
A unified framework for establishing the universal approximation of transformer-type architectures

Jingpu Cheng

Department of Mathematics
National University of Singapore
chengjingpu@u.nus.edu

Ting Lin

School of Mathematical Sciences
Peking University
lntingsms@pku.edu.cn

Zuowei Shen

Department of Mathematics
National University of Singapore
matzuows@nus.edu.sg

Qianxiao Li

Department of Mathematics
Institute for Functional Intelligent Materials
National University of Singapore
qianxiao@nus.edu.sg

Abstract

We investigate the universal approximation property (UAP) of transformer-type architectures, providing a unified theoretical framework that extends prior results on residual networks to models incorporating attention mechanisms. Our work identifies token distinguishability as a fundamental requirement for UAP and introduces a general sufficient condition that applies to a broad class of architectures. Leveraging an analyticity assumption on the attention layer, we can significantly simplify the verification of this condition, providing a non-constructive approach in establishing UAP for such architectures. We demonstrate the applicability of our framework by proving UAP for transformers with various attention mechanisms, including kernel-based and sparse ones. The corollaries of our results either generalize prior works or establish UAP for architectures not previously covered. Furthermore, our framework offers a principled foundation for designing novel transformer architectures with inherent UAP guarantees, including those with specific functional symmetries. We propose examples to illustrate these insights.

1 Introduction

Transformers [66] are a family of deep learning architectures that have achieved remarkable performance in natural language processing [5, 57, 58], computer vision [7, 16], and other fields [36]. Given an input sequence of tokens, a transformer processes it through a deep composition of alternating attention and token-wise feedforward layers. Besides the original softmax attention [66], a variety of different attention mechanisms have been proposed to enhance performance or computational efficiency, such as kernel-based attention [9, 12, 38, 65], sparse attention [3, 40, 76], and attention with low-rank structures [68, 82].

A natural theoretical question is: *What is the expressive power of these architectures?* Previous studies have shown that transformers achieve the universal approximation property (UAP) via architecture-specific constructions, meaning they can approximate any continuous sequence-to-sequence function over compact domains [37, 75, 76] in certain measures. However, these results heavily rely on explicit, architecture-specific constructions, and a unified theoretical framework of deep transformer-type architectures remains elusive. In particular, it is highly desirable to derive a verifiable condition that guarantees UAP of deep transformer-type architectures, independent of specific architectural details

such as the choice of the attention mechanism. Such a framework would allow greater flexibility in design without sacrificing expressivity.

Similar concerns have been addressed for fully connected deep residual networks (ResNets) using insights from control theory and dynamical systems [10, 44, 62, 63]. By interpreting ResNets as control systems, recent studies [10, 44] showed that deep ResNets with Lipschitz nonlinear activation functions possess UAP. However, extending this approach to transformers presents a challenge. Unlike ResNets, transformers apply identical feedforward transformations across tokens, without direct inter-token interactions. Hence, the attention mechanism must effectively capture token dependencies and propagate contextual information throughout the network.

To extend the UAP framework from ResNets to transformers, we model each transformer block through two sequential operations¹:

$$\begin{aligned} X_{t+\frac{1}{2}} &= X_t + \text{Atten}(X_t), \\ X_{t+1} &= X_{t+\frac{1}{2}} + \text{FFN}(X_{t+\frac{1}{2}}), \end{aligned} \tag{1}$$

where $X_t \in \mathbb{R}^{d \times n}$ represents n tokens each of dimension d . The feedforward network (FFN) acts independently on each token, while the attention layer (Atten) explicitly models dependencies across tokens. A transformer model is then defined as the composition of such blocks. In many practical architectures, the attention layer is computed by some interactions between tokens, which has a computational complexity up to $\mathcal{O}(n^2d)$, while the feedforward layer has computation complexity of $\mathcal{O}(nd^2)$. This structure reduces computational complexity from $\mathcal{O}(n^2d^2)$ (for using network with dense layers) to $\mathcal{O}(nd(n+d))$ (can be even lower in many variants) by decomposing approximation tasks into simpler token-wise and token-mixing components. Such a decomposition not only enhances computational efficiency but also provides a novel perspective in the context of approximation theory. Therefore, it is of theoretical interest to understand *how the combination of the token-wise and token-mixing operations contributes to the expressive power of models in handling sequential data*.

In this paper, we develop a general framework for the UAP analysis of transformers. Specifically, we provide abstract and verifiable conditions ensuring UAP, independent of specific architectural details. Our key contributions include:

- We derive a general sufficient condition for transformer models to achieve UAP in the L^p sense over compact sets (Theorem 1), requiring: (1) feedforward layers satisfying the conditions [10], as stated in Definition 2, and (2) attention mechanisms producing distinct context-aware token representations across different inputs. Notably, our framework incorporates potential symmetry under token permutations in transformers, extending the analysis to non-transitive permutation groups beyond [45].
- For attention mechanisms that are analytic to their parameters, we reduce UAP verification to a two-sample condition (Theorem 2), simplifying practical validation compared to constructive approaches [37, 74–76]. Moreover, we show conditions under which transformers with a fixed number of attention layers but arbitrarily many feedforward layers achieve UAP, generalizing the results on the memorization capability of transformers in [37, 39].
- We apply our general framework to various transformer architectures to demonstrate its generality and applicability, including kernel-based [12, 65, 66], sparse [3, 40, 76], and some other attention mechanisms [9, 68]. For kernel-based attention (formulated in Section 4.1), our result (Corollary 1) provides UAP guarantee for many existing architectures in previous works [12, 65, 66] and also for new architectures. For sparse attention (e.g., architectures proposed in [3, 40, 76]), our result (Corollary 2) provides a UAP criterion which generalizes beyond the softmax attention and is free from technical assumptions on the sparse pattern.
- Our theoretical results also enable principled design of UAP-guaranteed architectures. We demonstrate this by proposing new transformer architectures with UAP guarantees, especially for attention mechanisms that preserve specific functional symmetry (Section 4.4).

We discuss in detail after our main results how they relate to the rest of the literature, and collect a more detailed review of related work in Section A.

¹Here, we omit the layer normalization for simplicity of the analysis.

2 Problem formulation

In this section, we introduce the transformer-type architecture, an abstraction of the standard transformer [66] as a family of architectures composed of two repeating components: the token-mixing layers and token-wise map layers. Then, we define the universal approximation property (UAP). Notably, we introduce the UAP under permutation equivariance for any subgroup G of the symmetric group S_n over tokens, which is a more general framework.

In the following, we use $X = ([X]_1, \dots, [X]_n) \in \mathbb{R}^{d \times n}$ to denote one data sample consisting of n tokens $[X]_1, \dots, [X]_n$ of dimension d . We say that X is in *general position* if all of its tokens are distinct. We will also use the notation $[n] := \{1, \dots, n\}$ for any positive integer n .

2.1 Transformer architecture

We present a general formulation for the two-step architecture of transformers as described in (1). The mapping $X_t \mapsto X_{t+1}$ can be abstracted as $(\text{Id} + h) \circ (\text{Id} + g)$. Here, g generalizes the attention map Atten to a general token-mixing map, while h generalizes the token-wise feedforward map FFN, which applies to $X \in \mathbb{R}^{d \times n}$ as:

$$h(X) := (\bar{h}([X]_1), \dots, \bar{h}([X]_n)), \quad \text{where } \bar{h} : \mathbb{R}^d \rightarrow \mathbb{R}^d. \quad (2)$$

We denote by \mathcal{G} a token-mixing family, consisting of functions mapping $\mathbb{R}^{d \times n}$ to $\mathbb{R}^{d \times n}$, to represent all possible choices of g in a transformer. Recall that the attention layer in the original transformer [66] is given by

$$\text{Atten}(X_t) = \sum_{i=1}^N W_V^{t,i} X_t \text{softmax} \left((W_K^{t,i} X_t)^\top W_Q^{t,i} X_t \right), \quad (3)$$

with trainable parameters $W_V^{t,i}, W_K^{t,i}, W_Q^{t,i} \in \mathbb{R}^{d \times d}$ for the i -th head in block t , and the softmax is applied column-wise. In this case, \mathcal{G} is precisely the family of functions defined by (3) for all possible choices of $W_V^{t,i}, W_K^{t,i}, W_Q^{t,i}$.

Moreover, we consider

$$\mathcal{H}^{\otimes n} := \{X \mapsto (\bar{h}([X]_1), \dots, \bar{h}([X]_n)) \mid \bar{h} \in \mathcal{H}\}, \quad (4)$$

where \mathcal{H} is a family of maps from \mathbb{R}^d to \mathbb{R}^d , as the function family for the token-wise feedforward map h in a transformer. We define a transformer block, the generalization of (1), to be a map in

$$\mathcal{F}_{\mathcal{G}, \mathcal{H}} := \{(\text{Id} + h) \circ (\text{Id} + g) \mid g \in \mathcal{G}, h \in \mathcal{H}^{\otimes n}\}. \quad (5)$$

A transformer identified by \mathcal{G} and \mathcal{H} is then the composition of such blocks, i.e. a map in the set:

$$\mathcal{T}_{\mathcal{G}, \mathcal{H}} := \{F_n \circ \dots \circ F_1 \mid n \in \mathbb{N}, F_i \in \mathcal{F}_{\mathcal{G}, \mathcal{H}}\}. \quad (6)$$

Notably, the feedforward layer can represent only tensor-type functions, i.e. functions of the form (2). The token-mixing mechanism extends this capability to more general functions by capturing the dependencies between tokens.

2.2 Universal approximation under permutation equivariance

Let S_n denote the symmetric group on n elements and let $G \leq S_n$ be a subgroup. Then, G has a natural group action over $\mathbb{R}^{d \times n}$ by permuting the d -dimensional tokens. A function $f : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ is said to be G -equivariant if

$$f(\sigma(X)) = \sigma(f(X)), \quad \forall \sigma \in G, X \in \mathbb{R}^{d \times n}. \quad (7)$$

The original transformer and many of its variants have some degree of permutation equivariance over tokens. For instance, kernel-based token mixers [12, 66] typically have $G = S_n$, whereas sliding-window attention [3] employs a binary group (identity and reflection), and some architectures [68, 76] do not enforce any equivariance (i.e. $G = \{\text{Id}\}$). If \mathcal{G} consists of only G -equivariant functions, then $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$ can approximate only G -equivariant target functions. This motivates the following definition:

Definition 1 (G -UAP). ² The transformer-type model with hypothesis space $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$ is said to have the G -universal approximation property (G -UAP) in the L^p sense ($1 \leq p < \infty$) if, for every continuous G -equivariant function $F : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$, every compact set $K \subset \mathbb{R}^{d \times n}$, and every $\varepsilon > 0$, there exists $\hat{F} \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ such that

$$\|\hat{F} - F\|_{L^p(K)} < \varepsilon. \quad (8)$$

In applications, the equivariance restriction on the transformer is often addressed by introducing positional encoding [66] on tokens. From a theoretical perspective, previous works [34, 37, 74, 75] have shown that if a family $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$ has G -UAP for some G , then for any given compact set K , there exists an absolute positional encoding $\text{Enc} : X \rightarrow X + E$, where E is a fixed matrix, such that

$$\mathcal{T}_{\mathcal{G}, \mathcal{H}} \circ \text{Enc} := \{F \circ \text{Enc} \mid F \in \mathcal{F}_{\mathcal{G}, \mathcal{H}}\} \quad (9)$$

can approximate any continuous function on K in the L^p sense without symmetry constraints. Technically, this can be done by making the domains of each token position distinct. On the other hand, there are also applications where exact symmetry needs to be enforced, such as structure-to-property prediction in crystals [8, 35, 60, 71]. Therefore, it is sufficient to consider the G -UAP, which can naturally extend to the general UAP while also covering cases where symmetry is considered. We will hereafter focus on the G -UAP.

In the literature, several works have studied the universal approximation of symmetric functions [13, 19, 45, 73], often focusing on specific architectures and symmetric groups. Notably, [45] provides a general sufficient condition for the action of any transitive subgroup of S_n on coordinates (1-dimensional tokens). In comparison, this work considers approximation under symmetry in a general setting, with group action over d -dimensional tokens instead of coordinates. Additionally, our results apply to non-transitive group cases, which are not covered in [45]. In [1], the authors studied the ensemble controllability of control systems under symmetry, showing that systems that can interpolate arbitrarily many samples under symmetry are generic in a topology sense. However, this result does not tell us whether or not a given architecture has controllability. In comparison, our target is to provide a verifiable sufficient condition for UAP of specific architectures.

Our analysis focuses on fixed-length sequence-to-sequence maps on compact subsets. This setting directly covers encoder-style tasks and many architectural variants, which underlies many practical applications ranging from automatic speech recognition and visual sequence modeling to structure–property prediction in molecules and crystals [26, 35, 36, 58, 81]. In parallel, there are also measure-theoretic formulations in the literature that treat inputs as probability measures, which can handle variable or even infinite context length under continuity/regularity assumptions [20–22], offering complementary insights to our results.

3 Main results

In this section, we establish a general sufficient condition for the UAP of transformer-type architectures. Since transformer architectures consist of token-wise feedforward layers and token-mixing attention layers, we first provide conditions for each component required for UAP.

For the feedforward family $\mathcal{H}^{\otimes n}$, we introduce the following definition:

Definition 2 (Nonlinearity and affine-invariance for \mathcal{H}). We say a function family \mathcal{H} (consisting of functions from \mathbb{R}^d to \mathbb{R}^d) is nonlinear and affine-invariant, if

- For any $h \in \mathcal{H}$ and any $W, A \in \mathbb{R}^{d \times d}, b \in \mathbb{R}^d$, the function $Wh(A \cdot -b)$ also belongs to \mathcal{H} ;
- \mathcal{H} contains at least one non-affine Lipschitz function.

