwise, $w_1(t) = z_1(t), w_2(t) = z_2(t)$.
- $w_i(t_i) = y_i, i = 1, ..., s; j = 1, 2.$
- $w_j(t_i^*) = x^{(i)}, i = 2, ..., D; j = 1, 2.$
- For all other t, $w_i(t) = x^{(D)}$.

Difference of W1, W2 **applied to target function** Denote by I_1 the set of all indices t with $z_1(t) \neq z_2(t)$, and $I_2 = [T_0] - I_1$, $I_3 = [T] - I_1$. It is clear from the difference of Z_1, Z_2 that $I_1 \neq \emptyset$.

We then define the following notations for the simplicity of calculation (defined for each head $i = 1, \ldots, s$):

- $Q_{1,i} = \sum_{t \in I_1} \lambda_i(w_1(t), t)$.
- $Q_{2,i} = \sum_{t \in I_1} \lambda_i(w_2(t), t)$.
- $V_{1,i} = (\sum_{t \in I_1} \lambda_i(w_1(t), t) v_i(w_1(t), t)) / Q_{1,i}$.
- $V_{2,i} = (\sum_{t \in I_1} \lambda_i(w_2(t), t) v_i(w_2(t), t)) / Q_{2,i}$.
- $Q_{3,i} = \sum_{t \in I_2} \lambda_i(z_1(t), t)$, which is also the same if defined on Z_2 .
- $V_{3,i}=(\sum_{t\in I_2}\lambda_i(z_1(t),t)v_i(z_1(t),t))/Q_{3,i}$, which is the same if defined on Z_2 .
- $Q_{4,i} = \sum_{t \in I_3} \lambda_i(w_1(t),t)$, which is the same if defined on W_2 .
- $V_{4,i}=(\sum_{t\in I_3}\lambda_i(w_1(t),t)v_i(w_1(t),t))/Q_{4,i}$, which is the same if defined on W_2 .

As $\lambda_i()$ maps to positive values, $V_{j,i}$ are convex combinations of $v_i()$, whose norm is bounded by 1 according to the constraint section 1. Therefore $||V_{j,i}|| \le 1, j = 1, 2, 3, 4$.

As $f_1 \circ \eta$ is monotone on [0,1], let $\tilde{t} = \max_{t \in I_1} t$, then we have

- $\max_{t \in S_1} f_1(w_1(t)) = f_1(w_1(\tilde{t})).$
- $\max_{t \in S_1} f_1(w_2(t)) = f_1(w_2(\tilde{t})).$

And by construction we know that

$$\|(w_1(\tilde{t})) - (w_2(\tilde{t}))\| \ge \frac{r}{M}$$
 (22)

which is the minimal distance for any two points in $U_{\tilde{t}}$. Then we have

$$|f_1(w_1(\tilde{t})) - f_1(w_2(\tilde{t}))| \ge \frac{rL}{M}$$
 (23)

As we have for $i = 2, \dots, D$

• $\max_{t \in S_i} f_i(w_1(t)) = z^{(i)}$.

 • $\max_{t \in S_i} f_i(w_2(t)) = z^{(i)}$.

Then following the perturbation property of F_0 defined above we have that the difference of output between the two sequence to be at least $\frac{rL^2}{M}$, which is greater than 3ϵ . Then ϵ -approximation requires that $|Model(W_1) - Model(W_2)| \ge \epsilon$.

 W_1 and W_2 are close after attention layer For any given head i, we consider the two cases given in 2.1.

Case 1 Case 1 can be rewritten as follows:

- $\bullet \ \| \frac{Q_{1,i}V_{1,i} + Q_{3,i}V_{3,i}}{Q_{1,i} + Q_{3,i}} \frac{Q_{2,i}V_{2,i} + Q_{3,i}V_{3,i}}{Q_{2,i} + Q_{3,i}} \|_2 \le \frac{\epsilon^{k+1}}{3T_0}.$
- $\frac{Q_{1,i}+Q_{3,i}}{Q_{2,i}+Q_{3,i}} \in \left[1/(1+\frac{\epsilon^{k+1}}{12T_0^2}), 1+\frac{\epsilon^{k+1}}{12T_0^2}\right].$

Without loss of generality, we assume $Q_{1,i} \geq Q_{2,i}$. By calculation, we have

$$\frac{Q_{1,i}V_{1,i} + Q_{3,i}V_{3,i}}{Q_{1,i} + Q_{3,i}} - \frac{Q_{2,i}V_{2,i} + Q_{3,i}V_{3,i}}{Q_{2,i} + Q_{3,i}}$$
(24)

$$= \frac{Q_{3,i}(Q_{2,i} - Q_{1,i})(V_{3,i} - V_{2,i})}{(Q_{1,i} + Q_{3,i})(Q_{2,i} + Q_{3,i})} + \frac{Q_{1,i}}{Q_{1,i} + Q_{3,i}}(V_{1,i} - V_{2,i}).$$
(25)

