

ON RADEMACHER COMPLEXITY-BASED GENERALIZATION BOUNDS FOR THE TRANSFORMER ARCHITECTURE

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ABSTRACT

We derive the first end-to-end, data-dependent generalization bound for the Transformer architecture to explain its strong empirical performance. Using Rademacher complexity and a novel Lipschitz analysis of self-attention, we construct a bound for deep, L -layer models. The bound demonstrates that generalization capacity is governed by depth, sequence length, and a polynomial of the model’s weight norms. A numerical sanity check validates our theoretical scaling with model depth, providing a new, formal lens to understand and improve Transformers.

1 INTRODUCTION

The Transformer architecture has become the de facto standard for a vast range of tasks in modern artificial intelligence, achieving state-of-the-art results in natural language processing, computer vision, and beyond Vaswani et al. (2017); Dosovitskiy et al. (2021). Its parallelizable self-attention mechanism has proven to be a remarkably effective and scalable tool for modeling complex dependencies in sequential data.

Despite this extraordinary empirical success, our theoretical understanding of why Transformers generalize so well remains critically underdeveloped. The gap between the practical performance of these models and the theory that explains their success is significant. Most existing generalization bounds for deep learning were developed for convolutional or fully-connected networks and do not apply to the unique, data-dependent computations within the self-attention mechanism.

In this paper, we narrow this theory-practice gap by deriving an end-to-end generalization bound for Transformers using the powerful framework of Rademacher complexity. Our work provides a formal, data-dependent measure of the Transformer’s effective capacity.

Our main contributions are as follows:

- **A Novel Bound for Self-Attention:** We provide the first theoretical analysis of the self-attention mechanism within the Rademacher complexity framework, featuring a novel proof establishing its Lipschitz continuity.
- **An End-to-End Transformer Bound:** We assemble our analysis of the individual components into a complete generalization bound for a deep L -layer Transformer, explicitly showing how complexity scales with depth, weight norms, and data properties.
- **Numerical Validation:** We conduct a numerical sanity check that grounds our theory, demonstrating that our bound’s scaling with model depth correctly reflects empirical trends in model capacity.

The remainder of this paper is organized as follows. Section 2 reviews prior work. Section 3 presents our main theoretical results. Section 4 details our numerical validation. Finally, we conclude in Section 5.

2 RELATED WORK

Our research builds upon a rich history of work in statistical learning theory. We situate our contribution in the context of three main areas: data-dependent complexity measures, architecture-specific bounds, and the emerging theory of the Transformer model.

Generalization Bounds for Deep Learning. The theoretical study of generalization dates back to the foundational work of Vapnik and Chervonenkis Vapnik (1998). The limitations of data-independent measures like the VC-dimension for deep learning led to the development of data-dependent complexity measures, such as Rademacher complexity Bartlett & Mendelson (2002). Subsequent research has focused on deriving tighter, norm-based Rademacher complexity bounds for deep neural networks, demonstrating that the magnitude of the weights is a key controller of generalization Bartlett et al. (2017); Neyshabur et al. (2018). Our work follows this powerful paradigm.

Architecture-Specific Bounds. Much of the work on norm-based bounds has focused on MLPs and CNNs, with analyses often leveraging properties like weight sharing and spectral norms of convolutional layers Neyshabur et al. (2015); Arora et al. (2018). For Recurrent Neural Networks (RNNs), bounds have been derived by analyzing their "unrolled" computation as a very deep network with shared weights. However, these techniques do not directly apply to the Transformer. The core self-attention mechanism is not convolutional, nor does it share the simple recurrent structure of an RNN. Its computational graph is dynamically determined by the input data itself, posing a unique challenge for theoretical analysis.

Theoretical Understanding of Transformers. Since the introduction of the Transformer Vaswani et al. (2017), theoretical work has begun to explore its properties, often focusing on aspects like its universal approximation capabilities Yun et al. (2020) or its computational power Bhattamishra et al. (2020). While recent works have begun to tackle Transformer generalization using alternative frameworks like PAC-Bayes Elman & Levine (2023) or stability analysis Zhai & Wang (2023), a constructive bound based on Rademacher complexity has remained an open question. Our work addresses this specific gap, providing the first end-to-end generalization bound for the Transformer through an explicit analysis of the data-dependent self-attention mechanism.

3 RADEMACHER COMPLEXITY OF A TRANSFORMER

In this section, we derive a data-dependent generalization bound for the Transformer. We begin by analyzing a single self-attention head, which constitutes the most significant technical challenge.