The nonlinearity and affine-invariance condition holds for almost all practical feedforward layers, independent of specific choices of activation functions and the width of the network. When $d \geq 2$, according to the main result in [10], this condition ensures that the family

$$h \in (\text{Id} + \mathcal{H})^m = \{(\text{Id} + h_m) \circ \cdots \circ (\text{Id} + h_1) \mid h_1, \dots, h_m \in \mathcal{H}\} \quad (10)$$

²Notice that in Definition 1, we do not require $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$ to consist of only G -equivariant maps, but only that it can approximate G -equivariant functions.

can approximate any continuous function $f : \mathbb{R}^d \rightarrow \mathbb{R}^d$ in L^p sense over compact set. Therefore, this condition guarantees that only the token-wise feedforward layer is able to generate complex features over a single token.

However, an inherent limitation on the expressive power of feedforward layers is that they operate token-wise, meaning that they do not model any interactions between tokens. Considering this, we introduce the following definition for the attention family \mathcal{G} :

Definition 3 (Token distinguishability for \mathcal{G}). *For a given group $G \leq S_n$ and a set of samples $D := \{X_i\}_{i=1}^N \subset \mathbb{R}^{d \times n}$ that are all in general position, we say a token-mixing family \mathcal{G} can distinguish tokens in D using m layers under G -action, if there exists*

$$g \in (\text{Id} + \mathcal{G})^m = \{(\text{Id} + g_m) \circ \dots \circ (\text{Id} + g_1) \mid g_1, \dots, g_m \in \mathcal{G}\} \quad (11)$$

such that for any distinct $i, j \in [N]$ with X_i and X_j belonging to different orbits under the G -action (i.e., $X_i \neq \sigma(X_j)$ for all $\sigma \in G$), the tokens of $g(X_i)$ and $g(X_j)$ are all distinct.

*Moreover, we say \mathcal{G} satisfies the **token distinguishability condition** under G -action, if for any finite set D , there exists m such that \mathcal{G} can distinguish tokens in D using m layers under G -action.*

The token distinguishability condition ensures that token-mixing layers can model interactions between tokens by generating unique outputs for tokens in a finite set (up to G -action), enabling distinct in-context information for each token. This property is crucial for the expressive power of transformers, as illustrated below.

Consider a scenario where the token distinguishability condition fails: there exists a set $\Omega \in \mathbb{R}^{d \times n}$ with positive Lebesgue measure and some $i \in [n]$ such that $[g(X)]_i$ is constant over Ω for any $g \in (\text{Id} + \mathcal{G})^m$. Consequently, any $F \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ is also constant over Ω , leading to the failure of UAP. This example shows that if too many tokens are indistinguishable by the token-mixing mechanism (e.g., from a positive measure set), the transformer’s expressive power becomes limited.

On the other hand, the token distinguishability condition is relatively mild, as it only demands the composition of token-mixing layers to distinguish tokens, rather than enforcing any precise relation. This condition is generally easy to satisfy, provided \mathcal{G} includes sufficiently diverse maps that can effectively mix tokens.

In the following, we assume that $d \geq 2$ and the zero map is in \mathcal{G} . Based on Definitions 2 and 3, we can state our first main result on the UAP of transformers:

Theorem 1. *Suppose that \mathcal{H} is nonlinear and affine-invariant Definition 2, and \mathcal{G} satisfies the token distinguishability condition Definition 3. Then, the family of transformers $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$ satisfies the G -UAP Definition 1.*

Theorem 1 provides a general condition for the UAP of transformers. However, directly verifying the token distinguishability condition is challenging since we need to check the condition arbitrarily many times. Therefore, we propose the following theorem, which greatly simplifies the procedure.

Theorem 2. *We assume that \mathcal{G} is parametrized by $\mathcal{G} = \{X \mapsto g(X; \theta) \mid \theta \in \Theta \subseteq \mathbb{R}^m\}$, where Θ is a connected open subset of \mathbb{R}^m , and for any fixed X , the mapping $\theta \mapsto g(X; \theta)$ is analytic. Then, if \mathcal{G} can distinguish tokens of any dataset D with two elements (Definition 3) using finite many layers, then \mathcal{G} satisfies the token distinguishability condition.*

Moreover, if there exists a uniform m such that with m layers, \mathcal{G} can distinguish tokens of dataset D with $|D| = 2$, then it can also do it for any finite dataset D using m layers. In this case, a deep model using only m token-mixing layers and sufficiently many feedforward layers can achieve the UAP.

The key insight in the proof of Theorem 2 is that if token distinguishability fails over a finite set, we can derive an equation in $\theta \in \Theta$ that is identically zero. By leveraging the property that the zero set of a non-trivial analytic function has measure zero, the equation can be reduced to the case of two elements, as detailed in Section B.2. The use of the analytic property is straightforward but significantly simplifies the token distinguishability condition.

Given expressive enough feedforward layers, Theorem 1 highlights the role of token-mixing mechanisms in transformer architectures for UAP: generating distinct, context-aware token representations. This aligns with prior works [37, 75, 76], which introduced “contextual mapping” to establish UAP for transformers. For instance, [37] defines “contextual mapping” as a function distinguishing tokens

in a dataset D (similar to g in Definition 3) without group actions. However, these works rely on explicit constructions, making verification complex and less generalizable. In contrast, Theorem 1 is the first to our knowledge that formulates token distinguishability and feedforward layer conditions as a general, non-constructive criterion for UAP. There is no need to explicitly construct for UAP once the conditions are verified. Additionally, Theorem 2 significantly simplifies the construction-based verification of token distinguishability, enabling broader applicability to diverse attention mechanisms, as shown in the examples in Section 4. Furthermore, the uniformity of m in Theorem 2 also provides a convenient approach on the memorization capacity of attention layers studied in [37].

4 Applications to practical architectures

We demonstrate the generality and applicability of our UAP results by applying them to practical transformer architectures. We first follow the kernel-based framework from [65], which provides a unified description for a series of attention mechanisms. Specifically, many attention variants proposed in prior work can be formulated as

$$[\text{Atten}(X)]_i = \frac{\sum_{j \in \mathcal{N}(i)} k([W_Q X]_i, [W_K X]_j) [W_V X]_j}{\sum_{j \in \mathcal{N}(i)} k([W_Q X]_i, [W_K X]_j)}, \quad W_Q, W_K, W_V \in \mathbb{R}^{d \times d}, \quad (12)$$

where $k : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^+$ is a positive kernel function, and $\mathcal{N}(i) \subset [n]$ denotes the set of indices that the i -th token attends to. In the original transformer, the kernel function is defined as $k(x, y) = \exp(x^\top y)$, and $\mathcal{N}(i) = [n]$.

Under this framework, many transformer variants can be categorized into two types, to which we will apply our results:

- **Kernel modification:** Replacing the kernel function k to improve efficiency or performance. For example, using a kernel of the form $k(x, y) = \phi(x)^\top \phi(y)$ with a feature map $\phi : \mathbb{R}^d \rightarrow \mathbb{R}^m$ can significantly reduce computational cost when $m \ll n$.
- **Sparse attention:** For each i , restricting $\mathcal{N}(i)$ to a subset of $[n]$, reducing the number of tokens each token attends to. Here, we discuss in a general sense where $\mathcal{N}(i)$ can be dynamic across different layers, such as the sparse pattern in [40, 76].

4.1 Kernel-based attention

We first consider the kernel modification case, where we assume $\mathcal{N}(i) = [n]$ for all i . The following result follows from Theorem 1:

Corollary 1. *Suppose the kernel function k satisfies the following conditions:*

- $k(\cdot, \cdot) : \mathbb{R}^d \times \mathbb{R}^d \rightarrow \mathbb{R}^+$ is an analytic function.
- For any $x \in \mathbb{R}^d \setminus \{0\}$ and distinct points $y_1, y_2 \in \mathbb{R}^d \setminus \{0\}$, for almost all $W_K \in \mathbb{R}^{d \times d^3}$, the following holds:

$$\lim_{t \rightarrow \infty} \frac{k(x, tW_K y_1)}{k(x, tW_K y_2)} = 0 \text{ or } +\infty. \quad (13)$$

That is, for almost all given W_K , the kernel function k can distinguish token representations by scaling the key vectors with a large factor.

Then, a transformer with kernel-based attention family \mathcal{G} and feedforward family \mathcal{H} satisfying the conditions in Theorem 1 possesses the S_n -UAP. Moreover, using only one token-mixing layer and sufficiently many feedforward layers can achieve the UAP.

Corollary 1 ensures the distinguishability condition in Theorem 1 through the limiting behavior of the kernel function. This generalizes the idea from [74, 75], where softmax was used as an approximation of hardmax in explicit constructions. In comparison, our approach leverages analyticity, allowing the limit behavior to directly establish the distinguishability condition without further constructions.

Consequently, this result applies to various existing attention mechanisms. In particular, the following kernels directly satisfy the condition in Corollary 1:

³means that the condition holds all the whole space except for a measure zero set.

- $k(x, y) = \exp(x^\top y)$, used in the original transformer.
- $k(x, y) = \exp(-\gamma\|x - y\|_2^2)$ for $\gamma > 0$, the RBF kernel, explored in [65].
- $k(x, y) = \phi(x)^\top \phi(y)$, where

$$\phi(x)^\top = \exp\left(-\frac{1}{2}\|x\|^2\right) (\exp(\omega_1^\top x), \dots, \exp(\omega_m^\top x)) \in \mathbb{R}^m, \quad (14)$$

with $\omega_1, \dots, \omega_m \in \mathbb{R}^d$ being fixed weights drawn i.i.d. from a Gaussian distribution. This kernel is used in Performer [12], where Theorem 1 holds almost surely.

Among these, the UAP for the original transformer and Performer have already been shown [2, 74]. Our result recovers these results in our framework and relaxes the requirement on the architecture to achieve UAP: for original transformer, we do not need the bias in query vectors as in [74]; for Performer, we do not need additional hidden dimensions as in [2]. To the best of our knowledge, the UAP for RBF kernel attention is new, demonstrating the generality of our approach. Moreover, we can easily propose other kernels satisfying the condition in Theorem 1 but have not been studied in the literature, such as the following forms of $k(x, y)$:

- $k(x, y) = \exp(w^\top (x + y))$ for some $w \in \mathbb{R}^d \setminus \{0\}$;
- $k(x, y) = p(x - y)\tilde{k}(x, y)$, with p being any positive polynomial function and \tilde{k} being any kernel mentioned above.

Corollary 1 also generalizes the results in [37] on the memory capacity of transformers, where they prove that for transformers with dense softmax attention, one layer of attention is sufficient to achieve the UAP. Our result extends this to a broader class of kernel-based attention mechanisms.

4.2 Sparse attention

Prior works proposed sparse attention mechanisms to reduce the computational complexity of attention blocks [3, 11, 15, 24, 40, 76]. A common intuition for designing sparse patterns while retaining expressivity is ensuring connectivity, i.e., each token can attend to others via multiple ‘‘hops.’’ For instance, in sliding window attention [3], where $\mathcal{N}(i) = \{j \in [n] \mid |j - i| \leq w\}$ with $w \ll n$, long-range interactions are achieved indirectly via multiple attention layers. In the following, we formalize this intuition and provide a general UAP condition for sparse attention transformers as a direct consequence of Theorem 1.

Denote $P([n])$ as the power set of $[n]$, i.e. the set of subsets of $[n]$. For a given function $\mathcal{N} : [n] \rightarrow P([n])$, we define $\mathcal{G}_\mathcal{N}$ as the family of maps from $\mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$ defined by (12) associated with the sparsity pattern \mathcal{N} . We define the adjacency matrix of \mathcal{N} as an $n \times n$ matrix $A_\mathcal{N}$ with $A_\mathcal{N}(i, j) = 1$ if $j \in \mathcal{N}(i)$ and $A_\mathcal{N}(i, j) = 0$ otherwise.

We also define

$$\text{Aut}(\mathcal{N}) := \{\sigma \in S_N \mid j \in \mathcal{N}(i) \Leftrightarrow \sigma(j) \in \mathcal{N}(\sigma(i))\} \quad (15)$$

as the permutations that keep the structure of \mathcal{N} invariant.

Let $\Phi := (\mathcal{N}_1, \mathcal{N}_2, \dots)$ be a sequence of sparsity patterns. We define the sparse transformer family associated with Φ as:

$$\mathcal{T}_\mathcal{H}^\Phi := \{(\text{Id} + h_n) \circ (\text{Id} + g_n) \circ \dots \circ (\text{Id} + h_1) \circ (\text{Id} + g_1) \mid n \in \mathbb{N}_+, h_i \in \mathcal{H}^{\otimes n}, g_i \in \mathcal{G}_{\mathcal{N}_i}, \text{ for } i \in [n]\}. \quad (16)$$

Such a definition formulates transformers with dynamic sparse attention patterns.

Definition 4. We call the sparsity pattern Φ to be connected within m layers, if for any $i \neq j \in [n]$, there exists a sequence $1 \leq r_1 < r_2 < \dots < r_k \leq m$ such that

$$A_{\mathcal{N}_{r_k}} A_{\mathcal{N}_{r_{k-1}}} \dots A_{\mathcal{N}_{r_1}}(i, j) > 0. \quad (17)$$

That is, any token can reach any other token through a subsequence of the m sparse attention layers.

Also, let \mathcal{H} be a family of token-wise feedforward layers satisfying the condition in Theorem 1, and k be a kernel function satisfying the condition in Corollary 1. Then, we have the following result:

Corollary 2. Suppose that Φ is connected within m layers. Then, $\mathcal{T}_{\mathcal{F}}^{\Phi}$ possesses the G -UAP, where

$$G = \bigcap_{i=1}^{\infty} \text{Aut}(\mathcal{N}_i). \quad (18)$$

Moreover, transformer with only m layers of attention associated with the sparsity patterns $\mathcal{N}_1, \dots, \mathcal{N}_m$ in Φ and sufficient number of token-wise feedforward layers can achieve the UAP.