We have already known that $Q_{4,i} \ge \frac{Q_{1,i} + Q_{2,i}}{T_0}$ (As $Q_{4,i}$ has the max weight of each head in it). Then

$$\left\| \frac{Q_{4,i}(Q_{2,i} - Q_{1,i})(V_{4,i} - V_{2,i})}{(Q_{1,i} + Q_{4,i})(Q_{2,i} + Q_{4,i})} \right\|$$
 (26)

$$\leq \left\| \frac{(Q_{2,i} - Q_{1,i})(V_{4,i} - V_{2,i})}{(Q_{1,i} + Q_{4,i})} \right\| \tag{27}$$

$$\leq \left\| \frac{T_0(Q_{2,i} - Q_{1,i})(V_{4,i} - V_{2,i})}{(Q_{1,i} + Q_{3,i})} \right\| \tag{28}$$

$$\leq \|\frac{T_0 \epsilon^{k+1} (V_{4,i} - V_{2,i})}{12T_0^2}\| \tag{29}$$

$$\leq \frac{\epsilon^{k+1}}{6T_0} \tag{30}$$

Similarly, we also have

$$\left\| \frac{Q_{3,i}(Q_{2,i} - Q_{1,i})(V_{3,i} - V_{2,i})}{(Q_{1,i} + Q_{3,i})(Q_{2,i} + Q_{3,i})} \right\| \le \frac{\epsilon^{k+1}}{6T_0}$$
(31)

From inequality 26 and substituting equation 24, we have

$$\left\| \frac{Q_{1,i}}{Q_{1,i} + Q_{3,i}} (V_{1,i} - V_{2,i}) \right\| \le \frac{\epsilon^{k+1}}{6T_0} + \frac{\epsilon^{k+1}}{3T_0} = \frac{\epsilon^{k+1}}{2T_0}$$
(32)

Therefore

$$\|\frac{Q_{1,i}}{Q_{1,i} + Q_{4,i}} (V_{1,i} - V_{2,i})\|$$
(33)

$$\leq \|\frac{T_0 Q_{1,i}}{Q_{1,i} + Q_{3,i}} (V_{1,i} - V_{2,i})\| \tag{34}$$

$$\leq \frac{\epsilon^{k+1}}{2} \tag{35}$$

Thus

$$\|\frac{Q_{1,i}V_{1,i} + Q_{4,i}V_{4,i}}{Q_{1,i} + Q_{4,i}} - \frac{Q_{2,i}V_{2,i} + Q_{4,i}V_{4,i}}{Q_{2,i} + Q_{4,i}}\|_{2}$$
(36)

$$\leq \left\| \frac{Q_{4,i}(Q_{2,i} - Q_{1,i})(V_{4,i} - V_{2,i})}{(Q_{1,i} + Q_{4,i})(Q_{2,i} + Q_{4,i})} \right\| + \left\| \frac{Q_{1,i}}{Q_{1,i} + Q_{4,i}}(V_{1,i} - V_{2,i}) \right\|$$
(37)

$$\leq \frac{\epsilon^{k+1}}{6T_0} + \frac{\epsilon^{k+1}}{2} \tag{38}$$

$$\leq \epsilon^{k+1}$$
 (39)

Case 2 Case 2 can be rewritten as follows:

$$\bullet \ \| \frac{Q_{1,i}V_{1,i} + Q_{3,i}V_{3,i}}{Q_{1,i} + Q_{3,i}} - \frac{Q_{2,i}V_{2,i} + Q_{3,i}V_{3,i}}{Q_{2,i} + Q_{3,i}} \|_2 \leq \frac{\epsilon^{k+1}}{3T_0}.$$

•
$$Q_{1,i} + Q_{3,i} \le \frac{\epsilon^{k+1}}{4} \sum_{w=1}^{s} \lambda_i(y_w, t_w) \le \frac{\epsilon^{k+1}}{4} Q_{4,i}$$
.

•
$$Q_{2,i} + Q_{3,i} \le \frac{\epsilon^{k+1}}{4} \sum_{w=1}^{s} \lambda_i(y_w, t_w) \le \frac{\epsilon^{k+1}}{4} Q_{4,i}$$
.

Thus

$$\|\frac{Q_{1,i}V_{1,i} + Q_{4,i}V_{4,i}}{Q_{1,i} + Q_{4,i}} - \frac{Q_{2,i}V_{2,i} + Q_{4,i}V_{4,i}}{Q_{2,i} + Q_{4,i}}\|_{2}$$

$$(40)$$

$$\leq \left\| \frac{Q_{4,i}(Q_{2,i} - Q_{1,i})(V_{4,i} - V_{2,i})}{(Q_{1,i} + Q_{4,i})(Q_{2,i} + Q_{4,i})} \right\| + \left\| \frac{Q_{1,i}}{Q_{1,i} + Q_{4,i}}(V_{1,i} - V_{2,i}) \right\| \tag{41}$$

$$\leq \|\frac{Q_{4,i}(Q_{2,i} - Q_{1,i})(V_{4,i} - V_{2,i})}{(Q_{1,i} + Q_{4,i})(Q_{2,i} + Q_{4,i})}\| + \|\frac{Q_{1,i}}{Q_{1,i} + Q_{4,i}}(V_{1,i} - V_{2,i})\|
\leq \|\frac{(Q_{2,i} - Q_{1,i})(V_{4,i} - V_{2,i})}{(Q_{2,i} + Q_{4,i})}\| + \|\frac{Q_{1,i}}{Q_{1,i} + Q_{4,i}}(V_{1,i} - V_{2,i})\|$$
(41)

$$\leq \|\frac{\epsilon^{k+1}(V_{4,i} - V_{2,i})}{4}\| + \|\frac{\epsilon^{k+1}}{4}(V_{1,i} - V_{2,i})\| \tag{43}$$

$$\leq \epsilon^{k+1}$$
 (44)