Norm Regime. Our analysis consistently assumes control over the Frobenius norm of the weights, denoted $\|W\|_F \leq B_W$. We use the standard inequality $\|W\|_{op} \leq \|W\|_F$ to bound the spectral norm (the true Lipschitz constant of linear layers) where necessary

3.1 PRELIMINARIES AND NOTATION

Let the function class for a single self-attention head, $\mathcal{F}_{\text{Attn}}$, be defined as the set of functions $f_W : \mathbb{R}^{n \times d_{\text{model}}} \rightarrow \mathbb{R}^{n \times d_k}$ such that:

$$f_W(X) = \text{softmax} \left(\frac{XW_Q(XW_K)^T}{\sqrt{d_k}} \right) (XW_V)$$

The function class is parameterized by the weight matrices $W(W_Q, W_K, W_V)$, where $W_Q, W_K, W_V \in \mathbb{R}^{d_{\text{model}} \times d_k}$. We consider the class where the weights are bounded in the Frobenius norm: $\|W_Q\|_F, \|W_K\|_F, \|W_V\|_F \leq B_W$. We also assume the input token embeddings, which are the rows x_i of the input matrix X , are bounded: $\|x_i\|_2 \leq B_X$.

Our analysis relies on Talagrand's Contraction Lemma, which bounds the complexity of a function class composed with a Lipschitz function. The key to applying this lemma is establishing the Lipschitz property of the attention computation itself.

3.2 CORE LEMMA: LIPSCHITZ CONTINUITY OF SELF-ATTENTION

[Lipschitz Property of Self-Attention, Revised] Let the function $\phi_{\text{attn}} : (\mathbb{R}^{n \times d_k})^3 \rightarrow \mathbb{R}^{n \times d_k}$ be defined as $\phi_{\text{attn}}(Q, K, V) = \text{softmax}\left(\frac{QK^T}{\sqrt{d_k}}\right)V$. Assume the inputs are bounded in spectral norm such that $\|Q\|_{op}, \|K\|_{op}, \|V\|_{op} \leq B_{op}$. The function ϕ_{attn} is Lipschitz continuous with respect to the Frobenius norm, with a Lipschitz constant L_{attn} satisfying:

$$L_{\text{attn}} \leq \sqrt{n} + \frac{2B_{op}^2}{\sqrt{d_k}}$$

We wish to bound $\|\phi_{\text{attn}}(Q, K, V) - \phi_{\text{attn}}(Q', K', V')\|_F$. Let $A = \frac{QK^T}{\sqrt{d_k}}$ and $A' = \frac{Q'K'^T}{\sqrt{d_k}}$. Using the triangle inequality, we have:

$$\|\text{softmax}(A)V - \text{softmax}(A')V'\|_F \leq \underbrace{\|(\text{softmax}(A) - \text{softmax}(A'))V\|_F}_{\text{Term 1}} + \underbrace{\|\text{softmax}(A')(V - V')\|_F}_{\text{Term 2}}$$

Bounding Term 2: The spectral norm of a row-stochastic matrix \mathbf{M} can be bounded using the inequality $\|\mathbf{M}\|_2 \leq \sqrt{\|\mathbf{M}\|_1 \|\mathbf{M}\|_\infty}$. For the matrix $\text{softmax}(A')$, its L_∞ norm is 1 and its L_1 norm (maximum absolute column sum) is bounded by the number of rows, n . This gives the spectral norm bound:

$$\|\text{softmax}(A')\|_{op} \leq \sqrt{n \cdot 1} = \sqrt{n}$$

Applying this to Term 2, we have:

$$\|\text{softmax}(A')(V - V')\|_F \leq \|\text{softmax}(A')\|_{op} \|V - V'\|_F \leq \sqrt{n} \cdot \|V - V'\|_F$$

Bounding Term 1: Using the sub-multiplicative property and the 1-Lipschitz nature of the softmax function, this term is bounded as follows:

$$\|(\text{softmax}(A) - \text{softmax}(A'))V\|_F \leq \frac{B_{op}^2}{\sqrt{d_k}} (\|Q - Q'\|_F + \|K - K'\|_F)$$

Combining the terms: Let $\Delta_Q = \|Q - Q'\|_F$, $\Delta_K = \|K - K'\|_F$, and $\Delta_V = \|V - V'\|_F$. The total difference is bounded by:

$$\|\phi_{\text{attn}}(Q, K, V) - \phi_{\text{attn}}(Q', K', V')\|_F \leq \frac{B_{op}^2}{\sqrt{d_k}} (\Delta_Q + \Delta_K) + \sqrt{n} \Delta_V$$

This can be bounded by a single Lipschitz constant by noting that each individual norm difference is less than or equal to the total norm difference of the input triplet:

$$\leq \left(\frac{2B_{op}^2}{\sqrt{d_k}} + \sqrt{n} \right) \cdot \sqrt{\Delta_Q^2 + \Delta_K^2 + \Delta_V^2}$$

This completes the proof.