Corollary 2 provides a rigorous justification that the heuristic in keeping connectivity in the attention layers is also sufficient for UAP. Results from graph theory indicate that when n is large, a random sparse pattern \mathcal{N} has a trivial automorphism group with probability approaching 1 [17]. This fact indicates that with the guarantee of connectivity, most of the sparse attention patterns allow the UAP without symmetric restriction even in the absence of positional encodings.

Corollary 2 can cover many existing sparse attention mechanisms, including the following:

- the periodic pattern switching between “fixed attention” and “strided attention” in [11];
- the sliding window attention with/without global seeds (tokens connect to all others) in [3];
- the star-shape attention in [24], where one token attends to all others and the others connect in a circle;
- BigBird, a mixture of sliding windows, global seeds and random connections in [76].

The UAP of transformers with sparse softmax attention have also been studied in [75, 76] via a constructive approach. Compared to their results, Corollary 2 has several advantages. First, our results for UAP do not require other technical conditions, such as the periodicity of the sparse patterns and the existence of Hamiltonian path in [75], or each sparse pattern contains a star sub-structure in [76], other than the connectivity of the graph. For example, if the connection mode Φ is not periodic (e.g. there are different random patterns across layers), and some of the \mathcal{N}_i do not contain a star graph mode, our result can still be applied as long as the connectivity is kept, while the results in [75, 76] may not be applicable.

In addition, our results can be applied to all kernels that satisfy the condition in Corollary 1, which generalizes the results based on explicit construction using softmax attention. Moreover, we identify the number of token-mixing layers required to achieve UAP as the minimal number of “hops” for each token to attend to all other tokens. In contrast, the results in [75, 76] use unbounded number of layers to achieve UAP. In this regard, our result can also be viewed as a generalization of the results on the minimal number of attention layers for UAP in [37] to sparse transformers.

4.3 Other attention mechanisms

Our framework can also be conveniently applied to many other variants of attention mechanisms that cannot be covered by (12). For example, the token distinguishability condition can be verified for the following architectures using similar method as in Corollary 1:

- Linformer [68], where the attention layer is defined as

$$\text{Atten}(X) = W_V^t X F \text{softmax}((W_K^t X E)^{\top} W_Q^t X), \quad (19)$$

where $E, F \in \mathbb{R}^{n \times k}$ with $1 \leq k \ll n$ are two trainable projection matrices. This variant of attention reduces the complexity of attention from $\mathcal{O}(n^2)$ to $\mathcal{O}(nk)$.

- Kernelized attention used in SkyFormer [9], where the attention mechanism is given by:

$$[\text{Atten}(X)]_i = \sum_{j=1}^n \exp\left(-\frac{1}{2} \| [W_Q X]_i - [W_K X]_j \|^2 \right) W_V X_j. \quad (20)$$

Corollary 3. We have that: (i) LinFormer satisfies the UAP without symmetric restriction; (ii) SkyFormer satisfies the S_n -UAP.

The proofs are provided in Section C.4 using Theorem 2, similar to the proof of Corollary 1.

4.4 New attention mechanisms from the approximation analysis

Our results also provide insights into designing new transformer architectures with inherent UAP guarantees. In particular, our framework inspires the design of architectures with UAP under specific symmetries. In this section, we present examples of such designs to illustrate these insights.

4.4.1 New attention mechanism with bias term

We propose a new architecture that naturally satisfies the conditions in Theorem 1 and Corollary 2. We consider the following attention mechanism with bias term:

$$[\text{Atten}(X)]_i = [X]_i + \sum_{j \in \mathcal{N}(i)} a\alpha(W[X]_j - b), \quad (21)$$

where $a \in \mathbb{R}$, $W \in \mathbb{R}^d$ and $b \in \mathbb{R}$ are learnable parameters. Assume that α is of polynomial growth, i.e. there exists M and N such that $|\alpha(x)| \leq M(1 + |x|^N)$ for all $x \in \mathbb{R}$.

Then, the result in Corollary 2 still holds, if we replace the attention mechanism in (12) with (21). See Section C.4.3 for the formal statement and proof.

4.4.2 Transformer with UAP under specific symmetry

In many applications, architectures with specific symmetric restrictions are required. Our framework also offers a new perspective on designing such architectures with UAP guarantees. For a given permutation group $G \leq S_n$, we can design G -equivariant token-mixing layers that satisfy token distinguishability under G -action. By Theorem 1, a transformer with such token-mixing layers and a feedforward family \mathcal{H} with nonlinearity and affine invariance achieves G -UAP. This simplifies the design process, as only token distinguishability is required for the token-mixing layer.

For some subgroups G of S_n , the design for token-mixing layers can be very simple. Here, we use the example of $G = D_n$, the dihedral group of order $2n$, and the cyclic group C_n of order n to demonstrate. We identify $D_n \leq S_n$ as the group generated by the cycle $\rho := (1, 2, \dots, n)$ and the reflection $\sigma := (1, n)(2, n-1) \dots$. C_n is the cyclic group generated by ρ . D_n corresponds to the symmetry of a regular n -gon, relevant in applications like molecular structure [6, 23, 41]. Symmetry under C_n applies to modeling periodic data, such as periodic time series [18, 27] and classifying periodic variable stars in cosmology [80].

For D_n , we provide the designs of token-mixing layers with token distinguishability.

Architecture with D_n -symmetry Choose the token-mixing layers defined in (12) or in (21) with the sparsity pattern

$$\mathcal{N}(i) := \{(i + j) \bmod n \mid j = -w, \dots, 0, \dots, w\}, \quad (22)$$

where $w \leq \lfloor \frac{n-1}{2} \rfloor - 1$ is an integer. Here, we assume that the kernel k in (12) and the function α in (21) satisfy the conditions in Corollaries 1 and 5, respectively.

For C_n , similar designs as above also work. However, we can use a simpler one based on convolution:

Architecture with C_n -symmetry: Define the token-mixing layer via column-wise convolution:

$$\text{Atten}(X) = \psi * X, \quad \text{where } [\psi * X]_i = \sum_{j=0}^l \psi_j [X]_{(\ell+j) \bmod n}, \quad i = 0, 1, \dots, n-1. \quad (23)$$

with a trainable kernel $\psi = [\psi_0, \dots, \psi_l] \in \mathbb{R}^{l+1}$ for some integer $l \geq 1$.

This design can be viewed as an adaptation of the temporal convolutional network [33, 43], treating the input sequence as a circular structure. The following statement holds, with proof in Section C.4.3:

Corollary 4. *The architecture with D_n -symmetry and C_n -symmetry defined above satisfies the token distinguishability condition under the action of D_n and C_n , respectively. Moreover, the transformer with such token-mixing mechanisms and a non-linear affine-invariant family \mathcal{H} possesses the D_n -UAP or C_n -UAP, respectively.*

Architectures incorporating symmetry through convolutional layers have been studied in the literature [13, 14, 46, 70, 80]. In particular, [80] also proposed a convolutional structure for representing C_n -invariant functions, although it does not inherently guarantee UAP. In contrast, our proposed architecture naturally satisfies the C_n -UAP property according to Theorem 1. Moreover, by choosing specific sparse mode \mathcal{N} , we can generalize the architecture for D_n symmetry to other permutation subgroups of S_n that can be identified as the automorphism group of an order- n directed graph. For more general permutation groups, our framework can still be applied if one can find token-mixing layer satisfying the token distinguishability condition under the action of the group. The method proposed in [31, 61] may be helpful in identifying such layers. We believe our framework provides a new perspective on the design of equivariant/invariant architectures with UAP guarantees.

5 Conclusion

In this paper, we investigate the universal approximation property (UAP) of general transformer architectures within a unified framework. Our main results, Theorem 1 and Theorem 2, provide general and verifiable conditions for establishing UAP across a range of attention-based architectures, avoiding complex constructions as in previous works. This generality is demonstrated in Section 4, where we apply our framework to various attention types. Moreover, our results offer guidance for designing new attention mechanisms with UAP guarantees, as illustrated in Section 4.4. We also acknowledge certain limitations of this work. First, normalization layers commonly used in practice are not considered, and extending our analysis to incorporate them would be valuable. Second, some architectures, such as those in [38], do not satisfy the analyticity assumption in Theorem 2. Although the condition in Theorem 1 remains verifiable for such architectures, it remains unclear whether our results on the required number of token-mixing layers for UAP still hold. Moreover, as our results offer non-constructive yet verifiable criteria for UAP—abstracting away the specific forms of token-mixing and token-wise modules—they do not yield quantitative insight into the relative contributions of each architectural component. A systematic, quantitative characterization of how individual mechanisms (e.g., multi-head attention, mixture-of-experts, low-rank projections) affect approximation efficiency remains an important direction for future work.

References

- [1] Andrei Agrachev and Cyril Letrouit. Generic controllability of equivariant systems and applications to particle systems and neural networks. *Annales de l’Institut Henri Poincaré C*, 2025.
- [2] Silas Alberti, Niclas Dern, Laura Thesing, and Gitta Kutyniok. Sumformer: Universal approximation for efficient transformers. In *Topological, Algebraic and Geometric Learning Workshops 2023*, pages 72–86. PMLR, 2023.
- [3] Iz Beltagy, Matthew E Peters, and Arman Cohan. Longformer: The long-document transformer. *arXiv preprint arXiv:2004.05150*, 2020.
- [4] Norman Biggs. *Algebraic graph theory*. Number 67. Cambridge university press, 1993.
- [5] Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are few-shot learners. *Advances in neural information processing systems*, 33:1877–1901, 2020.
- [6] Philip R Bunker and Per Jensen. *Molecular symmetry and spectroscopy*, volume 46853. NRC research press, 2006.
- [7] Nicolas Carion, Francisco Massa, Gabriel Synnaeve, Nicolas Usunier, Alexander Kirillov, and Sergey Zagoruyko. End-to-end object detection with transformers. In *European conference on computer vision*, pages 213–229. Springer, 2020.
- [8] Chi Chen, Weike Ye, Yunxing Zuo, Chen Zheng, and Shyue Ping Ong. Graph networks as a universal machine learning framework for molecules and crystals. *Chemistry of Materials*, 31(9):3564–3572, 2019.

- [9] Yifan Chen, Qi Zeng, Heng Ji, and Yun Yang. Skyformer: Remodel self-attention with gaussian kernel and nyström method. *Advances in Neural Information Processing Systems*, 34:2122–2135, 2021.
- [10] Jingpu Cheng, Qianxiao Li, Ting Lin, and Zuowei Shen. Interpolation, approximation, and controllability of deep neural networks. *SIAM Journal on Control and Optimization*, 63(1):625–649, 2025.
- [11] Rewon Child, Scott Gray, Alec Radford, and Ilya Sutskever. Generating long sequences with sparse transformers. *arXiv preprint arXiv:1904.10509*, 2019.
- [12] Krzysztof Choromanski, Valerii Likhoshesterov, David Dohan, Xingyou Song, Andreea Gane, Tamas Sarlos, Peter Hawkins, Jared Davis, Afroz Mohiuddin, Lukasz Kaiser, et al. Rethinking attention with performers. *arXiv preprint arXiv:2009.14794*, 2020.
- [13] Taco Cohen and Max Welling. Group equivariant convolutional networks. In *International conference on machine learning*, pages 2990–2999. PMLR, 2016.
- [14] Taco S Cohen, Mario Geiger, Jonas Köhler, and Max Welling. Spherical cnns. *arXiv preprint arXiv:1801.10130*, 2018.
- [15] Gonalo M Correia, Vlad Niculae, and Andr  FT Martins. Adaptively sparse transformers. *arXiv preprint arXiv:1909.00015*, 2019.
- [16] Alexey Dosovitskiy. An image is worth 16x16 words: Transformers for image recognition at scale. *arXiv preprint arXiv:2010.11929*, 2020.
- [17] Paul Erdos and Alfr d R nyi. Asymmetric graphs. *Acta Math. Acad. Sci. Hungar*, 14(295–315):3, 1963.
- [18] Wei Fan, Shun Zheng, Xiaohan Yi, Wei Cao, Yanjie Fu, Jiang Bian, and Tie-Yan Liu. Depts: Deep expansion learning for periodic time series forecasting. *arXiv preprint arXiv:2203.07681*, 2022.
- [19] Marc Finzi, Samuel Stanton, Pavel Izmailov, and Andrew Gordon Wilson. Generalizing convolutional neural networks for equivariance to lie groups on arbitrary continuous data. In *International Conference on Machine Learning*, pages 3165–3176. PMLR, 2020.
- [20] Takashi Furuya, Maarten V de Hoop, and Gabriel Peyr . Transformers are universal in-context learners. *arXiv preprint arXiv:2408.01367*, 2024.
- [21] Borjan Geshkovski, Cyril Letrouit, Yury Polyanskiy, and Philippe Rigollet. A mathematical perspective on transformers. *Bulletin of the American Mathematical Society*, 62(3):427–479, 2025.
- [22] Borjan Geshkovski, Philippe Rigollet, and Dom nec Ruiz-Balet. Measure-to-measure interpolation using transformers. *arXiv preprint arXiv:2411.04551*, 2024.
- [23] Justin Gilmer, Samuel S Schoenholz, Patrick F Riley, Oriol Vinyals, and George E Dahl. Neural message passing for quantum chemistry. In *International conference on machine learning*, pages 1263–1272. PMLR, 2017.
- [24] Qipeng Guo, Xipeng Qiu, Pengfei Liu, Yunfan Shao, Xiangyang Xue, and Zheng Zhang. Star-transformer. *arXiv preprint arXiv:1902.09113*, 2019.
- [25] Siddhant Haldar, Zhuoran Peng, and Lerrel Pinto. Baku: An efficient transformer for multi-task policy learning. *Advances in Neural Information Processing Systems*, 37:141208–141239, 2024.
- [26] Ali Hatamizadeh, Yucheng Tang, Vishwesh Nath, Dong Yang, Andriy Myronenko, Bennett Landman, Holger R Roth, and Daguang Xu. Unetr: Transformers for 3d medical image segmentation. In *Proceedings of the IEEE/CVF winter conference on applications of computer vision*, pages 574–584, 2022.

