Generalization bound for a Shallow Transformer trained using Gradient Descent

Anonymous authors Paper under double-blind review

Abstract

In this work, we establish a **norm-based generalization bound** for a *shallow Transformer model* trained via gradient descent under the *bounded-drift* (*lazy training*) regime, where model parameters remain close to their initialization throughout training. Our analysis proceeds in three stages: (a) we formally define a hypothesis class of Transformer models constrained to remain within a small neighborhood of their initialization; (b) we derive an **upper bound on the Rademacher complexity** of this class, quantifying its effective capacity; and (c) we establish an **upper bound on the empirical loss** achieved by gradient descent under suitable assumptions on model width, learning rate, and data structure. Combining these results, we obtain a **high-probability bound on the true loss** that decays sublinearly with the number of training samples N and depends explicitly on model and data parameters. The resulting bound demonstrates that, in the lazy regime, wide and shallow Transformers generalize similarly to their linearized (NTK) counterparts. Empirical evaluations on both text and image datasets support the theoretical findings.

1 Introduction

The deep learning community has achieved outstanding performance on language and vision tasks which were once considered very complex for neural network models. Transformers have played a central role in the development of highly impressive conversational large language models (LLMs) like GPT-4 (Achiam et al., 2023), LLaMA (Touvron et al., 2023) and Gemini (Team et al., 2023). Vision transformers (Dosovitskiy et al., 2020) have similarly achieved outstanding results in image generation and classification. This tremendous success of transformer models has led to anticipation of early Artificial General Intelligence (AGI). However, theoretical understanding of transformer models is still limited. It is very crucial to develop mathematical theorems which give some guarantees on the generalization abilities of transformers and other modern neural network architectures.

Various generalization bounds have been proposed for transformer models (Edelman et al., 2021; Trauger & Tewari, 2024; Fu et al., 2024). The researchers compute an upper bound on the difference between the true loss and the empirical loss i.e., $[\mathcal{L}_{\mathcal{D}}(f) - \mathcal{L}_{\mathcal{S}}(f)]$ for all $f \in \mathcal{F}$ where \mathcal{F} is some class of transformer models. With this kind of bound, if we wish to analyze the model's true loss $\mathcal{L}_{\mathcal{D}}(f)$, we need to first perform training and obtain the final empirical loss $\mathcal{L}_{\mathcal{S}}(f)$. In another approach of presenting generalization bounds, researchers directly upper bound the true loss $\mathcal{L}_{\mathcal{D}}(f)$. With this type of bound, we can analyze the model's true loss without having to first obtain the empirical loss $\mathcal{L}_{\mathcal{S}}(f)$ through training. Arora et al. (2019) and Cao & Gu (2019) presented an upper bound on the true loss $\mathcal{L}_{\mathcal{D}}(f)$ for a 2-layer fully connected ReLU neural network and a deep L-layer fully connected neural network respectively. In this work, we extend this approach of directly upper bounding the true loss to transformer models.

We develop a generalization bound for a class of transformers whose weights remain very close to their initialization during training. In other-words, we assume that the difference between the transformer's weights at any training step and the transformer's weights at initialization is bounded. This is mostly true especially in modern networks which are considered to be highly over-parameterized i.e., having significantly more number of parameters than number of training examples required to generalize well. After defining this class of transformer models, we then proceed to compute an upper bound on the Rademacher complexity for the above defined class of transformer models. Constructing this upper bound on the Rademacher complexity involves employing the concept of covering numbers. Lastly we

utilize the convergence theorem proposed by Wu et al. (2024) to derive an upper bound on the empirical loss for all transformer models belonging to the class defined above.

Specifically, our main contribution is developing an upper bound on the true loss for a class of transformer models whose weights remain close to their initialization during training. We find that this bound tightens sublinearly with increasing number of training examples N for all values of model dimension d_m .

2 Related Work

Researchers have developed several generalization bounds for neural networks (Bartlett et al., 2017; Neyshabur et al., 2015; 2017; 2018; Pitas et al., 2018; Golowich et al., 2017; Li et al., 2018; Arora et al., 2018; Dziugaite & Roy, 2017; Zhou et al., 2018a; Chen et al., 2019; Long & Sedghi, 2019). Norm-based generalization bounds have also been developed for transformer models. Edelman et al. (2021) derived a norm-based generalization bound for transformers which scales logarithmically with sequence length of the input. Trauger & Tewari (2024) also presented another bound for transformers which is independent of the sequence length of the input. All these results involve computing an upper bound on the difference between true loss and empirical loss i.e., $[\mathcal{L}_{\mathcal{D}}(f) - \mathcal{L}_{S}(f)]$ for all $f \in \mathcal{F}$. As mentioned earlier, this means that in order to study the true loss of the neural network, training must first be completed to obtain the final $\mathcal{L}_{S}(f)$.