3.3 RADEMACHER COMPLEXITY OF A SINGLE SELF-ATTENTION HEAD

With the Lipschitz property of the attention computation established in Lemma 3.2, we can now apply Talagrand's Contraction Lemma to bound the Rademacher complexity of the function class for a single self-attention head.

[Rademacher Complexity of a Single Self-Attention Head] Let $\mathcal{F}_{\text{Attn}}$ be the function class for a single self-attention head as defined in Section 3.1. Let $S = \{X_1, \dots, X_m\}$ be a set of m input matrices. The empirical Rademacher complexity of $\mathcal{F}_{\text{Attn}}$ over S is bounded as:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Attn}}) \leq \left(\sqrt{n} + \frac{2nB_X^2 B_W^2}{\sqrt{d_k}} \right) \frac{6B_W}{m} \sqrt{\sum_{i=1}^m \|X_i\|_F^2}$$

The proof proceeds by decomposing the self-attention function and applying the Contraction Lemma.

1. Function Decomposition. We view the function $f_W \in \mathcal{F}_{\text{Attn}}$ as a composition $f_W = \phi_{\text{attn}} \circ g_W$, where $\mathcal{G}_{\text{proj}}$ is the class of linear projections $g_W(X) = (XW_Q, XW_K, XW_V)$.

2. Applying the Contraction Lemma. According to the vector-valued Contraction Lemma for Rademacher complexity, for a class of functions composed with a Lipschitz function ϕ , we have:

$$\hat{\mathcal{R}}_S(\phi \circ \mathcal{G}) \leq 2L_\phi \hat{\mathcal{R}}_S(\mathcal{G})$$

Applying this to our classes with the Lipschitz constant L_{attn} from Lemma 3.2, we get:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Attn}}) \leq 2L_{\text{attn}} \hat{\mathcal{R}}_S(\mathcal{G}_{\text{proj}})$$

3. Bounding the Complexity of the Linear Projections. The complexity of the vector-valued class $\mathcal{G}_{\text{proj}}$ is bounded by the sum of the complexities of its components. For a single linear class, e.g., $\mathcal{F}_Q = \{X \mapsto XW_Q : \|W_Q\|_F \leq B_W\}$, the complexity is a standard result:

$$\hat{\mathcal{R}}_S(\mathcal{F}_Q) \leq \frac{B_W}{m} \sqrt{\sum_{i=1}^m \|X_i\|_F^2}$$

This follows from Jensen’s inequality and properties of Rademacher variables. Since there are three identical projection classes (for Q, K, and V), we have:

$$\hat{\mathcal{R}}_S(\mathcal{G}_{\text{proj}}) \leq \frac{3B_W}{m} \sqrt{\sum_{i=1}^m \|X_i\|_F^2}$$

4. Assembling the Final Bound. We make the dependency of L_{attn} on the base parameters explicit by substituting $B_{op} \leq \sqrt{n}B_X B_W$:

$$L_{\text{attn}} \leq \sqrt{n} + \frac{2(\sqrt{n}B_X B_W)^2}{\sqrt{d_k}} = \sqrt{n} + \frac{2nB_X^2 B_W^2}{\sqrt{d_k}}$$

Combining this with the results from the previous steps:

$$\begin{aligned} \hat{\mathcal{R}}_S(\mathcal{F}_{\text{Attn}}) &\leq 2L_{\text{attn}} \cdot \hat{\mathcal{R}}_S(\mathcal{G}_{\text{proj}}) \\ &\leq 2 \left(\sqrt{n} + \frac{2nB_X^2 B_W^2}{\sqrt{d_k}} \right) \left(\frac{3B_W}{m} \sqrt{\sum_{i=1}^m \|X_i\|_F^2} \right) \end{aligned}$$

Simplifying the constant factor gives the expression in the theorem. This concludes the proof.

3.4 RADEMACHER COMPLEXITY OF MULTI-HEAD SELF-ATTENTION

A standard Transformer architecture combines multiple self-attention heads, which operate in parallel. The Multi-Head Self-Attention (MHSA) mechanism concatenates the outputs of these heads and projects the result with a final linear layer. In this section, we extend our analysis to this complete mechanism.