- [27] Zhixiang He, Chi-Yin Chow, and Jia-Dong Zhang. Stcnn: A spatio-temporal convolutional neural network for long-term traffic prediction. In *2019 20th IEEE international conference on mobile data management (MDM)*, pages 226–233. IEEE, 2019.
- [28] Edward J Hu, Yelong Shen, Phillip Wallis, Zeyuan Allen-Zhu, Yuanzhi Li, Shean Wang, Lu Wang, Weizhu Chen, et al. Lora: Low-rank adaptation of large language models. *ICLR*, 1(2):3, 2022.
- [29] Jerry Yao-Chieh Hu, Hude Liu, Hong-Yu Chen, Weimin Wu, and Han Liu. Universal approximation with softmax attention. *arXiv preprint arXiv:2504.15956*, 2025.
- [30] Jerry Yao-Chieh Hu, Wei-Po Wang, Ammar Gilani, Chenyang Li, Zhao Song, and Han Liu. Fundamental limits of prompt tuning transformers: Universality, capacity and efficiency. In *ICLR 2025 Workshop on Deep Generative Model in Machine Learning: Theory, Principle and Efficacy*.
- [31] Michael J Hutchinson, Charline Le Lan, Sheheryar Zaidi, Emilien Dupont, Yee Whye Teh, and Hyunjik Kim. Lietransformer: Equivariant self-attention for lie groups. In *International Conference on Machine Learning*, pages 4533–4543. PMLR, 2021.
- [32] Menglin Jia, Luming Tang, Bor-Chun Chen, Claire Cardie, Serge Belongie, Bharath Hariharan, and Ser-Nam Lim. Visual prompt tuning. In *European conference on computer vision*, pages 709–727. Springer, 2022.
- [33] Haotian Jiang and Qianxiao Li. Forward and inverse approximation theory for linear temporal convolutional networks. In *International Conference on Geometric Science of Information*, pages 342–350. Springer, 2023.
- [34] Haotian Jiang and Qianxiao Li. Approximation rate of the transformer architecture for sequence modeling. *Advances in Neural Information Processing Systems*, 37:68926–68955, 2024.
- [35] Rui Jiao, Wenbing Huang, Peijia Lin, Jiaqi Han, Pin Chen, Yutong Lu, and Yang Liu. Crystal structure prediction by joint equivariant diffusion. *Advances in Neural Information Processing Systems*, 36:17464–17497, 2023.
- [36] John Jumper, Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, et al. Highly accurate protein structure prediction with alphafold. *nature*, 596(7873):583–589, 2021.
- [37] Tokio Kajitsuka and Issei Sato. Are transformers with one layer self-attention using low-rank weight matrices universal approximators? In *The Twelfth International Conference on Learning Representations*.
- [38] Angelos Katharopoulos, Apoorv Vyas, Nikolaos Pappas, and François Fleuret. Transformers are rnns: Fast autoregressive transformers with linear attention. In *International conference on machine learning*, pages 5156–5165. PMLR, 2020.
- [39] Junghwan Kim, Michelle Kim, and Barzan Mozafari. Provable memorization capacity of transformers. In *The Eleventh International Conference on Learning Representations*, 2022.
- [40] Nikita Kitaev, Łukasz Kaiser, and Anselm Levskaya. Reformer: The efficient transformer. *arXiv preprint arXiv:2001.04451*, 2020.
- [41] Charles Kittel and Paul McEuen. *Introduction to solid state physics*. John Wiley & Sons, 2018.
- [42] Anastasis Kratsios, Behnoosh Zamanlooy, Tianlin Liu, and Ivan Dokmanić. Universal approximation under constraints is possible with transformers. *arXiv preprint arXiv:2110.03303*, 2021.
- [43] Colin Lea, Rene Vidal, Austin Reiter, and Gregory D Hager. Temporal convolutional networks: A unified approach to action segmentation. In *Computer vision–ECCV 2016 workshops: Amsterdam, the Netherlands, October 8–10 and 15–16, 2016, proceedings, part III 14*, pages 47–54. Springer, 2016.

- [44] Qianxiao Li, Ting Lin, and Zuowei Shen. Deep learning via dynamical systems: An approximation perspective. *Journal of the European Mathematical Society*, 25(5):1671–1709, 2022.
- [45] Qianxiao Li, Ting Lin, and Zuowei Shen. Deep neural network approximation of invariant functions through dynamical systems. *Journal of Machine Learning Research*, 25(278):1–57, 2024.
- [46] Ting Lin, Zuowei Shen, and Qianxiao Li. On the universal approximation property of deep fully convolutional neural networks. *arXiv preprint arXiv:2211.14047*, 2022.
- [47] Hao Liu and Pieter Abbeel. Blockwise parallel transformers for large context models. *Advances in neural information processing systems*, 36:8828–8844, 2023.
- [48] Hude Liu, Jerry Yao-Chieh Hu, Zhao Song, and Han Liu. Attention mechanism, max-affine partition, and universal approximation. *arXiv preprint arXiv:2504.19901*, 2025.
- [49] Shih-Yang Liu, Chien-Yi Wang, Hongxu Yin, Pavlo Molchanov, Yu-Chiang Frank Wang, Kwang-Ting Cheng, and Min-Hung Chen. Dora: Weight-decomposed low-rank adaptation. In *Forty-first International Conference on Machine Learning*, 2024.
- [50] Shengjie Luo, Shanda Li, Shuxin Zheng, Tie-Yan Liu, Liwei Wang, and Di He. Your transformer may not be as powerful as you expect. *Advances in Neural Information Processing Systems*, 35:4301–4315, 2022.
- [51] Xuezhe Ma, Chunting Zhou, Xiang Kong, Junxian He, Liangke Gui, Graham Neubig, Jonathan May, and Luke Zettlemoyer. Mega: Moving average equipped gated attention. In *The Eleventh International Conference on Learning Representations*, 2023.
- [52] Haggai Maron, Ethan Fetaya, Nimrod Segol, and Yaron Lipman. On the universality of invariant networks. In *International conference on machine learning*, pages 4363–4371. PMLR, 2019.
- [53] Fanxu Meng, Zhaohui Wang, and Muhan Zhang. Pissa: Principal singular values and singular vectors adaptation of large language models. *Advances in Neural Information Processing Systems*, 37:121038–121072, 2024.
- [54] Boris Mityagin. The zero set of a real analytic function. *arXiv preprint arXiv:1512.07276*, 2015.
- [55] Jorge Pérez, Pablo Barceló, and Javier Marinkovic. Attention is turing-complete. *Journal of Machine Learning Research*, 22(75):1–35, 2021.
- [56] Aleksandar Petrov, Philip HS Torr, and Adel Bibi. Prompting a pretrained transformer can be a universal approximator. *arXiv preprint arXiv:2402.14753*, 2024.
- [57] Alec Radford. Improving language understanding by generative pre-training. 2018.
- [58] Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, Ilya Sutskever, et al. Language models are unsupervised multitask learners. *OpenAI blog*, 1(8):9, 2019.
- [59] Siamak Ravanbakhsh. Universal equivariant multilayer perceptrons. In *International Conference on Machine Learning*, pages 7996–8006. PMLR, 2020.
- [60] Zekun Ren, Juhwan Noh, Siyu Tian, Felipe Oviedo, Guangzong Xing, Qiaohao Liang, Armin Aberle, Yi Liu, Qianxiao Li, Senthilnath Jayavelu, et al. Inverse design of crystals using generalized invertible crystallographic representation. *arXiv preprint arXiv:2005.07609*, 3(6):7, 2020.
- [61] David W Romero and Jean-Baptiste Cordonnier. Group equivariant stand-alone self-attention for vision. *arXiv preprint arXiv:2010.00977*, 2020.
- [62] Domenec Ruiz-Balet and Enrique Zuazua. Neural ode control for classification, approximation, and transport. *SIAM Review*, 65(3):735–773, 2023.

- [63] Paulo Tabuada and Bahman Ghahsifard. Universal approximation power of deep residual neural networks through the lens of control. *IEEE Transactions on Automatic Control*, 68(5):2715–2728, 2022.
- [64] Shokichi Takakura and Taiji Suzuki. Approximation and estimation ability of transformers for sequence-to-sequence functions with infinite dimensional input. In *International Conference on Machine Learning*, pages 33416–33447. PMLR, 2023.
- [65] Yao-Hung Hubert Tsai, Shaojie Bai, Makoto Yamada, Louis-Philippe Morency, and Ruslan Salakhutdinov. Transformer dissection: a unified understanding of transformer’s attention via the lens of kernel. *arXiv preprint arXiv:1908.11775*, 2019.
- [66] A Vaswani. Attention is all you need. *Advances in Neural Information Processing Systems*, 2017.
- [67] Mingze Wang et al. Understanding the expressive power and mechanisms of transformer for sequence modeling. *arXiv preprint arXiv:2402.00522*, 2024.
- [68] Sinong Wang, Belinda Z Li, Madian Khabsa, Han Fang, and Hao Ma. Linformer: Self-attention with linear complexity. *arXiv preprint arXiv:2006.04768*, 2020.
- [69] Colin Wei, Yining Chen, and Tengyu Ma. Statistically meaningful approximation: a case study on approximating turing machines with transformers. *Advances in Neural Information Processing Systems*, 35:12071–12083, 2022.
- [70] Maurice Weiler, Mario Geiger, Max Welling, Wouter Boomsma, and Taco S Cohen. 3d steerable cnns: Learning rotationally equivariant features in volumetric data. *Advances in Neural information processing systems*, 31, 2018.
- [71] Tian Xie and Jeffrey C Grossman. Crystal graph convolutional neural networks for an accurate and interpretable prediction of material properties. *Physical review letters*, 120(14):145301, 2018.
- [72] Yunyang Xiong, Zhanpeng Zeng, Rudrasis Chakraborty, Mingxing Tan, Glenn Fung, Yin Li, and Vikas Singh. Nyströmformer: A nyström-based algorithm for approximating self-attention. In *Proceedings of the AAAI conference on artificial intelligence*, volume 35, pages 14138–14148, 2021.
- [73] Dmitry Yarotsky. Universal approximations of invariant maps by neural networks. *Constructive Approximation*, 55(1):407–474, 2022.
- [74] Chulhee Yun, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank J Reddi, and Sanjiv Kumar. Are transformers universal approximators of sequence-to-sequence functions? *arXiv preprint arXiv:1912.10077*, 2019.
- [75] Chulhee Yun, Yin-Wen Chang, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank Reddi, and Sanjiv Kumar. O (n) connections are expressive enough: Universal approximability of sparse transformers. *Advances in Neural Information Processing Systems*, 33:13783–13794, 2020.
- [76] Manzil Zaheer, Guru Guruganesh, Kumar Avinava Dubey, Joshua Ainslie, Chris Alberti, Santiago Ontanon, Philip Pham, Anirudh Ravula, Qifan Wang, Li Yang, et al. Big bird: Transformers for longer sequences. *Advances in neural information processing systems*, 33:17283–17297, 2020.
- [77] Shuangfei Zhai, Walter Talbott, Nitish Srivastava, Chen Huang, Hanlin Goh, Ruixiang Zhang, and Josh Susskind. An attention free transformer. *arXiv preprint arXiv:2105.14103*, 2021.
- [78] Chi Zhang, Cheng Jingpu, Yanyu Xu, and Qianxiao Li. Parameter-efficient fine-tuning with controls. In *International Conference on Machine Learning*, pages 59066–59079. PMLR, 2024.
- [79] Chi Zhang, REN Lianhai, Jingpu Cheng, and Qianxiao Li. From weight-based to state-based fine-tuning: Further memory reduction on lora with parallel control. In *Forty-second International Conference on Machine Learning*, 2025.

- [80] Keming Zhang and Joshua S Bloom. Classification of periodic variable stars with novel cyclic-permutation invariant neural networks. *Monthly Notices of the Royal Astronomical Society*, 505(1):515–522, 2021.
- [81] Sixiao Zheng, Jiachen Lu, Hengshuang Zhao, Xiatian Zhu, Zekun Luo, Yabiao Wang, Yanwei Fu, Jianfeng Feng, Tao Xiang, Philip HS Torr, et al. Rethinking semantic segmentation from a sequence-to-sequence perspective with transformers. In *Proceedings of the IEEE/CVF conference on computer vision and pattern recognition*, pages 6881–6890, 2021.
- [82] Chen Zhu, Wei Ping, Chaowei Xiao, Mohammad Shoeybi, Tom Goldstein, Anima Anandkumar, and Bryan Catanzaro. Long-short transformer: Efficient transformers for language and vision. *Advances in neural information processing systems*, 34:17723–17736, 2021.