And it can be seen from definition that

- $\frac{Q_{1,i}V_{1,i}+Q_{4,i}V_{4,i}}{Q_{1,i}+Q_{4,i}}$ is the output of the *i*-th head of the attention layer with input sequence W_1 . (which means $\frac{Q_{1,i}V_{1,i}+Q_{4,i}V_{4,i}}{Q_{1,i}+Q_{4,i}} = \sum_{t=1}^T \sigma \left[(W_{K,i}\hat{w}_1(t))^\top W_{Q,i}\hat{c}_0 \right] W_{V,i}\hat{w}_1(t)$).
- $\frac{Q_{2,i}V_{1,i}+Q_{4,i}V_{4,i}}{Q_{2,i}+Q_{4,i}}$ is the output of the *i*-th head of the attention layer with input sequence $\begin{array}{l} W_2, \text{ (which means } \frac{Q_{2,i}V_{2,i}+Q_{4,i}V_{4,i}}{Q_{2,i}+Q_{4,i}} = \sum_{t=1}^T \sigma \big[(W_{K,i}\hat{w_2}(t))^\top W_{Q,i}\hat{c}_0 \big] \ W_{V,i}\hat{w_2}(t)). \end{array}$

Then for each $i = 1, \ldots, s$, we have that

$$\|\sum_{t=1}^{T} \sigma \left[(W_{K,i} \hat{w}_1(t))^{\top} W_{Q,i} \hat{c}_0 \right] W_{V,i} \hat{w}_1(t) - \sum_{t=1}^{T} \sigma \left[(W_{K,i} \hat{w}_2(t))^{\top} W_{Q,i} \hat{c}_0 \right] W_{V,i} \hat{w}_2(t) \| \le \epsilon^{k+1}$$
(45)

Therefore, as W_O have entries bounded by 1, we have

$$\| \left[\hat{c}_0 + W_O \operatorname{Concat}_{i=1}^h \left(\sum_{t=1}^T \sigma \left[(W_{K,i} \hat{w}_1(t))^\top W_{Q,i} \hat{c}_0 \right] W_{V,i} \hat{w}_1(t) \right) \right]$$
(46)

$$-\left[\hat{c}_{0} + W_{O} \operatorname{Concat}_{i=1}^{h} \left(\sum_{t=1}^{T} \sigma \left[(W_{K,i} \hat{w}_{2}(t))^{\top} W_{Q,i} \hat{c}_{0} \right] W_{V,i} \hat{w}_{2}(t) \right) \right] \|$$
 (47)

$$\leq s\epsilon^{k+1}$$
 (48)

However, it has been proven above that we need $|Model(W_1) - Model(W_2)| \ge \epsilon$ to achieve ϵ -approximation of the target function. According to lemma 4, the required parameter count of the FFN \hat{F} is of order $\Omega(\epsilon/\epsilon^{k+1})$. Thus the parameter count required to achieve ϵ -approximation is $\Omega(1/\epsilon^k)$.

A.3 PROOF OF THEOREM 2 (3)

Proof Sketch. The argument is based on an explicit construction. We begin with trivial attention, so that the post-attention output is simply the averaged concatenation $\frac{1}{T}(x(1),\ldots,x(T)) \in \mathbb{R}^{Td}$. The feed-forward block can then be used to compute the transformations $f_i(x(t))$, perform the necessary comparisons, and approximate F_0 , as ensured by Lemmas 9 and 8.

Having outlined the main idea, we now proceed to the detailed proof. As a first step, we introduce several auxiliary lemmas that will be used in the argument.

Lemma 8. Fix a pointwise activation σ (e.g., ReLU or any activation used in this paper). Let $F_1: \mathbb{R}^{m_1} \to \mathbb{R}^{m_2}$ be a 2-layer fully connected network, $F_2: \mathbb{R}^{m_2} \to \mathbb{R}^{m_3}$ a 3-layer fully connected network, and $F_3: \mathbb{R}^{m_3} \to \mathbb{R}$ a 2-layer fully connected network. Let W_1, W_2, W_3 denote their respective (maximum) hidden widths, and set $W:=\max\{W_1,W_2,W_3\}$. Then there exists a 5-layer fully connected network $G: \mathbb{R}^{m_1} \to \mathbb{R}$ with activation σ and hidden width at most W such that

$$G(x) = F_3(F_2(F_1(x)))$$
 for all $x \in \mathbb{R}^{m_1}$.