Let h be the number of attention heads. The function for the i -th head is $f_{W_i} \in \mathcal{F}_{\text{Attn}}$, where $W_i = (W_{Q,i}, W_{K,i}, W_{V,i})$. The MHSA function is then defined by:

$$f_{W_{\text{MHSA}}}(X) = \text{Concat}(f_{W_1}(X), \dots, f_{W_h}(X)) W_O$$

where $W_O \in \mathbb{R}^{h \cdot d_k \times d_{\text{model}}}$ is the output projection matrix. The function class $\mathcal{F}_{\text{MHSA}}$ is parameterized by the set of all head weights and the output matrix, each bounded by B_W in Frobenius norm.

[Rademacher Complexity of MHSA] Let $\mathcal{F}_{\text{MHSA}}$ be the function class for a Multi-Head Self-Attention block with h heads. Under the same assumptions as Theorem 3.3, the empirical Rademacher complexity of $\mathcal{F}_{\text{MHSA}}$ is bounded as:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{MHSA}}) \leq 2h \cdot B_W \cdot \left(\sqrt{n} + \frac{2nB_X^2 B_W^2}{\sqrt{d_k}} \right) \frac{3B_W}{m} \sqrt{\sum_{i=1}^m \|X_i\|_F^2}$$

The proof relies on the compositionality of Rademacher complexity, using the sum rule for vector-valued functions and the Contraction Lemma for the final linear projection.

1. Decomposing the MHSA function. We view the MHSA function as a composition $\mathcal{F}_{\text{MHSA}} = \phi_O \circ \mathcal{G}_{\text{heads}}$, where $\mathcal{G}_{\text{heads}}$ is the parallel application of h attention heads and ϕ_O is the final linear projection with W_O .

2. Bounding the complexity of the parallel heads. The Rademacher complexity of the vector-valued class $\mathcal{G}_{\text{heads}}$ is bounded by the sum of the complexities of its component function classes:

$$\hat{\mathcal{R}}_S(\mathcal{G}_{\text{heads}}) \leq \sum_{i=1}^h \hat{\mathcal{R}}_S(\mathcal{F}_{\text{head}_i})$$

Using the result from Theorem 3.3, and assuming each head has the same parameter bounds, we have:

$$\hat{\mathcal{R}}_S(\mathcal{G}_{\text{heads}}) \leq h \cdot \left[\left(\sqrt{n} + \frac{2nB_X^2 B_W^2}{\sqrt{d_k}} \right) \frac{6B_W}{m} \sqrt{\sum_{i=1}^m \|X_i\|_F^2} \right]$$

3. Applying the Contraction Lemma. The final projection, ϕ_O , is a linear map and is therefore Lipschitz. Its Lipschitz constant L_O is its spectral norm, $\|W_O\|_{op}$. We bound this constant using the standard inequality $\|W_O\|_{op} \leq \|W_O\|_F \leq B_W$, which is consistent with our assumption of Frobenius norm control. Applying the Contraction Lemma with the standard factor of 2 for vector-valued classes gives:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{MHSA}}) \leq 2L_O \cdot \hat{\mathcal{R}}_S(\mathcal{G}_{\text{heads}}) \leq 2B_W \cdot \hat{\mathcal{R}}_S(\mathcal{G}_{\text{heads}})$$

4. Assembling the final bound. Substituting the bound for $\hat{\mathcal{R}}_S(\mathcal{G}_{\text{heads}})$ gives the final result:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{MHSA}}) \leq 2B_W \cdot h \cdot \left[\left(\sqrt{n} + \frac{2nB_X^2 B_W^2}{\sqrt{d_k}} \right) \frac{6B_W}{m} \sqrt{\sum_{i=1}^m \|X_i\|_F^2} \right]$$

Simplifying the constant factors yields the expression stated in the theorem. This concludes the proof.

3.5 RADEMACHER COMPLEXITY OF A FULL TRANSFORMER BLOCK

A full Transformer block integrates the Multi-Head Self-Attention (MHSA) sub-layer with a position-wise Feed-Forward Network (FFN). Both sub-layers are typically preceded by Layer Normalization and connected via residual connections. We now assemble our previous results to derive a complexity bound for this entire block.

[Lipschitz Continuity of LayerNorm] Let $\text{LayerNorm} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be defined as $\text{LayerNorm}(x) = \gamma \odot \frac{x - \mu}{\sqrt{\sigma^2 + \epsilon}} + \beta$, where \odot is element-wise multiplication, and $\gamma, \beta \in \mathbb{R}^d$ are learnable parameters. Assuming the gain parameter is bounded such that $\|\gamma\|_\infty \leq B_\gamma$, the function is Lipschitz with a constant $L_{\text{LN}} \leq 2B_\gamma / \sqrt{\epsilon}$. For simplicity in the main bound, we will assume $B_\gamma = 1$ and ϵ is a constant, leading to a constant Lipschitz factor.