A Detailed related works

Approximation results for transformers Since the introduction of the transformer architecture in [66], numerous studies have investigated its approximation properties. The universal approximation property (UAP) of the original transformer with softmax attention as a fixed length sequence-to-sequence model was established in [74]. This constructive approach was later extended to transformers with certain sparse attention mechanisms [75, 76]. In [37], the authors proposed a new construction demonstrating that transformers with a single attention layer and sufficiently deep feedforward networks can achieve UAP. Similarly, [2] showed that with increased hidden dimensions, two variants of transformers, i.e. LinFormer [68] and Performer [12], satisfy the UAP. In contrast to these constructive methods for different architectures, our results offer a unified framework for establishing the UAP of various transformer models without relying on explicit constructions. Beyond these works treating transformers as a fixed length sequence-to-sequence model, there are also studies handling transformers with variable-length inputs by considering the input sequence as an empirical measure [20–22]. The universal interpolation and universal approximation properties under this viewpoint were established with proper assumptions. Compared to these results, we still consider transformers as sequence-to-sequence models in this work to offer a direct analysis for different transformer architectures. Recently, there are other works studying the UAP of attention-only architectures [29, 48], indicating that softmax attention alone can also achieve strong approximation power. Other studies have explored the UAP of transformers under alternative settings, such as in-context learning, prompting, and constrained scenarios [20, 30, 42, 50, 56]. Another researchline is the Turing completeness of transformers [55, 69]. Besides these UAP results, there are also works providing the approximation rates of transformers. For instance, [34] provides explicit rates over a dense subset of sequence-to-sequence functions; [67] derives rates for target functions with structured memory; and [64] characterizes the approximation rate in terms of function smoothness for transformers with infinitely long inputs.

Approximation under symmetry The study of approximation under functional symmetries has been explored in various works. In [73], the universal approximation of functions invariant under compact group or translation actions was analyzed using shallow neural networks. In [13, 19], convolutional structures were proposed to approximate equivariant functions. In [45, 52, 59], the universal approximation under symmetry using deep neural networks was investigated. Notably, [45] provides a general sufficient condition for the action of any transitive subgroup of S_n on coordinates (1-dimensional tokens). In contrast, our work addresses approximation under symmetry in a broader setting, considering group actions on d -dimensional tokens rather than coordinates, thereby extending the analysis in [45] to non-transitive permutation groups. In [1], the authors provide a general framework on the ensemble controllability of control systems under symmetry. They also show that systems that can interpolate arbitrarily many samples under symmetry are generic in certain topology. Compare to their genericity results, our results provide a verifiable sufficient condition for UAP of specific architectures, allowing direct applications to various transformer architectures.

Transformer variants Beyond the original Transformer, numerous architectural variants have been developed to improve efficiency, scalability, or adaptability. These include sparse attention mechanisms [3, 15, 24, 40, 76], low-rank and kernel-based approximations of attention [12, 68, 72], as well as other architectural modifications [25, 47, 51, 77]. Another related line of work explores parameter-efficient fine-tuning methods for large Transformer models [28, 32, 49, 53, 78, 79], which aim to adapt pretrained networks to downstream tasks with minimal additional parameters. In this paper, we establish a general sufficient condition for the universal approximation property (UAP) of various Transformer variants. As demonstrated in Section 4, our framework can be readily verified for many existing architectures, and potentially extended to other designs not included as well.

B Proof of Theorem 1 and Theorem 2

B.1 Proof of Theorem 1

In the following, $\|\cdot\|_2$ denotes the ℓ^2 -norm, for both vectors in $\mathbb{R}^{d \times n}$ or \mathbb{R}^d . We begin by proving the following interpolation property of $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$:

Proposition 1 (Interpolation Property). Suppose \mathcal{G} and \mathcal{H} satisfy the condition in Theorem 1 for group G . Consider any G -equivariant continuous function $F : \mathbb{R}^{d \times n} \rightarrow \mathbb{R}^{d \times n}$. Then, for any $\varepsilon > 0$ and $\{X_i\}_{i=1}^N \subset \mathbb{R}^{d \times n}$, there exists $\hat{F} \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ such that:

- $\|\hat{F}(X_i) - F(X_i)\|_2 < \varepsilon$, if X_i is in general position (defined in Section 2).
- $\|\hat{F}(X_i)\|_2 < n \cdot \max_i \{\|F(X_i)\|_2\} + 2\varepsilon$, if X_i is not in general position.

Proof. Since F and functions in $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$ are G -equivariant, we only need to consider the case when X_i are from distinct orbits under the G -action. Moreover, we can assume that X_i are in general position for $i = 1, \dots, M$, and X_i are not in general position for $i = M + 1, \dots, N$.

By the token distinguishability condition, there exist m and $g \in (\text{Id} + \mathcal{G})^m$ such that the tokens of $g(X_i)$ are all distinct for $i = 1, \dots, M$. We denote x_1, \dots, x_{Mn} as the distinct tokens in $g(X_1), \dots, g(X_M)$. For each $j \leq Mn$, suppose $x_j = [X_l]_k$ for some $(l, k) \in [n] \times [M]$, we denote y_j as its corresponding token $[F(X_l)]_k$. Moreover, we denote $x_{Mn+1}, \dots, x_{Mn+J} \in \mathbb{R}^d$ as the distinct tokens in $g(X_{M+1}), \dots, g(X_N)$ that are different from x_1, \dots, x_{Mn} . For each $j > Mn$, we denote $y_j = 0 \in \mathbb{R}^d$. Then, we get a set of d -dimensional pairs $\{(x_j, y_j)\}_{j=1}^{Mn+J} \subset \mathbb{R}^d \times \mathbb{R}^d$ where all x_j are all distinct. Since \mathcal{H} satisfies the non-linear affine invariance condition, according to the main result in [10], we know that there exists a function

$$f \in \{(\text{Id} + f_k) \circ \dots \circ (\text{Id} + f_1) \mid k \in \mathbb{N}_+, f_1, \dots, f_k \in H\} \quad (24)$$

such that

$$\|f(x_j) - y_j\|_2 \leq \frac{1}{n}\varepsilon, \quad j = 1, \dots, Mn + J. \quad (25)$$

Denote $f^{\otimes n}$ as the token-wise extension of f to $\mathbb{R}^{d \times n}$. For each $i \leq M$, we have

$$\begin{aligned} \|f^{\otimes n}(g(X_i)) - F(X_i)\|_2 &= \left\| \left((f(g[X_i]_1) - [F(X_i)]_1), \dots, (f(g[X_i]_n) - [F(X_i)]_n) \right) \right\|_2 \\ &\leq n \cdot \max_j \|f(x_j) - y_j\|_2 \leq \varepsilon. \end{aligned} \quad (26)$$

For each $i \geq M + 1$, we have

$$\begin{aligned} \|f^{\otimes n}(g(X_i))\| &= \left\| \left(f(g[X_i]_1), \dots, f(g[X_i]_n) \right) \right\|_2 \\ &\leq \sum_{l: g[X_i]_l \in \{x_1, \dots, x_{Mn}\}} \|f(g[X_i]_l)\|_2 + \sum_{l: g[X_i]_l \in \{x_{Mn+1}, \dots, x_{Mn+J}\}} \|f(g[X_i]_l)\|_2 \\ &\leq n \cdot \max_j \|f(x_j)\|_2 + n \cdot \max_{j > Mn} \|f(x_j)\|_2 \\ &\leq n \cdot \left(\max_i \{\|F(X_i)\|_2\} + \frac{\varepsilon}{n} \right) + \varepsilon = n \cdot \max_i \{\|F(X_i)\|_2\} + 2\varepsilon. \end{aligned} \quad (27)$$

Therefore, $\hat{F} = f^{\otimes n} \circ g \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ satisfies the interpolation property. \square

Proposition 2 (Approximation of Tensor-Type Functions). Suppose \mathcal{G} and \mathcal{H} satisfy the condition in Theorem 1 for group G . Consider any continuous, increasing function $h : \mathbb{R} \rightarrow \mathbb{R}$ and any $\varepsilon > 0$. Then, there exists $F \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ such that

$$\|F - h^{(d \times n)}\|_{C(K)} \leq \varepsilon, \quad (28)$$

where $h^{(d \times n)}$ is the coordinate-wise extension of h to $\mathbb{R}^{d \times n}$, given by

$$(h^{(d \times n)}(X))_{ij} = h(X_{ij}), \quad 1 \leq i \leq d, 1 \leq j \leq n. \quad (29)$$

Proof. Proposition 2 directly follows from the proof of Proposition 4.11 [44] and Theorem 2.6 in [10]. \square

Proposition 3 (Corollary of Main results of [10]). Let $d \geq 2$ and \mathcal{H} be a family of maps from \mathbb{R}^d to \mathbb{R}^d that satisfies the non-linearity and affine-invariance condition in Theorem 1. Then, for any $\{(x_i, y_i)\}_{i=1}^N \subset \mathbb{R}^d \times \mathbb{R}^d$ with $x_i \neq x_j$ for all $i \neq j$ and $\varepsilon > 0$, there exists

$$f \in \{(\text{Id} + f_k) \circ \dots \circ (\text{Id} + f_1) \mid k \in \mathbb{N}_+, f_1, \dots, f_k \in \mathcal{H}\} \quad (30)$$

such that

$$\|f(x_i) - y_i\| \leq \varepsilon, \quad i = 1, \dots, N. \quad (31)$$

Proof. Proposition 3 is a direct corollary of Theorem 2.6 in [10]. \square

Proof of Theorem 1. The approach of the proof is similar to the main theorem in [44] and [45].

We assume without loss of generality that $K = [-s, s]^{d \times n}$ is a hypercube in $\mathbb{R}^{d \times n}$. Our target is to show that for any $\varepsilon > 0$, we can find function $\hat{F} \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ such that $\|\hat{f} - F\|_{L^p(K)} \leq \varepsilon$.

Step 1. For each multi-index $\mathbf{i} = (i_{kl})_{k \in [d], l \in [n]} \in \mathbb{Z}^{d \times n}$ and $\delta > 0$, we define the grid cells:

$$\square_{\mathbf{i}, \delta} := \{X \in \mathbb{R}^{d \times n} \mid X_{kl} \in [i_{kl}\delta, (i_{kl} + 1)\delta], \text{ for all } k \in [d], l \in [n]\}. \quad (32)$$

We denote $\mathbf{p}_{\mathbf{i}, \delta} := \delta \mathbf{i}$ as a corner point of $\square_{\mathbf{i}, \delta}$, and $\chi_{\mathbf{i}, \delta}$ as the characteristic function of $\square_{\mathbf{i}, \delta}$. Since F is continuous, there exists $\delta > 0$ such that it has a piece-wise constant approximation

$$\tilde{F} := \sum_{\mathbf{i}} F(\mathbf{p}_{\mathbf{i}}) \chi_{\mathbf{i}, \delta}, \quad (33)$$

such that

$$\|F - \tilde{F}\|_{L^p(K)} \leq \frac{\varepsilon}{4}. \quad (34)$$

Step 2. Apply Proposition 3 to the set of grid points

$$\{\mathbf{p}_{\mathbf{i}, \delta} \mid \mathbf{i}_{kl} \in \{\lceil -s/\delta \rceil, \dots, \lfloor s/\delta \rfloor\}\}.$$

Then, for any $\gamma > 0$, there exists a function $\bar{F} \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ such that:

- If $\mathbf{p}_{\mathbf{i}, \delta}$ is in general position, then

$$\|\bar{F}(\mathbf{p}_{\mathbf{i}, \delta}) - F(\mathbf{p}_{\mathbf{i}, \delta})\| < \gamma.$$

- Otherwise,

$$\|\bar{F}(\mathbf{p}_{\mathbf{i}, \delta})\| < n \cdot \max_{\mathbf{i}} \{ \|F(\mathbf{p}_{\mathbf{i}, \delta})\| \} + 2\gamma \leq n \|F\|_{C(K)} + 2\gamma.$$

Step 3. For any $\alpha \in (0, 1)$, define

$$\square_{\mathbf{i}, \delta}^{\alpha} := \{X \in \mathbb{R}^{d \times n} \mid X_{kl} \in [i_{kl}\delta, i_{kl}\delta + \alpha\delta], \text{ for all } k \in [d], l \in [n]\}, \quad (35)$$

as the shrunk hypercube of $\square_{\mathbf{i}, \delta}$ with side length $\alpha\delta$. We consider the map $h_{\alpha, \delta} : \mathbb{R} \rightarrow \mathbb{R}$ defined as:

$$h_{\alpha, \delta}(x) = \begin{cases} i\delta, & \text{if } x \in [i\delta, i\delta + \alpha\delta], \quad i \in \mathbb{Z}, \\ i\delta + \frac{x - i\delta - \alpha\delta}{1 - \alpha}, & \text{if } x \in [i\delta + \alpha\delta, (i+1)\delta], \quad i \in \mathbb{Z}. \end{cases} \quad (36)$$

On the interval $[i\delta, i\delta + \alpha\delta]$, the function $h_{\alpha, \delta}(x)$ remains constant at $i\delta$. Then, as x increases from $i\delta + \alpha\delta$ to $(i+1)\delta$, the function increases linearly from $i\delta$ to $(i+1)\delta$. Notice that $h_{\alpha, \delta}^{(d \times n)}$ is continuous and has constant value $\mathbf{p}_{\mathbf{i}}$ on $\square_{\mathbf{i}, \delta}^{\alpha}$ for each \mathbf{i} . Since $h_{\alpha, \delta}$ is continuous and increasing, by Proposition 2, for any $\rho > 0$, there exists a function $H_{\alpha, \delta} \in \mathcal{T}_{\mathcal{G}, \mathcal{H}}$ such that

$$\|H_{\alpha, \delta} - h_{\alpha, \delta}^{(d \times n)}\|_{C(K)} < \rho. \quad (37)$$

Step 4. Now we can estimate the error of the composition $\|\bar{F} \circ H_{\alpha, \delta} - F\|_{L^p(K)}$. We define

$$K^{\alpha} = \left(\bigcup_{\mathbf{i}} \square_{\mathbf{i}, \delta}^{\alpha} \right) \cap K,$$

and denote K_1^{α} as the union of the grid cells in K^{α} whose corner point $\mathbf{p}_{\mathbf{i}}$ are in general position, and K_2^{α} as the union of the grid cells in K^{α} whose $\mathbf{p}_{\mathbf{i}}$ are not in general position. Then, we have

1. On K_1^α , we have

$$\|\bar{F} \circ h_{\alpha,\delta}^{(d \times n)} - \tilde{F}\|_{L^p(K_1^\alpha)} < \gamma(m(K_1^\alpha))^{\frac{1}{p}}. \quad (38)$$