Proof. Proof of Lemma 8 Write the three networks in affine–nonlinearity form (with a pointwise activation σ):

$$F_{1}(x) = A_{1} \sigma(B_{1}x + b_{1}) + a_{1}, \qquad x \in \mathbb{R}^{m_{1}}, \ F_{1}(x) \in \mathbb{R}^{m_{2}},$$

$$F_{2}(u) = C_{2} \sigma(D_{2} \sigma(E_{2}u + e_{2}) + d_{2}) + c_{2}, \quad u \in \mathbb{R}^{m_{2}}, \ F_{2}(u) \in \mathbb{R}^{m_{3}},$$

$$F_{3}(v) = p_{3} \sigma(Q_{3}v + q_{3}) + r_{3}, \qquad v \in \mathbb{R}^{m_{3}}, \ F_{3}(v) \in \mathbb{R}.$$

Define a 5-layer fully connected network $G: \mathbb{R}^{m_1} \to \mathbb{R}$ by stacking the hidden layers of F_1 (one), F_2 (two), and F_3 (one), keeping their original widths:

$$h_1(x) := \sigma(B_1x + b_1),$$

$$u(x) := A_1h_1(x) + a_1,$$

$$h_2(x) := \sigma(E_2u(x) + e_2),$$

$$h_3(x) := \sigma(D_2h_2(x) + d_2),$$

$$v(x) := C_2h_3(x) + c_2,$$

$$h_4(x) := \sigma(Q_3v(x) + q_3),$$

$$G(x) := p_3h_4(x) + r_3.$$

By construction,

$$G(x) = p_3 \sigma \Big(Q_3 \Big(C_2 \sigma (D_2 \sigma (E_2(A_1 \sigma (B_1 x + b_1) + a_1) + e_2) + d_2) + c_2 \Big) + q_3 \Big) + r_3 = F_3 \Big(F_2 \Big(F_1(x) \Big) \Big).$$

Thus G realizes the composition exactly, has 4 hidden layers (hence 5 layers total), and its hidden widths are precisely those of the constituent hidden layers of F_1 , F_2 , and F_3 .

Lemma 9 (Approximating max with a shallow ReLU network). Let $f:[0,1]^T \to \mathbb{R}$ be $f(x_1,\ldots,x_T)=\max\{x_1,\ldots,x_T\}$. For any $\epsilon\in(0,1]$, there exists a fully connected ReLU network \hat{f} with three layers (i.e., two hidden layers and one output layer), whose hidden-layer widths are each at most $2T[1/\epsilon]$, such that \hat{f} ϵ -approximates f.

Proof. Proof of Lemma 9 Let

$$n = \lceil 1/\epsilon \rceil$$
.

For each coordinate $t \in [T]$ and each grid index $i = 0, 1, \dots, n-1$, define the first hidden layer neurons by

$$h_1(t,i) = \text{ReLU}\left(x_t - \frac{i}{n}\right).$$

For each $j = 0, 1, \dots, n-1$, define the second hidden layer neurons by

$$h_2(j) = \text{ReLU}\left(\sum_{t=1}^T h_1(t,j)\right) - \text{ReLU}\left(\sum_{t=1}^T h_1(t,j) - \frac{1}{n}\right).$$

Finally, the output of the network is given by

$$\hat{f}(x_1, \dots, x_T) = \sum_{j=0}^{n-1} h_2(j).$$

Claim. Fix $j \in \{0, \dots, n-1\}$ and set

$$S_j = \sum_{t=1}^T h_1(t,j) = \sum_{t=1}^T \text{ReLU}\left(x_t - \frac{j}{n}\right).$$

By definition,

$$h_2(j) = \text{ReLU}(S_j) - \text{ReLU}(S_j - \frac{1}{n}).$$

1) If $h_2(j) > 0$, then necessarily $S_j > 0$ (since $\mathrm{ReLU}(z) > 0$ iff z > 0), hence there exists some t with

$$\operatorname{ReLU}\left(x_t - \frac{j}{n}\right) > 0 \iff x_t > \frac{j}{n}.$$

Thus $h_2(j) > 0$ only if $\exists t$ with $x_t > j/n$.

2) If there exists t with $x_t > (j+1)/n$, then

$$S_j \ge \text{ReLU}\left(x_t - \frac{j}{n}\right) > \frac{1}{n}.$$

Therefore $S_j \geq \frac{1}{n}$, and we get

$$h_2(j) = S_j - \left(S_j - \frac{1}{n}\right) = \frac{1}{n}.$$

Fix $x \in [0,1]^T$ and let j be such that $\max_t x_t \in (j/n,(j+1)/n]$. By construction,

$$h_2(k) = 0$$
 for $k \ge j + 1$, $h_2(k) = \frac{1}{n}$ for $k \le j - 1$,

and for k = j we have

$$0 \le h_2(j) = \text{ReLU}(S_j) - \text{ReLU}\left(S_j - \frac{1}{n}\right) \le \frac{1}{n}, \quad S_j := \sum_{t=1}^T \text{ReLU}\left(x_t - \frac{j}{n}\right).$$

Hence

$$\hat{f}(x) = \sum_{k=0}^{n-1} h_2(k) = \sum_{k=0}^{j-1} \frac{1}{n} + h_2(j) \in \left[\frac{j}{n}, \frac{j}{n} + \frac{1}{n}\right] = \left[\frac{j}{n}, \frac{j+1}{n}\right].$$

Since $\max_t x_t \in (j/n, (j+1)/n]$, it follows that

$$0 \le |\hat{f}(x) - \max_{t} x_t| \le \frac{1}{n} \le \epsilon.$$

Therefore \hat{f} ϵ -approximates $f(x) = \max_t x_t$ on $[0, 1]^T$.