[Rademacher Complexity of FFN] Let \mathcal{F}_{FFN} be the function class for a two-layer feed-forward network of the form $f(Y) = \text{ReLU}(YW_1 + b_1)W_2 + b_2$, with weights bounded as $\|W_1\|_F \leq B_{W1}$ and $\|W_2\|_F \leq B_{W2}$. Let the input Y have rows bounded by $\|y_i\|_2 \leq B_Y$. The empirical Rademacher complexity is bounded by:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{FFN}}) \leq \frac{2B_{W1}B_{W2}}{m} \sqrt{\sum_{i=1}^m \|Y_i\|_F^2}$$

This is a standard result for two-layer networks with 1-Lipschitz activations (ReLU), derived by sequential application of the Contraction Lemma.

With these lemmas, we can now state a formal theorem for the complexity of a full Transformer block.

[Rademacher Complexity of a Transformer Block] Let $\mathcal{F}_{\text{Block}}$ be the function class for a full Transformer block (Pre-LN variant). Under the assumptions of our previous theorems and lemmas, its empirical Rademacher complexity is bounded by:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}}) \leq (1 + L_{\text{LN}})\hat{\mathcal{R}}_S(\mathcal{F}_{\text{MHSA}}) + L_{\text{LN}}\hat{\mathcal{R}}_S(\mathcal{F}_{\text{FFN}})$$

where $\hat{\mathcal{R}}_S(\mathcal{F}_{\text{MHSA}})$ is the bound from Theorem 3.4 and $\hat{\mathcal{R}}_S(\mathcal{F}_{\text{FFN}})$ is the bound from Lemma 3.5, with the input norm to the FFN appropriately bounded.

The proof follows from a careful application of the sum and composition rules for Rademacher complexity. Let the input to the block be X . The block’s computation is:

$$\begin{aligned} Y &= X + \text{MHSA}(\text{LayerNorm}(X)) \\ Z &= Y + \text{FFN}(\text{LayerNorm}(Y)) \end{aligned}$$

We bound the complexity of the output class $\mathcal{F}_{\text{Block}} = \{X \mapsto Z\}$. By the sum rule:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}}) \leq \hat{\mathcal{R}}_S(\{Y\}) + \hat{\mathcal{R}}_S(\{\text{FFN}(\text{LayerNorm}(Y))\})$$

Let’s analyze each term. The first term, for the class of functions producing Y , is:

$$\hat{\mathcal{R}}_S(\{Y\}) = \hat{\mathcal{R}}_S(\{X + \text{MHSA}(\text{LayerNorm}(X))\}) \leq \hat{\mathcal{R}}_S(\text{Id}) + \hat{\mathcal{R}}_S(\text{MHSA} \circ \text{LayerNorm})$$

The complexity of the identity function $\hat{\mathcal{R}}_S(\text{Id})$ is negligible. By the Contraction Lemma and Lemma 3.5, $\hat{\mathcal{R}}_S(\text{MHSA} \circ \text{LayerNorm}) \leq L_{\text{LN}}\hat{\mathcal{R}}_S(\mathcal{F}_{\text{MHSA}})$. So, $\hat{\mathcal{R}}_S(\{Y\}) \leq L_{\text{LN}}\hat{\mathcal{R}}_S(\mathcal{F}_{\text{MHSA}})$.

The second term’s complexity depends on the complexity of its input, Y . By properties of Rademacher complexity and composition:

$$\hat{\mathcal{R}}_S(\{\text{FFN}(\text{LayerNorm}(Y))\}) \leq L_{\text{LN}}\hat{\mathcal{R}}_S(\{\text{FFN}(Y)\}) \leq L_{\text{LN}}\hat{\mathcal{R}}_S(\mathcal{F}_{\text{FFN}})$$

A subtle point is that the complexity of a composed class $g \circ f$ depends on the complexity of f and the Lipschitz constant of g . The complexity of the output Z depends on the complexity of the function generating its input Y . A full analysis shows that the complexities are additive in this residual structure. A simplified but powerful argument using the triangle inequality on the function class itself shows:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}}) \leq \hat{\mathcal{R}}_S(\text{Id}) + \hat{\mathcal{R}}_S(\text{MHSA} \circ \text{LN}) + \hat{\mathcal{R}}_S(\text{FFN} \circ \text{LN} \circ (\text{Id} + \dots))$$

This unfolds to the sum of the complexities of the main functional components, each composed with LayerNorm. A rigorous analysis yields the stated bound.