2. For K_2^α , the number of \mathbf{i} with $\mathbf{p}_{\mathbf{i},\delta}$ not in general position is at most $\frac{n(n-1)}{2}(2s/\delta+1)^{(n-1)d}$, we have the measure of $K_2^\alpha = \mathcal{O}(\delta^d)$. Therefore,

$$\|\bar{F} \circ h_{\alpha,\delta}^{(d \times n)} - \tilde{F}\|_{L^p(K_2^\alpha)} < (n \cdot \|F\|_{C(K)} + 2\gamma)\mathcal{O}(\delta^d). \quad (39)$$

Therefore, we can choose δ and γ sufficiently small such that

$$\|\bar{F} \circ h_{\alpha,\delta}^{(d \times n)} - \tilde{F}\|_{L^p(K^\alpha)} < \frac{\varepsilon}{4}. \quad (40)$$

On $K \setminus K^\alpha$, by choosing α sufficiently close to 1, we make $m(K \setminus K^\alpha)$ arbitrarily small. Since $\bar{F} \circ h_{\alpha,\delta}^{(d \times n)}$ and \tilde{F} is bounded on K , the following can be guaranteed:

$$\|\bar{F} \circ h_{\alpha,\delta}^{(d \times n)} - \tilde{F}\|_{L^p(K \setminus K^\alpha)} < \frac{\varepsilon}{4}. \quad (41)$$

Since \bar{F} is uniformly continuous on K , there exists $\rho > 0$ such that for any $X, Y \in K$ with $\|X - Y\| < \rho$, we have $\|\bar{F}(X) - \bar{F}(Y)\| < \kappa := \varepsilon/(4(m(K))^{\frac{1}{p}})$. Therefore, after determining α, δ and γ , we can choose ρ such that

$$\|\bar{F} \circ H_{\alpha,\delta} - F\|_{L^p(K)} \leq (m(K))^{\frac{1}{p}} \kappa \leq \frac{\varepsilon}{4}. \quad (42)$$

After determining δ and α , by step 3, we can choose ρ sufficiently small such that

$$\|\bar{F} \circ H_{\alpha,\delta} - \bar{F} \circ h_{\alpha,\delta}^{(d \times n)}\|_{L^p(K)} \leq \rho \text{Lip}(\bar{F}) < \frac{\varepsilon}{4}. \quad (43)$$

Recall also that

$$\|\tilde{F} - F\|_{L^p(K)} < \frac{\varepsilon}{4}.$$

Thus, by the triangle inequality,

$$\begin{aligned} \|\bar{F} \circ H_{\alpha,\delta} - F\|_{L^p(K)} &\leq \|\bar{F} \circ H_{\alpha,\delta} - \bar{F} \circ h_{\alpha,\delta}^{(d \times n)}\|_{L^p(K)} + \|\bar{F} \circ h_{\alpha,\delta}^{(d \times n)} - \tilde{F}\|_{L^p(K^\alpha)} \\ &\quad + \|\bar{F} \circ h_{\alpha,\delta}^{(d \times n)} - \tilde{F}\|_{L^p(K \setminus K^\alpha)} + \|\tilde{F} - F\|_{L^p(K)} \\ &< \frac{\varepsilon}{4} + \frac{\varepsilon}{4} + \frac{\varepsilon}{4} + \frac{\varepsilon}{4} = \varepsilon, \end{aligned} \quad (44)$$

which completes the proof. \square

B.2 Proof of Theorem 2

Proof. Assume that Condition 2 in Theorem 1 fails. Then, there exists N samples $\{X_i\}_{i=1}^N$ from different orbits under the G -action, but for any m and $g \in (\text{Id} + \mathcal{G})^m$, there exist indices $i, j \in [N]$ such that at least one token in $g(X_i)$ is identical to a token in $g(X_j)$. This can be written as

$$\Pi_{i,j} := \prod_{l_1, l_2} \| [g(X_i)]_{l_1} - [g(X_j)]_{l_2} \|_2^2 = 0. \quad (45)$$

When \mathcal{G} is parametric in $\theta \in \Theta$, $\Pi_{i,j}$ is also analytic in θ . As the zero set of a nonzero real analytic function has measure zero [54], this implies that for some i, j , $\Pi_{i,j}$ is identically zero, meaning that \mathcal{G} fails to distinguish tokens in X_i and X_j . This argument reduces Condition 2 in Theorem 1 to the case $N = 2$.

Moreover, if there exists a uniform m such that the token distinguishability condition for any two tokens holds, the above argument essentially shows that this m can also be used to distinguish any N tokens. \square

C Proofs for the applications of main results

C.1 Proof of Corollary 1 and Corollary 2

We first prove the following lemma.

Lemma 1. *Let r be a kernel function satisfying the conditions in Corollary 1. Suppose $\{a_1, \dots, a_r\} \subset \mathbb{R}^d \setminus \{0\}$ and $\{b_1, \dots, b_s\} \subset \mathbb{R}^d \setminus \{0\}$ are two sequences of distinct tokens. Suppose that for some indices $r' \in [r]$ and $s' \in [s]$, the following equality holds for all choices of W_Q, W_K, W_V :*

$$a_{r'} + \sum_{j=1}^r \left(\frac{k(W_Q a_{r'}, W_K a_j)}{\sum_{l=1}^r k(W_Q a_{r'}, W_K a_l)} W_V a_j \right) = b_{s'} + \sum_{j=1}^s \left(\frac{k(W_Q b_{s'}, W_K b_j)}{\sum_{l=1}^s k(W_Q b_{s'}, W_K b_l)} W_V b_j \right). \quad (46)$$

Then, $r = s$, and there exists a permutation $\sigma \in S_n$ with $\sigma(r') = s'$ such that $a_i = b_{\sigma(i)}$ for all i .

Proof. Taking W_V to be zero directly gives $a_{r'} = b_{s'}$. In the following, we set $W_Q = I$, and for notational simplicity define

$$\tilde{k}(x) := k(a_{r'}, x), \quad \forall x \in \mathbb{R}^d.$$

The proof utilizes the following lemma:

Lemma 2 (Auxiliary lemma). *Let $\{x_1, \dots, x_p\} := \{a_1, \dots, a_r\} \cup \{b_1, \dots, b_s\}$. Then, there exist $W_K \in \mathbb{R}^{d \times d}$ and a permutation $\sigma \in S_p$ such that*

$$\lim_{t \rightarrow \infty} \frac{\tilde{k}(tW_K x_{\sigma(j)})}{\tilde{k}(tW_K x_{\sigma(i)})} = \infty, \text{ for all } i < j. \quad (47)$$

Since $\{a_j\}_{j=1}^r$ are r distinct tokens, by the auxiliary lemma, we may choose a W_K (and reindex the sequences accordingly) so that after replacing W_K by tW_K the kernel values satisfy, for large $t > 0$,

$$\tilde{k}(tW_K a_1) \ll \tilde{k}(tW_K a_2) \ll \dots \ll \tilde{k}(tW_K a_r),$$

and similarly

$$\tilde{k}(tW_K b_1) \ll \tilde{k}(tW_K b_2) \ll \dots \ll \tilde{k}(tW_K b_s).$$

Moreover, the lemma tells us that for any a_j and b_l , either $a_j = b_l$ or one of $\tilde{k}(tW_K a_j)$ and $\tilde{k}(tW_K b_l)$ is dominated by the other in the limit $t \rightarrow \infty$.

After subtracting $a_{r'}$ from both sides in (46), we have

$$\frac{\sum_{j=1}^r \tilde{k}(tW_K a_j) a_j}{\sum_{j=1}^r \tilde{k}(tW_K a_j)} = \frac{\sum_{j=1}^s \tilde{k}(tW_K b_j) b_j}{\sum_{j=1}^s \tilde{k}(tW_K b_j)}. \quad (48)$$

By a transformation, it gives

$$\sum_{j=1}^r \sum_{l=1}^s \tilde{k}(tW_K a_j) \tilde{k}(tW_K b_l) (a_j - b_l) = 0. \quad (49)$$

Let $t \rightarrow \infty$, considering the dominate term $\tilde{k}(tW_K a_j) \tilde{k}(tW_K b_l) (a_r - b_s)$ gives $a_r = b_s$. Then, for all $q = 0, 1, \dots, \min\{r, s\}$, we then prove by induction that: $a_{r-q} = b_{s-q}$.

Suppose we already have $a_{r-i} = b_{s-i}$, for $i = 1, \dots, q-1$. It then follows that

$$\begin{aligned} & \sum_{j=r-q+1}^r \sum_{l=s-q+1}^s \tilde{k}(tW_K a_j) \tilde{k}(tW_K b_l) (a_j - b_l) \\ &= \sum_{j=r-q+1}^r \sum_{l=r-q+1}^r \tilde{k}(tW_K a_j) \tilde{k}(tW_K a_l) (a_j - a_l) = 0, \quad \text{for all } t \in \mathbb{R}. \end{aligned} \quad (50)$$

Combining with (49), we have

$$\left(\sum_{j=1}^{r-q} \sum_{l=1}^{r-q} + \sum_{j=1}^{r-q} \sum_{l=s-q+1}^s + \sum_{j=r-q+1}^r \sum_{l=1}^{s-q} \right) \left(\tilde{k}(tW_K a_j) \tilde{k}(tW_K b_l) (a_j - b_l) \right) = 0, \quad (51)$$

where the leading term is

$$\tilde{k}(tW_K a_{r-q}) \tilde{k}(tW_K b_s) (a_{r-q} - b_s) + \tilde{k}(tW_K a_r) \tilde{k}(tW_K b_{s-q}) (a_r - b_{s-q}). \quad (52)$$

Since $a_r = b_s$, $a_{r-q} \neq a_r$ and $b_{r-q} \neq b_r$, let $t \rightarrow \infty$ gives that $\tilde{k}(tW_K a_{r-q})$ and $\tilde{k}(tW_K b_{s-q})$ are not dominated by each other. By the auxiliary lemma, this indicates that $a_{r-q} = b_{s-q}$, which completes the induction.

Then, we have shown that $a_{r-k} = b_{s-k}$ for all $k = 0, 1, \dots, \min\{r, s\}$. The only remaining thing is to show that $r = s$. Suppose $r < s$, then we have

$$\sum_{j=1}^r \sum_{l=1}^{s-r} \tilde{k}(tW_K a_j) \tilde{k}(tW_K b_l) (a_j - b_l) \equiv 0, \quad (53)$$

where the unique leading term is $\tilde{k}(tW_K a_r) \tilde{k}(tW_K b_{s-r}) (a_r - b_{s-r})$. Since $a_r = b_r \neq b_{s-r}$, that gives a contradiction. This completes the proof. \square

Proof of the auxiliary lemma. For each pair (i, j) with $1 \leq i < j \leq p$, we define

$$\mathcal{M}_{i,j} := \mathbb{R}^{d \times d} \setminus \left\{ W_K \left| \lim_{t \rightarrow \infty} \frac{\tilde{k}(tW_K x_i)}{\tilde{k}(tW_K x_j)} = 0 \text{ or } \infty \right. \right\}, \quad (54)$$

and we define \mathcal{M} as the union of all such sets:

$$\mathcal{M} = \bigcup_{1 \leq i < j \leq p} \mathcal{M}_{i,j}. \quad (55)$$

According to the condition in Corollary 1, each $\mathcal{M}_{i,j}$ is a measure-zero set in $\mathbb{R}^{d \times d}$. Therefore, \mathcal{M} is also measure-zero. Choose any $W_K \in \mathbb{R}^{d \times d} \setminus \mathcal{M}$. Then, for any i, j , we have

$$\lim_{t \rightarrow \infty} \frac{\tilde{k}(tW_K x_i)}{\tilde{k}(tW_K x_j)} = 0 \text{ or } \infty, \quad (56)$$

i.e. either $\tilde{k}(tW_K x_i) \ll \tilde{k}(tW_K x_j)$ or $\tilde{k}(tW_K x_i) \gg \tilde{k}(tW_K x_j)$ for large t . This indicates that there exists a permutation $\sigma \in S_p$ such that

$$\lim_{t \rightarrow \infty} \frac{\tilde{k}(tW_K x_{\sigma_1(j)})}{\tilde{k}(tW_K x_{\sigma_1(i)})} = \infty, \text{ for all } i < j, \quad (57)$$

which completes the proof. \square

Proof of Corollary 1. Lemma 1 shows the token-distinguishability condition over X with non-zero tokens. This indicates the interpolation property over the region when X has non-zero tokens. Since the set

$$\{X \in \mathbb{R}^{d \times n} \mid [X]_i = 0 \text{ for some } i \in [n]\} \quad (58)$$

is a measure-zero set, the S_n -UAP holds for $\mathcal{T}_{\mathcal{G}, \mathcal{H}}$ by the same argument as Theorem 1. \square

C.2 Verification of conditions in Corollary 1 on practical attention mechanisms

We verify the conditions in Corollary 1 for the following kernel functions:

- $k(x, y) = \exp(x^\top y)$, used in the original transformer [66].

Verification: For any given $x \neq 0$ and distinct $y_1, y_2 \in \mathbb{R}^d \setminus \{0\}$, the set

$$\mathcal{P} := \{W_K \mid x^\top W_K y_1 = x^\top W_K y_2\} \quad (59)$$

is a hyperplane in $\mathbb{R}^{d \times d}$, which has zero measure. Notice that for any W_K in $\mathbb{R}^{d \times n} \setminus \mathcal{P}$,

$$\lim_{t \rightarrow \infty} \frac{\exp(tx^\top W_K y_1)}{\exp(tx^\top W_K y_2)} = \lim_{t \rightarrow \infty} \exp(t(x^\top W_K(y_1 - y_2))) = \infty \text{ or } 0. \quad (60)$$

This indicates that the condition in Corollary 1 holds.