Proof. Theorem 2 (3)

We begin by fixing the embedding with positional information. Let $P_{\phi}:[0,1]^d\times [T]\to \mathbb{R}^{dT}$ be defined by

$$P_{\phi}(x(t),t) = (0,\ldots,0,x(t),0,\ldots,0),$$

where the vector x(t) occupies the t-th block of dimension d, and all other blocks are zero. With the classification token $\hat{c}_0 = 0$, the attention layer reduces to a trivial aggregation, and the output (prior to the feed-forward network) is

$$\frac{1}{T}(x(1),\ldots,x(T)) \in [0,1]^{dT}.$$

Given a target accuracy $\epsilon > 0$, we construct three feed-forward networks F_1, F_2, F_3 as follows.

where each $u(t) \in \mathbb{R}^D$ satisfies count $O(1/\epsilon^{\gamma})$.

Step 1: Approximating the component functions. Define

$$F_1: \frac{1}{T}[0,1]^{d \times T} \to \mathbb{R}^{D \times T}, \qquad F_1(\frac{1}{T}x(1), \dots, \frac{1}{T}x(T)) = (u(1), \dots, u(T)),$$

$$|u(t)_i - f_i(x(t))| \le \epsilon$$
 for all $i = 1, \dots, D$.

By Assumption 3, such an approximation can be implemented by a two-layer FFN with parameter

Step 2: Approximating the minimization. Let $F_2':\mathbb{R}^{D imes T} o \mathbb{R}^D$ be defined by

$$F'_2(u(1), \dots, u(T)) = (u_1, \dots, u_D), \qquad u_i = \min_{t \in S_i} u(t)_i.$$

By Lemma 9 (which works the same for taking minimum), there exists a three-layer ReLU network with $O(1/\epsilon)$ parameters that ϵ -approximates F_2' . We denote this approximation by F_2 .

Step 3: Approximating the outer function. Finally, let $F_3: \mathbb{R}^D \to \mathbb{R}$ be a two-layer FFN that ϵ -approximates F_0 , with parameter count $O(1/\epsilon^{\gamma})$.

Composition. Since F_0 is C^1 on a compact domain, it is Lipschitz with constant L, and the min operator is 1-Lipschitz. Therefore, the composed network

$$F_3 \circ F_2 \circ F_1$$

provides an $L\epsilon$ -approximation of the target function, with total parameter count

$$O(1/\epsilon^{\gamma+1}).$$

According to lemma 8, $F_3 \circ F_2 \circ F_1$ can be written equivalently as a five-layer FFN.

B EXPERIMENT DETAILS

B.1 Details for Experiment 1

B.1.1 EXPERIMENTAL DETAILS FOR SECTION 6.1

Data generation. The intrinsic dimension of the synthetic task is D=4. For each sequence length $T \in \{8, 16, 32, 64, 128\}$ we generate 8000 training and 2000 validation examples. The inputs are i.i.d. Gaussian samples $x(t) \sim \mathcal{N}(0, I_4)$.

Model architecture. Each input vector x(t) is first mapped to \mathbb{R}^{8h} by a two-layer feed-forward network with hidden dimension N and ReLU activations, ensuring a per-head embedding dimension of 8. A trainable classification token c_0 is appended, and no positional encoding is used since the task is permutation invariant. The sequence is processed by a single-layer multi-head attention block without residual connections or layer normalization, consistent with the theoretical setting. The output is concatenated and passed through a two-layer GeLU-activated feed-forward network with hidden dimension N, yielding the final scalar prediction. The fixed hidden size ensures comparability of parameter counts across different h.

Training protocol. Each configuration (h,T) is trained separately under multiple random seeds. To reduce the effect of optimization variance, we report the *minimal validation error* achieved across seeds. This choice isolates expressivity limitations of the architecture from randomness in training dynamics.

Evaluation metric. We adopt the normalized mean squared error (NMSE), defined as mean squared error divided by the variance of the targets. As T increases, maxima of Gaussian samples concentrate, shrinking target variance and making trivial predictors appear competitive under raw MSE. Normalization by variance corrects this effect and ensures comparability across lengths. NMSE is also equivalent to $1-R^2$, where R^2 is the standard coefficient of determination.

Variance across seeds. While mean performance across seeds is also informative, reporting the minimal validation NMSE highlights the best achievable accuracy for a given architecture. This emphasizes limitations due to model capacity rather than training noise. Tables showing seed variance are included for completeness (Table 1).