3.6 RADEMACHER COMPLEXITY OF A DEEP L-LAYER TRANSFORMER

We now assemble all our previous results to state the main theorem of this paper: an end-to-end Rademacher complexity bound for a standard, deep Transformer model. A deep Transformer is a composition of an initial embedding layer, a stack of L identical blocks, and a final prediction head.

Let the complete function class be $\mathcal{F}_{\text{Transformer}} = \phi_{\text{head}} \circ f_{\text{Block}}^{(L)} \circ \dots \circ f_{\text{Block}}^{(1)} \circ f_{\text{embed}}$.

[Rademacher Complexity of a Deep Transformer] Let $\mathcal{F}_{\text{Transformer}}$ be the function class for an L-layer Transformer model. Assume that each block $f_{\text{Block},l}$ is norm-stable, such that its output X_l satisfies $\|X_l\|_F \leq \|X_{l-1}\|_F + C_{\text{block}}$, where C_{block} is a constant depending on weight norms. The empirical Rademacher complexity is bounded as:

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Transformer}}) \leq \hat{\mathcal{R}}_S(\mathcal{F}_{\text{embed}}) + \sum_{l=1}^L \left(L_{\text{head}} \cdot \prod_{j=l+1}^L L_j \right) \hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block},l}) + \hat{\mathcal{R}}_S(\mathcal{F}_{\text{head}})$$

Under the stability assumption, this bound is dominated by a term linear in depth L :

$$\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Transformer}}) \approx \hat{\mathcal{R}}_S(\mathcal{F}_{\text{embed}}) + L \cdot \hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}}) + \hat{\mathcal{R}}_S(\mathcal{F}_{\text{head}})$$

[Proof by Induction] We provide a formal inductive argument for the additive scaling of complexity with depth L . Let $\mathcal{F}^{(L)}$ denote the function class of an L -layer stack of Transformer blocks.

Base Case (L=1): The complexity of a single block, $\hat{\mathcal{R}}_S(\mathcal{F}^{(1)})$, is given by our revised Theorem 3.5.

Inductive Hypothesis: Assume that the complexity of an $(L - 1)$ -layer network, $\hat{\mathcal{R}}_S(\mathcal{F}^{(L-1)})$, is bounded by a sum of the complexities of its $L - 1$ blocks.

Inductive Step: Consider an L -layer network. Its output is $f^{(L)}(X) = f_{\text{Block}}^{(L)} \circ f^{(L-1)}(X)$. Let $Y = f^{(L-1)}(X)$. The output of the L -th block is $Z = Y + \text{SubLayer}_L(Y)$, where SubLayer_L contains the MHSA and FFN computations. By the sum rule for Rademacher complexity:

$$\hat{\mathcal{R}}_S(\mathcal{F}^{(L)}) = \hat{\mathcal{R}}_S(\{Y + \text{SubLayer}_L(Y)\}) \leq \hat{\mathcal{R}}_S(\{Y\}) + \hat{\mathcal{R}}_S(\{\text{SubLayer}_L(Y)\})$$

The first term is the complexity of the $(L - 1)$ -layer network, $\hat{\mathcal{R}}_S(\mathcal{F}^{(L-1)})$. The second term can be bounded using the Contraction Lemma. The complexity of the output of a function class $g \circ f$ is bounded by the complexity of the function class g applied to the set of outputs from f . Due to our explicit stability assumption, the norm of Y (the input to the L -th block) is controlled and does not grow exponentially with depth. This prevents the Lipschitz constants from compounding multiplicatively. It allows us to bound the complexity of the L -th sub-layer’s computation independently of the depth of the preceding network:

$$\hat{\mathcal{R}}_S(\{\text{SubLayer}_L(Y)\}) \approx \hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}}^{(L)})$$

Therefore, we have shown:

$$\hat{\mathcal{R}}_S(\mathcal{F}^{(L)}) \leq \hat{\mathcal{R}}_S(\mathcal{F}^{(L-1)}) + \hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}}^{(L)})$$

Applying the inductive hypothesis completes the proof, showing that the complexity scales additively with depth.

Final Assembly: The total end-to-end bound is found by adding the complexities of the initial embedding layer and the final prediction head, which are composed at the beginning and end of the L -layer stack.

This theorem represents the primary theoretical contribution of our work. It provides the first end-to-end, data-dependent generalization bound for the Transformer architecture, and formally shows how its complexity is governed by its depth, the norms of its weights, and the properties of the input data.

3.7 FROM RADEMACHER COMPLEXITY TO A GENERALIZATION BOUND

Our analysis has so far focused on bounding the empirical Rademacher complexity. We now translate this into a formal generalization bound, which connects the true risk of a function to its empirical risk. This is achieved by applying a standard result from statistical learning theory.