- $k(x, y) = \exp(-\gamma\|x - y\|_2^2)$, the RBF kernel, explored in [65].

Verification: Notice that

$$\frac{\exp(-\gamma\|x - tW_K y_1\|_2^2)}{\exp(-\gamma\|x - tW_K y_2\|_2^2)} = \exp(-\gamma(\|tW_K y_1\|_2^2 - \|tW_K y_2\|_2^2) + 2tx^\top W_K(y_2 - y_1)). \quad (61)$$

Therefore, any W_K such that $\|W_K y_1\|_2 \neq \|W_K y_2\|_2$ satisfies the condition in Corollary 1. Since for distinct y_1 and y_2 ,

$$\|W_K y_1\|_2^2 - \|W_K y_2\|_2^2 = 0, \quad (62)$$

is a non-zero quadratic equation on W_K , whose solution set has zero measure. Therefore, the condition in Corollary 1 holds.

- $k(x, y) = \phi(x)^\top \phi(y)$, where

$$\phi(x)^\top = \exp\left(-\frac{1}{2}\|x\|^2\right) (\exp(\omega_1^\top x), \dots, \exp(\omega_m^\top x)) \in \mathbb{R}^m, \quad (63)$$

with $\omega_1, \dots, \omega_m \in \mathbb{R}^d$ drawn i.i.d. from a Gaussian distribution. This kernel is used in Performer [12], and Corollary 1 holds almost surely in this case.

Verification: We have

$$\begin{aligned} \frac{k(x, tW_K y_1)}{k(x, tW_K y_2)} &= \frac{\phi(x)^\top \phi(tW_K y_1)}{\phi(x)^\top \phi(tW_K y_2)} \\ &= \exp\left(\frac{t^2}{2}(\|W_K y_2\|_2^2 - \|W_K y_1\|_2^2)\right) \frac{\sum_{i=1}^m \exp(\omega_i^\top x) \exp(t\omega_i^\top W_K y_1)}{\sum_{i=1}^m \exp(\omega_i^\top x) \exp(t\omega_i^\top W_K y_2)} \end{aligned} \quad (64)$$

We claim that if w_i are pair-wise linear independent, i.e. there does not exist $i \neq j$ such that $w_i = \alpha w_j$ for some $\alpha \in \mathbb{R}$, the condition in Corollary 1 holds. This almost surely holds when w_i are drawn i.i.d. from a Gaussian distribution.

If when $t \rightarrow \infty$, the ratio in (64) do not goes to infinity or zero, it must hold that

$$\|W_K y_1\|_2 = \|W_K y_2\|_2, \text{ and } \max_i \{\omega_i^\top W_K y_1\} = \max_i \{\omega_i^\top W_K y_2\}. \quad (65)$$

When w_i are pair-wise linear independent, we have that $y_1 w_i^\top \neq y_2 w_j^\top$ for all $i \neq j \in [m]$. Also, since $y_1 \neq y_2$ and w_i are non-zero (by the pair-wise independent condition), we have $y_1 w_i^\top \neq y_2 w_i^\top$ for all $i \in [m]$. Therefore, we have that all the sets

$$\{W_K \mid \omega_i^\top W_K y_1 = \omega_j^\top W_K y_1\} = \{W_K \mid \langle W_K, y_1 w_i^\top - y_2 w_j^\top \rangle_F = 0\}, \quad (66)$$

where $\langle \cdot, \cdot \rangle_F$ denotes the Frobenius inner product, are hyperplanes in $\mathbb{R}^{d \times d}$, which has zero measure. That is, equation (65) only holds for a measure-zero set of W_K , which completes the verification.

- $k(x, y) = \exp(w^\top x) + \exp(w^\top y)$, where $w \in \mathbb{R}^d$.

Verification: We have

$$\frac{k(x, tW_K y_1)}{k(x, tW_K y_2)} = \frac{\exp(w^\top (x + tW_K y_1))}{\exp(w^\top (x + tW_K y_2))} = \exp(tw^\top W_K(y_1 - y_2)). \quad (67)$$

When $y_1 \neq y_2$, for almost all W_K , we have $w^\top W_K(y_1 - y_2) \neq 0$. Therefore, the condition in Corollary 1 holds.

- $k(x, y) = p(x - y)\tilde{k}(x, y)$, with p being any positive polynomial function and \tilde{k} being any kernel satisfies the condition in Corollary 1.

Verification: Just need to notice that for almost all W_k , it holds that

$$\lim_{t \rightarrow \infty} \frac{p(x - tW_K y_1)}{p(x - ptW_K y_2)} \quad (68)$$

is a constant indicating that the condition in Corollary 1 still holds.

C.3 Proof of Corollary 2

Proof. We only need to prove the token distinguishability condition for two samples:

- For any X and Y that are in general positions and from different orbits of G (defined in (18)), there exists

$$g \in \mathcal{G}_m^\Phi := \{(\text{Id} + g_m) \circ \dots \circ (\text{Id} + g_1) \mid g_i \in \mathcal{G}_{\mathcal{N}_i}, \text{ for } i \in [m]\} \quad (69)$$

such that the tokens of $g(X)$ and $g(Y)$ are all distinct.

We prove this claim by contradiction. Assume that, there exist X and Y that are in general positions and from different orbits of G , but for any $g \in \mathcal{G}_m^\Phi$, there exist indices $i, j \in [n]$ such that at least one token in $g(X)$ is identical to a token in $g(Y)$. Then, according to the analyticity, there exist indices i_1 and i_2 such that, $[g(X)]_{i_1} = [g(Y)]_{i_2}$ always hold. For a given $p_1 \in [m]$, we first consider $g \in \text{Id} + \mathcal{G}_{\mathcal{N}_{p_1}}$. Then, $[g(X)]_{i_1} = [g(Y)]_{i_2}$ gives:

$$[X]_{i_1} + \frac{\sum_{j \in \mathcal{N}_{p_1}(i_1)} k([W_Q X]_{i_1}, [W_K X]_j) [W_V X]_j}{\sum_{j \in \mathcal{N}_{p_1}(i_1)} k([W_Q X]_{i_1}, [W_K X]_j)} = [Y]_{i_2} + \frac{\sum_{l \in \mathcal{N}_{p_1}(i_2)} k([W_Q Y]_{i_2}, [W_K Y]_l) [W_V Y]_l}{\sum_{j \in \mathcal{N}_{p_1}(i_2)} k([W_Q Y]_{i_2}, [W_K Y]_l)}, \quad (70)$$

for any $W_Q, W_K, W_V \in \mathbb{R}^{d \times d}$. According to Lemma 1, we can deduce that $|\mathcal{N}_{p_1}(i_1)| = |\mathcal{N}_{p_1}(i_2)|$, $[X]_{i_1} = [Y]_{i_2}$, and

$$\{[X]_q \mid q \in \mathcal{N}_{p_1}(i_1)\} = \{[Y]_q \mid q \in \mathcal{N}_{p_1}(i_2)\}. \quad (71)$$

Therefore, choose any $q_1 \in \mathcal{N}_{p_1}(i_1)$, we can find $q_2 \in \mathcal{N}_{p_1}(i_2)$ such that $[X]_{q_1} = [Y]_{q_2}$.

Now, we claim that for any $p_2 < p_1$ and $g \in \text{Id} + \mathcal{G}_{\mathcal{N}_{p_2}}$ (a layer before the p_1 -th layer), $[g(X)]_{q_1} = [g(Y)]_{q_2}$. Otherwise, suppose there exists $g_1 \in \text{Id} + \mathcal{G}_{p_2}$ with $[g_1(X)]_{q_1} \neq [g_1(Y)]_{q_2}$. By scaling the W_V matrix to be small enough, we can assume g_1 satisfies that

$$\|g_1(X) - X\|_2 < \frac{1}{2} \min_{i \neq j} \{\|[X]_i - [X]_j\|_2\}. \quad (72)$$

Then, we have that $[g_1(X)]_{q_1} \neq [g_1(Y)]_{q_2}$, and by equation (72), for any $q \neq q_2$ in $\mathcal{N}(i_2)$, we have

$$\begin{aligned} \|[g_1(X)]_{q_1} - [g_1(Y)]_q\|_2 &= \|([g_1(X)]_{q_1} - [X]_{q_1}) + ([X]_{q_1} - [Y]_q) + ([Y]_q - [g_1(Y)]_q)\|_2 \\ &\geq \|[X]_{q_1} - [Y]_q\|_2 - \|[g_1(X)]_{q_1} - [X]_{q_1}\|_2 - \|[Y]_q - [g_1(Y)]_q\|_2 > 0. \end{aligned} \quad (73)$$

Therefore, $[g_1(X)]_{q_1}$ does not appear in the tokens of $g_1(Y)$, i.e. the sets

$$\{[g_1(X)]_j \mid j \in \mathcal{N}(i_1)\} \quad \text{and} \quad \{[g_1(Y)]_l \mid l \in \mathcal{N}(i_2)\} \quad (74)$$

must be different. By applying Lemma 1 to $[g_1(X)]_{q_1}$ and $[g_1(Y)]_{q_2}$, we know that there exists $g_2 \in \text{Id} + \mathcal{G}_{\mathcal{N}_{p_1}}$ such that $[g_2(g_1(X))]_{q_1} \neq [g_2(g_1(Y))]_{q_2}$. Since $g_2 \circ g_1 \in (\text{Id} + \mathcal{G}_{\mathcal{N}_{p_2}}) \circ (\text{Id} + \mathcal{G}_{\mathcal{N}_{p_1}}) \subset \mathcal{G}_m^\Phi$ which can distinguish $[X]_{i_1}$ and $[Y]_{i_2}$, contradicting to our assumption.

Hence, we have shown that for $p_2 < p_1 \leq n$ and any $g \in \text{Id} + \mathcal{G}_{\mathcal{N}_{p_2}}$, $[g(X)]_{q_1} = [g(Y)]_{q_2}$. Then, we can apply Lemma 1 to $[X]_{q_1}$ and $[Y]_{q_2}$, and deduce that the set of tokens of X with indices in $\mathcal{N}_{p_s}(q_1)$ are the same as those of Y with indices in $\mathcal{N}_{p_3}(q_2)$. That is, the tokens where $[X]_{i_1}$ can attend to within two hops are the same as those where $[Y]_{i_2}$ can attend to within two hops.

The above process can be repeated. Since we assume that Φ is connected within m layers, we know that any indices in $[n]$ can be reached starting from i_1 and i_2 within m hops. Finally, the above discussion can cover all indices in $[n]$. Since X and Y are in general positions, the correspondence between their tokens is unique. Finally, this results in a permutation $\sigma \in S_n$, such that:

$$[X]_i = [Y]_{\sigma(i)}. \quad (75)$$

On the other hand, apply Lemma 1 again to eqch \mathcal{N}_p , $[X]_i$ and $[Y]_{\sigma(i)}$, we can deduce that

$$j \in \mathcal{N}_p(i) \Leftrightarrow \sigma(j) \in \mathcal{N}_p(\sigma(i)), \text{ for all } p \in [m]. \quad (76)$$

By the definition of $\text{Aut}(\mathcal{N})$, this means that σ belongs to each \mathcal{N}_p , indicating that $\sigma \in G$. However, this contradicts to our assumption that X and Y are from different orbits of $\text{Aut}(\Gamma)$, which completes the proof. \square

C.4 Verification of the UAP for other transformer variants

In this section, we verify the condition in Theorem 1 for the kernelized attention of SkyFormer [9] and the attention mechanism of the Linformer [68].

C.4.1 UAP for LinFormer

Linformer [68], where the attention layer is defined as

$$\text{Atten}(X) = X + W_V X F \text{softmax}((W_K X E)^\top W_Q X) \quad (77)$$

where $E, F \in \mathbb{R}^{n \times k}$ with $1 \leq k \ll n$ are two trainable projection matrices.

For LinFormer, we have the following lemma:

Lemma 3. *Let $X, Y \in \mathbb{R}^{d \times n}$ be two points that are in general positions. If for some $i_1, i_2 \in [n]$, the following equality holds for all $W_Q, W_K, W_V \in \mathbb{R}^{d \times d}$ and $E, F \in \mathbb{R}^{n \times k}$:*

$$[X]_{i_1} + [W_V X F \text{softmax}((W_K X E)^\top W_Q X)]_{i_1} = [Y]_{i_2} + [W_V Y F \text{softmax}((W_K Y E)^\top W_Q Y)]_{i_2}, \quad (78)$$

then we have $i_1 = i_2$ and $X = Y$.

Proof. Take $W_V = 0$ gives $[X]_{i_1} = [Y]_{i_2}$. Then, for any given $R = \{r_1, \dots, r_k\} \subset [n]$, we take

$$E = F = [e_{r_1}, \dots, e_{r_k}], \quad (79)$$

where e_{r_i} is the r_i -th column of the identity matrix. Equation (78) then gives that

$$\sum_{j \in R} \left(\frac{\exp(\langle W_Q[X]_{i_1}, W_K[X]_j \rangle)}{\sum_{l \in R} \exp(\langle W_Q[X]_{i_1}, W_K[X]_l \rangle)} W_V[X]_j \right) = \sum_{j \in R} \left(\frac{\exp(\langle W_Q[Y]_{i_2}, W_K[Y]_j \rangle)}{\sum_{l \in R} \exp(\langle W_Q[Y]_{i_2}, W_K[Y]_l \rangle)} W_V[Y]_j \right) \quad (80)$$

which reduces to the discussion in Lemma 1. Therefore, we have that the set $\{[X]_i \mid i \in R\}$ is the same as $\{[Y]_i \mid i \in R\}$. Since X and Y are in general positions, and R is arbitrary, this indicates that $X = Y$. \square

According to this lemma and the fact that (19) is analytic to all the parameters, we conclude by Theorem 2 that the UAP holds for LinFormer without symmetric restrictions. Furthermore, the same result can be generalized to the case where the softmax function in (19) is replaced by a kernel-based form with a kernel satisfying the condition in Corollary 1.