B.1.2 FIGURES AND TABLES FOR SYNTHETIC EXPERIMENT 6.1

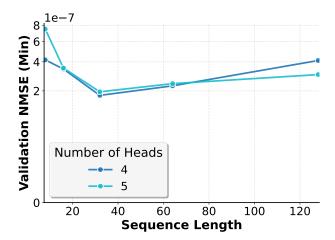


Figure 3: A zoom in plot of Figure 1, which shows that when the number of head is enough, the loss first decreases and then increases, as explained in the remark 6.1

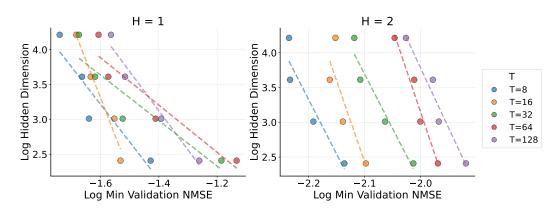


Figure 4: Additional plot of 1b for H = 1 and H = 2.

Heads	T=8	T=16	T=32	T=64	T=128
		$1.09 \times 10^{-1} \pm 9.93 \times 10^{-2}$			
2	$7.31 \times 10^{-3} \pm 4.75 \times 10^{-4}$	$8.41 \times 10^{-3} \pm 7.97 \times 10^{-4}$	$9.42 \times 10^{-3} \pm 6.42 \times 10^{-4}$	$1.31 \times 10^{-2} \pm 1.16 \times 10^{-2}$	$1.47 \times 10^{-2} \pm 1.21 \times 10^{-2}$
3	$6.94 \times 10^{-4} \pm 2.90 \times 10^{-4}$	$6.40 \times 10^{-4} \pm 3.87 \times 10^{-4}$	$9.09 \times 10^{-4} \pm 4.31 \times 10^{-4}$	$1.31 \times 10^{-3} \pm 5.10 \times 10^{-4}$	$1.58 \times 10^{-3} \pm 5.21 \times 10^{-4}$
	$6.10 \times 10^{-5} \pm 1.52 \times 10^{-4}$	$4.36 \times 10^{-5} \pm 1.93 \times 10^{-4}$	$4.80 \times 10^{-5} \pm 2.30 \times 10^{-4}$		$5.23 \times 10^{-6} \pm 5.67 \times 10^{-6}$
5	$3.35 \times 10^{-5} \pm 5.84 \times 10^{-5}$	$1.10 \times 10^{-5} \pm 2.36 \times 10^{-5}$	$4.91 \times 10^{-6} \pm 6.32 \times 10^{-6}$	$4.19 \times 10^{-6} \pm 8.39 \times 10^{-6}$	$3.99 \times 10^{-6} \pm 4.29 \times 10^{-6}$

Table 1: Error bar for synthetic dataset. $NMSE(Mean \pm Standard Deviation)$ for different sequence lengths T and number of heads.

B.2 MS MARCO TEXT RETRIEVAL

B.2.1 EXPERIMENT DETAILS FOR MS MARCO (TEXT RETRIEVAL) EXPERIMENT

Dataset construction. We construct retrieval-style datasets from the MS MARCO passage ranking collection (Bajaj et al., 2018). Since the original dataset associates each query with only a few candidate passages, we enlarge the candidate set by mining hard negatives. Specifically, BM25 (Robertson & Zaragoza, 2009) is used to mine local negatives and FAISS (Johnson et al., 2017) similarity search to retrieve global negatives, reducing redundancy across queries. For each query, the sequence length T is defined as the total number of candidates (one positive and T-1 negatives), with $T \in \{8, 16, 32, 64\}$. We build datasets containing 28,000 training queries and 2,000 validation queries for each T.

Model and training setup. We evaluate a two-layer Transformer encoder with per-head embedding dimension fixed at 32, while varying the number of heads across $\{1, 2, 4, 6, 8, 10, 12, 14, 16\}$. Tokenization and input embeddings follow the BERT tokenizer and frozen BERT word, position, and segment embeddings (Devlin et al., 2019), projected to the model hidden size $h = \text{heads} \times 32$. Only the projection and Transformer layers are trained. We report training top-1 accuracy, focusing on training performance since MS MARCO with BM25-mined negatives is particularly challenging for validation, and the difference can be seen in training metrics. Training MRR is also reported in Fig 5, with similar trend as training accuracy.