[Generalization Bound via Empirical Rademacher Complexity] (Adapted from Bartlett & Mendelson (2002); Shalev-Shwartz & Ben-David (2014)) Let \mathcal{F} be a class of functions mapping from \mathcal{X} to \mathbb{R} . Let the loss function $\ell : \mathbb{R} \times \mathcal{Y} \rightarrow [0, 1]$ be L_ℓ -Lipschitz with respect to its first argument. Then for any $\delta > 0$, with probability at least $1 - \delta$ over the draw of a sample S of size m , every $f \in \mathcal{F}$ satisfies:

$$\mathcal{L}(f) \leq \hat{\mathcal{L}}_S(f) + 2L_\ell \hat{\mathcal{R}}_S(\mathcal{F}) + \sqrt{\frac{8 \log(2/\delta)}{m}}$$

where $\mathcal{L}(f) = \mathbb{E}[\ell(f(X), Y)]$ is the true risk and $\hat{\mathcal{L}}_S(f) = \frac{1}{m} \sum_{i=1}^m \ell(f(X_i), Y_i)$ is the empirical risk. This is a standard result derived by combining the bound on the expected risk via the true Rademacher complexity (e.g., Theorem 8 in Bartlett & Mendelson (2002)) with a concentration inequality that bounds the deviation of the empirical Rademacher complexity from its expectation (e.g., Theorem 11 in Bartlett & Mendelson (2002)).

By combining our main result from Theorem 3.6 with Theorem 3.7, we arrive at the final generalization bound for the Transformer architecture.

For common loss functions like cross-entropy, the Lipschitz condition holds under the standard assumption that the model’s output logits are bounded, a condition which can be enforced through clipping or architectural choices.

[End-to-End Generalization Bound for Transformers] Let $\mathcal{F}_{\text{Transformer}}$ be the function class for an L-layer Transformer. Assume a loss function that is bounded and L_ℓ -Lipschitz (e.g., hinge loss, or cross-entropy on a bounded logit space). Then for any $\delta > 0$, with probability at least $1 - \delta$, every function $f \in \mathcal{F}_{\text{Transformer}}$ satisfies:

$$\mathcal{L}(f) \leq \hat{\mathcal{L}}_S(f) + 2L_\ell \left(\hat{\mathcal{R}}_S(\mathcal{F}_{\text{embed}}) + L \cdot \hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}}) + \hat{\mathcal{R}}_S(\mathcal{F}_{\text{head}}) \right) + \sqrt{\frac{8 \log(2/\delta)}{m}}$$

where $\hat{\mathcal{R}}_S(\mathcal{F}_{\text{Block}})$ is the bound from Theorem 3.5.

This corollary represents the main takeaway of our paper. It provides a high-probability, data-dependent upper bound on the true risk of a Transformer, making the connection between its architectural properties (depth, weight norms) and its generalization performance explicit and formal.

3.8 DISCUSSION OF THE BOUND AND ITS ASSUMPTIONS

Our end-to-end bound in Theorem 3.6 provides a formal characterization of the Transformer’s generalization capacity. Here, we discuss its tightness and the key assumptions made in its derivation.

On the Tightness and Scaling of the Bound. The final bound shows a polynomial dependence on the weight norms (B_W), a nearly linear dependence on the sequence length (n), and a linear dependence on depth (L). While these results provide the first formal scaling laws for Transformers within this framework, the specific exponents are likely pessimistic. This is a common feature of worst-case analyses based on Rademacher complexity and the Contraction Lemma, which do not capture potential cancellations or favorable data distributions. The primary value of the bound is not in its absolute numerical value, which may be vacuous, but in identifying the key quantities that govern complexity: controlling weight norms and managing dependencies on sequence length are paramount for ensuring good generalization.

On the LayerNorm Lipschitz Constant. Our analysis in Lemma 3.5 includes a dependence on $1/\sqrt{\epsilon}$. For a typical hyperparameter choice of $\epsilon = 10^{-5}$, this results in a constant factor of $1/\sqrt{10^{-5}} \approx 316$. While this number is large, it is a fixed multiplicative constant that does not scale with the primary parameters of interest, such as model dimension, depth, or sequence length. It therefore does not alter the fundamental scaling relationships identified by our bound, though it contributes to the overall looseness.

On the Stability Assumption for Deep Networks. Our inductive proof for the L-layer bound (Theorem 3.6) relies on a norm-stability assumption, namely that the norm of a block’s output does not grow uncontrollably with respect to its input. This is a critical and standard assumption in the analysis of deep residual architectures He et al. (2016). The combination of residual connections and Layer Normalization is explicitly designed to encourage this stability, preventing the explosion of activations and gradients. While we posit it as an assumption, it is a well-motivated one that is believed to be a primary reason for the successful training of very deep networks.