C.4.2 UAP for SkyFormer

The kernelized attention used in SkyFormer [9], where the attention mechanism is given by:

$$[\text{Atten}(X)]_i = [X]_i + \sum_{j=1}^n \exp\left(-\frac{1}{2} \| [W_Q X]_i - [W_K X]_j \|^2 \right) W_V X_j. \quad (81)$$

The proof follows from the verification for the RBF kernel Section C.2, with the same argument to prove the token-distinguishability condition.

C.4.3 UAP for architecture proposed in (21)

More precisely, if we define $\tilde{\mathcal{G}}_{\mathcal{N}}$ as the family of token-mixing maps associated with the sparsity pattern \mathcal{N} , and the transformer family $\tilde{\mathcal{T}}_{\mathcal{H}}^\Phi$ associated with a sequence of sparse mode, just as $\mathcal{T}_{\mathcal{H}}^\Phi$ defined in Section 4.2. Then, under the same assumption on Φ as in Corollary 2, we have:

Corollary 5.

$\tilde{\mathcal{T}}_{\mathcal{H}}^\Phi$ possesses the G -UAP with G defined in (18).

Assume the condition in Theorem 2 fails. Then, there exists X and Y that are in general positions, and $i_1, i_2 \in [n]$ such that for all $W \in \mathbb{R}^{d \times d}$, $a \in \mathbb{R}$ and $b \in \mathbb{R}^d$, we have

$$[X]_{i_1} + \sum_{j \in \mathcal{N}(i_1)} a \alpha(W[X]_j - b) = [Y]_{i_2} + \sum_{j \in \mathcal{N}(i_2)} a \alpha(W[Y]_j - b). \quad (82)$$

It then follows that $[X]_{i_1} = [Y]_{i_2}$. Moreover, if the sets

$$\{[X]_j \mid j \in \mathcal{N}(i_1)\} \quad (83)$$

and

$$\{[Y]_j \mid j \in \mathcal{N}(i_2)\} \quad (84)$$

are not the same, we can then derive an identity

$$\sum_{l=1}^L c_l \alpha(Wx_l - b) = 0, \quad (85)$$

where x_l are the unique tokens appears in the two sets, c_i equals to 1 if x_l appears in the set of X , and -1 otherwise. Notice that the identity holds for all $W \in \mathbb{R}^{d \times d}$ and $b \in \mathbb{R}$, this gives a contradiction according to the proof of Theorem 1 in [10]. Specifically, since α is of polynomial growth, taking the Fourier transform(in distributional sense) on both side of (85) with respect to b gives:

$$\left(\sum_{l=1}^L c_l e^{i(Wx_l)^\top \xi}\right) \hat{\alpha}(\xi) = 0, \quad \text{for all } \xi \in \mathbb{R}^d, \quad (86)$$

where $\hat{\alpha}$ is the Fourier transform of α . Since α is not a polynomial, we have $\text{supp } \hat{\alpha}$ contains a non-zero value. This will lead to a contradiction. See Section 3.2 in [10] for more details.

C.4.4 Details for architecture proposed for D_n/C_n equivariant map

For architecture with D_n symmetry By choosing $\Phi = (\mathcal{N}, \mathcal{N}, \dots)$ as an invariant sequence of sparse mode, by Corollary 2, we have that the transformer with the first design satisfies the $\text{Aut}(\mathcal{N})$ -UAP. Therefore, we only need to prove that $\text{Aut}(\mathcal{N}) = D_n$.

First, it is easy to see that for any $g \in D_n$, we have $j \in \mathcal{N}(i)$ indicates that $g(j) \in \mathcal{N}(g(i))$. This implies that $N_n \in \text{Aut}(\mathcal{N})$. On the other hand, for any $g \in \text{Aut}(\mathcal{N})$, since D_n is transitive, there exists $h \in D_n$ such that $h(g(1)) = 1$. Now, we prove that $\gamma := h \circ g$ is either the identity or the reflection $\sigma = (1, n)(2, n-1) \dots$.

Since $\gamma \in \text{Aut}(\mathcal{N})$, we know that $\gamma(\mathcal{N}(i)) = \mathcal{N}(\gamma(i))$. Since $\gamma(1) = 1$, we have $\gamma(\mathcal{N}(1)) = \mathcal{N}(\gamma(1)) = \mathcal{N}(1)$ is invariant. This indicates that for any $i \in \mathcal{N}(1)$, $\gamma(i)$ is also in $\mathcal{N}(1)$. Now, we consider the value of $\mathcal{N}(2)$. We have that

$$2w = |\mathcal{N}(1) \cap \mathcal{N}(2)| = |\gamma(\mathcal{N}(1)) \cap \gamma(\mathcal{N}(2))| = |\mathcal{N}(1) \cap \mathcal{N}(\gamma(2))| \quad (87)$$

Since $2w + 1 \leq n - 2$, we have that in $\mathcal{N}(1)$, there are only two indices $j = n, 2$ such that

$$|\mathcal{N}(1) \cap \mathcal{N}(j)| = 2w. \quad (88)$$

Therefore, it follows that $\gamma(2) = n$ or 2 . If $\gamma(2) = 2$, we can then repeat the discussion to deduce that $\gamma(i) = i$ for $i = 2, 3, \dots, n$ sequentially, indicating that γ is the identity. If $\gamma(2) = n$. Then, we can repeat the discussion to deduce that $\gamma(i) = n + 2 - i \bmod n$ for $i = 2, 3, \dots, n$. This indicates that γ is a reflection $(2, n)(3, n-1) \dots$, which is in D_n .

Therefore, we have shown that $\text{Aut}(\mathcal{N}) = D_n$. This is actually a classical result on the automorphism group of the circulant graph [4].

Moreover, if we destroy the symmetry to reflection by defining

$$\mathcal{N}(i) := \{i, i+1, i+2, \dots, i+w \bmod n\} \text{ for } i = 1, 2, \dots, n, \quad (89)$$

with $w \leq \lfloor \frac{n-1}{2} \rfloor - 1$, we get a transformer that is C_n -equivariant and satisfies the C_n -UAP. For the proof, we only need to check that $\text{Aut}(\mathcal{N}) = C_n$, which can be done following the same approach as D_n .

For architecture with C_n symmetry For token-mixing layer defined by the convolution in (23), we first notice that it satisfies the C_n -equivariance. In fact, this follows from the fact that the convolutional operation is equivariant to translation.

Therefore, to prove the C_n -UAP, we only need to check the token distinguishability condition under C_n action. Specifically, suppose the condition in Theorem 2 fails. Then, there exists X and Y that

are in general positions, and $i_1, i_2 \in [n]$ such that the composition of token mixing layers cannot distinguish the i_1 -th token of X and the i_2 -th token of Y .

Considering using single layers, we have that for all $\psi \in \mathbb{R}^{l+1}$, it holds

$$[\psi * X]_{i_1} = [\psi * X]_{i_2}, \quad (90)$$

i.e.

$$\sum_{j=0}^l \psi_j [X]_{(i_1+j) \bmod n} = \sum_{j=0}^l \psi_j [Y]_{(i_2+j) \bmod n}, \quad (91)$$

which indicates that

$$\sum_{j=0}^l \psi_j ([X]_{(i_1+j) \bmod n} - [Y]_{(i_2+j) \bmod n}) = 0 \quad (92)$$

Since ψ is arbitrary, this indicates that

$$[X]_{(i_1+j) \bmod n} = [Y]_{(i_2+j) \bmod n}, \quad \text{for } j = 0, 1, \dots, l. \quad (93)$$

Then, we take the indices $i_1 + l \bmod n$ and $i_2 + l \bmod n$ of X, Y respectively, and consider using two layers. The process is essentially the same as the proof of Corollary 2. We can finally deduce that

$$[X]_{(i_1+j) \bmod n} = [Y]_{(i_2+j) \bmod n}, \quad \text{for } j = 0, 1, \dots, n. \quad (94)$$

That is, X and Y differs only a cyclic action on tokens, meaning that they are from the same C_n orbit, which is a contradiction, and completes the proof.

NeurIPS Paper Checklist

1. Claims

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

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

Justification: The claims made in the abstract and introduction accurately reflect the paper's contributions and scope.

Guidelines:

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

2. Limitations

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

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

Justification: We discuss the limitations of our work in the last section of the paper.

Guidelines:

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

3. Theory assumptions and proofs

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

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

Justification: We provide exact and complete assumptions and proofs for all theoretical results in the paper and the appendix.

Guidelines:

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

4. Experimental result reproducibility

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

Answer: [NA]

Justification: This paper does not include experiments.

Guidelines:

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

5. Open access to data and code

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

Answer: [NA]

Justification: This paper does not include experiments.

Guidelines:

- The answer NA means that paper does not include experiments requiring code.
- Please see the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- While we encourage the release of code and data, we understand that this might not be possible, so “No” is an acceptable answer. Papers cannot be rejected simply for not including code, unless this is central to the contribution (e.g., for a new open-source benchmark).
- The instructions should contain the exact command and environment needed to run to reproduce the results. See the NeurIPS code and data submission guidelines (<https://nips.cc/public/guides/CodeSubmissionPolicy>) for more details.
- The authors should provide instructions on data access and preparation, including how to access the raw data, preprocessed data, intermediate data, and generated data, etc.
- The authors should provide scripts to reproduce all experimental results for the new proposed method and baselines. If only a subset of experiments are reproducible, they should state which ones are omitted from the script and why.
- At submission time, to preserve anonymity, the authors should release anonymized versions (if applicable).
- Providing as much information as possible in supplemental material (appended to the paper) is recommended, but including URLs to data and code is permitted.

6. Experimental setting/details

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

Answer: [NA]

Justification: This paper does not include experiments.

Guidelines:

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

7. Experiment statistical significance

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

Answer: [NA]

Justification: This paper does not include experiments.

Guidelines:

- The answer NA means that the paper does not include experiments.
- The authors should answer "Yes" if the results are accompanied by error bars, confidence intervals, or statistical significance tests, at least for the experiments that support the main claims of the paper.
- The factors of variability that the error bars are capturing should be clearly stated (for example, train/test split, initialization, random drawing of some parameter, or overall run with given experimental conditions).
- The method for calculating the error bars should be explained (closed form formula, call to a library function, bootstrap, etc.)
- The assumptions made should be given (e.g., Normally distributed errors).
- It should be clear whether the error bar is the standard deviation or the standard error of the mean.

- It is OK to report 1-sigma error bars, but one should state it. The authors should preferably report a 2-sigma error bar than state that they have a 96% CI, if the hypothesis of Normality of errors is not verified.
- For asymmetric distributions, the authors should be careful not to show in tables or figures symmetric error bars that would yield results that are out of range (e.g. negative error rates).
- If error bars are reported in tables or plots, The authors should explain in the text how they were calculated and reference the corresponding figures or tables in the text.

8. Experiments compute resources

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

Answer: [NA]

Justification: This paper does not include experiments.

Guidelines:

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

9. Code of ethics

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

Answer: [Yes]

Justification: The research conducted in this paper conforms with the NeurIPS Code of Ethics.

Guidelines:

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

10. Broader impacts

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

Answer: [NA]

Justification: This is a theoretical paper and does not discuss societal impacts.

Guidelines:

- The answer NA means that there is no societal impact of the work performed.
- If the authors answer NA or No, they should explain why their work has no societal impact or why the paper does not address societal impact.
- Examples of negative societal impacts include potential malicious or unintended uses (e.g., disinformation, generating fake profiles, surveillance), fairness considerations (e.g., deployment of technologies that could make decisions that unfairly impact specific groups), privacy considerations, and security considerations.

- The conference expects that many papers will be foundational research and not tied to particular applications, let alone deployments. However, if there is a direct path to any negative applications, the authors should point it out. For example, it is legitimate to point out that an improvement in the quality of generative models could be used to generate deepfakes for disinformation. On the other hand, it is not needed to point out that a generic algorithm for optimizing neural networks could enable people to train models that generate Deepfakes faster.
- The authors should consider possible harms that could arise when the technology is being used as intended and functioning correctly, harms that could arise when the technology is being used as intended but gives incorrect results, and harms following from (intentional or unintentional) misuse of the technology.
- If there are negative societal impacts, the authors could also discuss possible mitigation strategies (e.g., gated release of models, providing defenses in addition to attacks, mechanisms for monitoring misuse, mechanisms to monitor how a system learns from feedback over time, improving the efficiency and accessibility of ML).

11. Safeguards

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

Answer: [NA]

Justification: The paper does not release any data or models that have a high risk for misuse.

Guidelines:

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

12. Licenses for existing assets

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

Answer: [NA]

Justification: The paper does not use existing assets.

Guidelines:

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

- If this information is not available online, the authors are encouraged to reach out to the asset’s creators.

13. **New assets**

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

Answer: [NA]

Justification: The paper does not release new assets.

Guidelines:

- The answer NA means that the paper does not release new assets.
- Researchers should communicate the details of the dataset/code/model as part of their submissions via structured templates. This includes details about training, license, limitations, etc.
- The paper should discuss whether and how consent was obtained from people whose asset is used.
- At submission time, remember to anonymize your assets (if applicable). You can either create an anonymized URL or include an anonymized zip file.

14. **Crowdsourcing and research with human subjects**

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

Answer: [NA]

Justification: The paper does not involve crowdsourcing nor research with human subjects.

Guidelines:

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

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

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

Answer: [NA]

Justification: The paper does not involve crowdsourcing nor research with human subjects.

Guidelines:

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

16. **Declaration of LLM usage**

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

Answer: [NA]

Justification: This paper does not involve LLMs as any important, original, or non-standard components.

Guidelines:

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