B.2.2 FIGURES AND TABLES FOR EXPERIMENT

B.3 CIFAR-10 IMAGE CLASSIFICATION

B.3.1 DATASET CONSTRUCTION

We create image classification datasets from the CIFAR-10 dataset using a padded preprocessing approach. The original CIFAR-10 images have dimensions of 32×32 pixels. To generate datasets with larger image sizes, we apply padding to achieve sizes in the set $\{32, 48, 64, 96, 128\}$. The original image is randomly positioned within the enlarged frame, with padding filled using the colors of the border pixels. An illustration is provided in Figure 6. By apply this padding method we are creating tasks with increasing difficulty. The background is enlarged, making models need more

Heads	T=8	T=16	T=32	T=64
1	0.597 ± 0.003	0.450 ± 0.005	0.303 ± 0.003	0.154 ± 0.002
2	0.771 ± 0.003	0.647 ± 0.003	0.486 ± 0.002	0.286 ± 0.002
4	0.956 ± 0.002	0.900 ± 0.002	0.793 ± 0.002	0.580 ± 0.004
6	0.992 ± 0.000	0.977 ± 0.001	0.937 ± 0.001	0.814 ± 0.002
8	0.998 ± 0.000	0.995 ± 0.000	0.983 ± 0.001	0.932 ± 0.002
12	1.000 ± 0.000	0.999 ± 0.000	0.998 ± 0.000	0.991 ± 0.001
16	1.000 ± 0.000	1.000 ± 0.000	0.999 ± 0.000	0.996 ± 0.000

Table 2: Error bar for MS Marco dataset. Accuracy (Mean \pm Standard Deviation) for different sequence lengths T and number of heads.

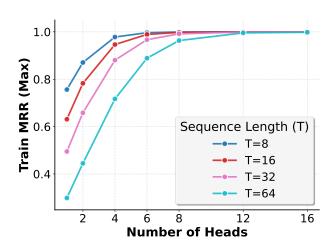


Figure 5: Plot of training mrr for MS MARCO dataset.

effort to learn how to extract useful information. The random placement make sure the padded outside aera cannot be simply ignored by position encodings.

Each image is divided into non-overlapping patches of size 8×8 pixels, resulting in a sequence of patches for each image. For each image size, the sequence length T is defined as the total number of patches plus one additional class token, with $T=\{17,37,65,145,257\}$. We adopt the standard CIFAR-10 data splits, which include 50,000 training images and 10,000 test images across 10 classes.

B.3.2 MODEL TRAINING SETUP

We evaluate a Vision Transformer (ViT) with four layers and a per-head embedding dimension of 16, while varying the number of attention heads in different configurations. Each image patch is embedded through a linear projection, and positional embeddings are added along with a learnable class token. No global convolutional embedding is used.

Input processing follows the standard ViT procedure, including patch embedding of size 8×8 , positional encoding, and aggregation of the class token for final classification. The model is trained using the AdamW optimizer with cosine annealing learning rate scheduling. Standard architectural techniques, such as layer normalization, residual connections, and dropout, are employed for regularization.

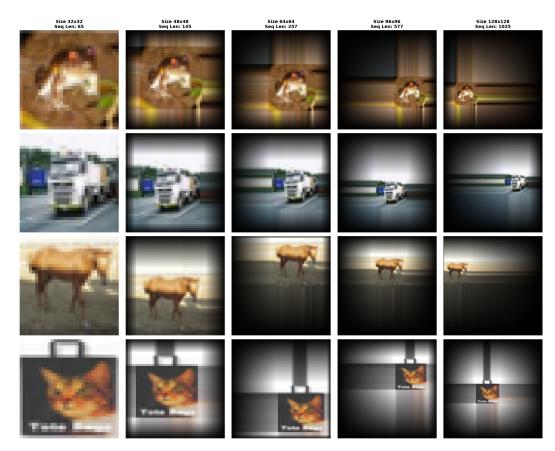


Figure 6: Examples of the padded images from the dataset.