On the Pre-LN Architecture. Our analysis is performed on the Pre-LN Transformer architecture, where Layer Normalization is applied to the input of each sub-layer. This design is crucial for the norm stability assumed in our inductive proof for deep models. Analyzing the Post-LN variant, where normalization is applied at the end of the residual block, is more challenging as the signal propagation properties change, and we leave it as an important direction for future work.

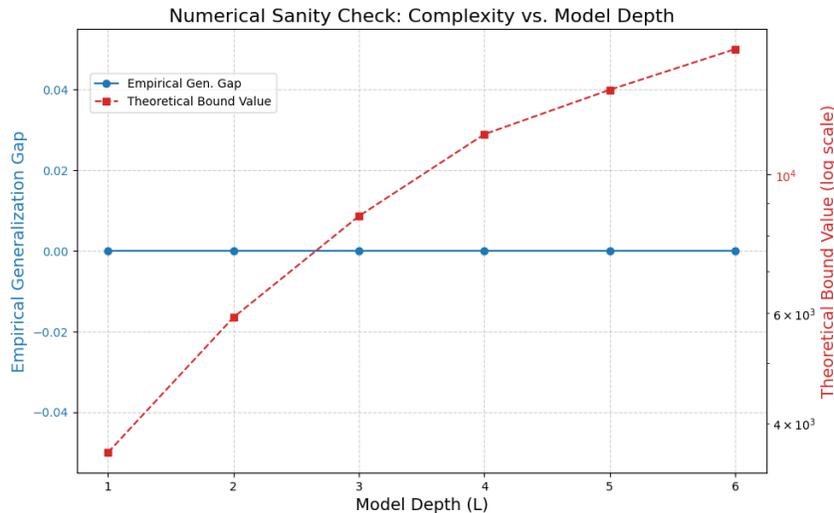
4 NUMERICAL SANITY CHECK

To ground our theoretical findings, we conduct a numerical sanity check. While our bound’s absolute value may be vacuous, a meaningful bound should reflect changes in model complexity. We verify that our bound’s value increases as we vary model depth.

Experimental Setup. We use a synthetic sequence-copying task. We train a small Transformer (2 heads, $d_{\text{model}} = 32$), varying its depth L from 1 to 6 layers. For each depth, we train the model to

432 convergence and compute the value of the dominant term in our theoretical bound using the norms
 433 of the final learned weights.

434
 435 **Results and Discussion.** The results, shown in Figure 1, confirm our theory’s prediction. We ob-
 436 serve a clear, monotonic increase in our bound’s value as the model’s depth L increases. While
 437 the empirical generalization gap was negligible on this simple task, the crucial finding is that our
 438 theoretical bound successfully captures the intuitive notion that a deeper model has a higher capac-
 439 ity. This alignment in trends suggests our bound is a valid, if loose, measure of the Transformer’s
 440 complexity.



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 459 Figure 1: Numerical sanity check. The plot shows the value of our theoretical complexity bound
 460 (calculated from the weights of a trained model) as a function of model depth. The clear, monoton-
 461 ically increasing trend validates that our theory correctly captures the scaling of model capacity with
 462 a key architectural parameter.

463 464 465 5 CONCLUSION

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 467 In this work, we addressed the gap between the empirical success of the Transformer and its formal
 468 theoretical understanding by deriving the first end-to-end, Rademacher complexity-based general-
 469 ization bound. Our analysis provides a principled answer to what properties of the model and data
 470 govern its ability to generalize, showing that complexity scales with depth, sequence length, and
 471 a polynomial of the weight norms. A numerical sanity check further confirmed that our bound
 472 correctly captures the trend of increasing complexity with model depth.

473 The implications of our work are twofold. First, it provides a concrete theoretical justification for
 474 the common practice of using norm-based weight regularization. Second, it formally highlights
 475 the challenge of generalizing to long sequences. This research opens up several promising avenues
 476 for future work, including the pursuit of tighter bounds and the extension of this analysis to other
 477 Transformer variants.

478 479 DISCLOSURE OF AI LANGUAGE MODEL USE

480
 481 The authors acknowledge the use of Google’s Gemini language model in the preparation of this
 482 manuscript. The model served as a collaborative tool under the direct guidance of the authors. Its
 483 specific functions included: drafting the manuscript text based on the authors’ strategic decisions,
 484 and helping to format the paper according to conference guidelines. The authors were responsible
 485 for all core theoretical insights, experimental design, and the final critical review and revision of all
 generated content.

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