Heads	Seq=65	Seq=145	Seq=257	Seq=577	Seq=1025
1	$4.78 \times 10^{1} \pm 4.50 \times 10^{-1}$	$4.37 \times 10^{1} \pm 4.70 \times 10^{-1}$	$4.20 \times 10^{1} \pm 5.00 \times 10^{-1}$	$4.08 \times 10^{1} \pm 6.50 \times 10^{-1}$	$4.00 \times 10^{1} \pm 7.20 \times 10^{-1}$
2	$5.97 \times 10^{1} \pm 4.50 \times 10^{-1}$	$5.52 \times 10^{1} \pm 3.80 \times 10^{-1}$	$5.34 \times 10^1 \pm 4.40 \times 10^{-1}$	$5.15 \times 10^{1} \pm 4.70 \times 10^{-1}$	$5.08 \times 10^{1} \pm 7.40 \times 10^{-1}$
4	$7.55 \times 10^{1} \pm 2.10 \times 10^{-1}$	$7.03 \times 10^1 \pm 3.20 \times 10^{-1}$	$6.85 \times 10^1 \pm 7.70 \times 10^{-1}$	$6.62 \times 10^{1} \pm 6.00 \times 10^{-1}$	$6.58 \times 10^{1} \pm 7.20 \times 10^{-1}$
8	$9.51 \times 10^{1} \pm 1.50 \times 10^{-1}$	$9.26 \times 10^{1} \pm 4.70 \times 10^{-1}$	$9.14 \times 10^{1} \pm 6.20 \times 10^{-1}$	$9.07 \times 10^1 \pm 1.02 \times 10^0$	$9.02 \times 10^1 \pm 1.00 \times 10^0$
10	$9.81 \times 10^{1} \pm 5.00 \times 10^{-2}$	$9.73 \times 10^{1} \pm 2.40 \times 10^{-1}$	$9.67 \times 10^1 \pm 4.60 \times 10^{-1}$	$9.65 \times 10^{1} \pm 3.20 \times 10^{-1}$	$9.67 \times 10^{1} \pm 7.30 \times 10^{-1}$
11	$9.88 \times 10^{1} \pm 1.20 \times 10^{-1}$	$9.83 \times 10^{1} \pm 1.20 \times 10^{-1}$	$9.81 \times 10^{1} \pm 2.40 \times 10^{-1}$	$9.77 \times 10^{1} \pm 2.10 \times 10^{-1}$	$9.79 \times 10^{1} \pm 2.20 \times 10^{-1}$
12	$9.92 \times 10^{1} \pm 3.00 \times 10^{-2}$	$9.89 \times 10^{1} \pm 1.60 \times 10^{-1}$	$9.86 \times 10^{1} \pm 2.40 \times 10^{-1}$	$9.86 \times 10^{1} \pm 1.90 \times 10^{-1}$	$9.86 \times 10^{1} \pm 2.90 \times 10^{-1}$
13	$9.94 \times 10^{1} \pm 6.00 \times 10^{-2}$	$9.93 \times 10^{1} \pm 6.00 \times 10^{-2}$	$9.91 \times 10^{1} \pm 1.10 \times 10^{-1}$	$9.90 \times 10^{1} \pm 2.00 \times 10^{-1}$	$9.91 \times 10^{1} \pm 2.50 \times 10^{-1}$
14	$9.96 \times 10^{1} \pm 3.00 \times 10^{-2}$	$9.94 \times 10^{1} \pm 9.00 \times 10^{-2}$	$9.93 \times 10^{1} \pm 1.00 \times 10^{-1}$	$9.93 \times 10^{1} \pm 1.70 \times 10^{-1}$	$9.93 \times 10^{1} \pm 2.30 \times 10^{-1}$
16	$9.97 \times 10^{1} \pm 3.00 \times 10^{-2}$	$9.96 \times 10^{1} \pm 2.00 \times 10^{-2}$	$9.95 \times 10^1 \pm 7.00 \times 10^{-2}$	$9.96 \times 10^{1} \pm 1.40 \times 10^{-1}$	$9.96 \times 10^{1} \pm 1.70 \times 10^{-1}$
20	$9.98 \times 10^{1} \pm 1.00 \times 10^{-2}$	$9.97 \times 10^{1} \pm 5.00 \times 10^{-2}$	$9.97 \times 10^{1} \pm 8.00 \times 10^{-2}$	$9.98 \times 10^{1} \pm 6.00 \times 10^{-2}$	$9.99 \times 10^{1} \pm 7.00 \times 10^{-2}$
24	$9.99 \times 10^{1} \pm 2.00 \times 10^{-2}$	$9.98 \times 10^{1} \pm 2.00 \times 10^{-2}$	$9.98 \times 10^{1} \pm 4.00 \times 10^{-2}$	$9.99 \times 10^{1} \pm 4.00 \times 10^{-2}$	$9.99 \times 10^{1} \pm 5.00 \times 10^{-2}$

Table 3: Error bar for Image task. Accuracy (Mean \pm Standard Deviation) for different sequence lengths and number of heads.

C LARGE LANGUAGE MODEL USAGE

Large language models were used only for linguistic refinement (e.g., polishing sentences and checking grammar). The core ideas, theoretical results, experimental design, and analyses presented in this paper were entirely developed by the authors without assistance from large language models.

Table 4: Hyperparameter settings of popular transformer models. Only d (embedding dimension), L (number of layers), and H (number of attention heads) are shown for brevity.

TT	M. J.1		T	X 7
H	Model	d	L	Year
8	Attention is all you need	512	6	2017
8	Gemma 2B	2,048	18	2024
12	GPT	768	12	2018
16	BERT-Large	1,024	24	2019
16	ViT-Huge	1,280	32	2021
16	Gemma 7B	3,072	28	2024
28	Turing-NLG	4,256	78	2020
32	LLaMA-7B	4,096	32	2023
32	Baichuan 2-7B	4,096	32	2023
32	Mistral 7B	4,096	32	2023
32	Yi-6B	4,096	32	2023
32	LLaMA 3-8B	4,096	32	2024
32	Mixtral 8x7B	4,096	32	2024
40	LLaMA-13B	5,120	40	2023
40	Baichuan 2-13B	5,120	40	2023
56	Yi-34B	7,168	60	2023
64	LLaMA-65B	8,192	80	2023
64	Llama-2-70B	8,192	80	2023
64	LLaMA 3-70B	8,192	80	2024
96	GPT-3	12,288	96	2020
96	Jurassic-1	13,824	76	2021
128	MT-NLG	20,480	105	2021
128	LaMDA	8,192	64	2022
128	LLaMA 3.1-405B	16,384	126	2024
128	DeepSeek-V2	5,120	60	2024