In another direction of computing generalization bounds, researchers directly upper-bound the true loss $\mathcal{L}_{\mathcal{D}}(f)$ for all $f \in \mathcal{F}$. This requires analysis of the convergence of the neural network optimization in order to obtain a bound on empirical loss $\mathcal{L}_S(f)$ which is then used to get the final bound on $\mathcal{L}_D(f)$. Once we have the final bound using this approach, we can directly analyze the true loss of the neural network without the need to first obtain empirical loss through training. Following this direction, Arora et al. (2019) presented a generalization bound for an over-parameterized two-layer ReLU fully connected neural network trained using gradient descent. In the overparameterization regime, the infinite-width neural tangent kernel (NTK) matrix was crucial in developing the bound. Cao & Gu (2019) also proposed a generalization bound for an over-parameterized deep L-layer fully connected neural network. The authors utilize Neural Tangent Random Features (NTRF) to develop this generalization bound. This second direction for computing generalization bounds by directly upper bounding the true loss $\mathcal{L}_{\mathcal{D}}(f)$ for all $f \in \mathcal{F}$ has not been explored for transformer models. Our paper focuses on closing this gap. In order to incorporate the training dynamics, we rely on the global convergence theorem of a shallow transformer presented by Wu et al. (2024). Other results on the convergence of transformers have also been proposed (Kohler & Krzyzak, 2023; Huang et al., 2024; Shen et al., 2024; Gurevych et al., 2022). It is important to note that our transformer generalization bound can not be directly compared to to the transformer generalization bounds proposed by Edelman et al. (2021) and Trauger & Tewari (2024). This is because their bound is on the difference between true loss and empirical loss i.e., $[\mathcal{L}_{\mathcal{D}}(f) - \mathcal{L}_{S}(f)]$ for all $f \in \mathcal{F}$ while our bound is on the true loss i.e., $\mathcal{L}_{\mathcal{D}}(f)$ for all $f \in \mathcal{F}$.

Beyond norm-based bounds: PAC-Bayes and stability perspectives. In addition to norm-based transformer bounds (Edelman et al., 2021; Trauger & Tewari, 2024), recent work has leveraged *PAC-Bayes/compression* and *algorithmic stability* frameworks to obtain guarantees that are directly relevant for Transformer and LLM settings. On the PAC-Bayes side, compression-based analyses yield non-vacuous bounds for pretrained large language models by explicitly relating generalization to compressibility under suitable priors/posteriors and prediction smoothing (Lotfi et al., 2023). More broadly, PAC-Bayes methods have been refined to produce tight bounds at scale through model compression and related parameterizations (Zhou et al., 2018b). On the stability side, Li et al. (2023) study in-context learning through the lens of multitask algorithmic stability and derive generalization bounds for attention/transformer architectures; complementary stability-style results for attention also appear in recent analyses of fine-tuning and self-attention dynamics (Yao et al., 2025; Deora, 2024; Deora et al., 2023). Conceptually, these frameworks bound the generalization gap via posterior complexity or stability coefficients, whereas our analysis (Theorem 5) *directly upper-bounds the true loss* by combining an empirical-loss bound (derived from an optimization convergence result for shallow Transformers) with a capacity term, thus tying generalization to lazy-regime training dynamics and initialization-dependent conditioning.

3 Preliminaries

3.1 Problem Setup

3.1.1 Training Examples

We are given N training examples $S = \{(\boldsymbol{X}_n, y_n)\}_{n=1}^N$ where $\{\boldsymbol{X}_n\}_{n=1}^N \in \mathbb{R}^{N \times d_s \times d}$ are the instances and $\boldsymbol{y} \triangleq \{y_n\}_{n=1}^N \in \mathbb{R}^N$ are the labels. d_s is the sequence length of the inputs and d is the input dimension.

3.1.2 Model

The model used in this work is a popular transformer encoder which is also used by Wu et al. (2024). Given an input $X \in \mathbb{R}^{d_s \times d}$, we define each of the transformer layers.

Self-attention layer

The self-attention layer is defined as follows;

$$oldsymbol{A}_1 riangleq \sigma_s \left(rac{(oldsymbol{X} oldsymbol{W}_Q^{\mathsf{T}})(oldsymbol{X} oldsymbol{W}_K^{\mathsf{T}})^{\mathsf{T}}}{\sqrt{d_m}}
ight) (oldsymbol{X} oldsymbol{W}_V^{\mathsf{T}})$$

where σ_s is the row-wise softmax, $W_Q, W_K, W_V \in \mathbb{R}^{d_m \times d}$ are the query, key and value matrices in the self-attention layer. d_m is the model dimension. We shall be interested in the effect of the self-attention layer on each row $X^{(i,:)}$ of the input X where $i \in [d_s]$. We therefore define β_i as the i-th row of the softmax output;

$$\beta_i = \sigma_s \left(\frac{\boldsymbol{X}^{(i,:)} \boldsymbol{W}_Q^{\mathrm{T}} \boldsymbol{W}_K \boldsymbol{X}^{\mathrm{T}}}{\sqrt{d_m}} \right)^{\mathrm{T}} = \sigma_s \left(\frac{\boldsymbol{X} \boldsymbol{W}_K^{\mathrm{T}} \boldsymbol{W}_Q (\boldsymbol{X}^{(i,:)})^{\mathrm{T}}}{\sqrt{d_m}} \right)$$

We also define z_i as the final output of the self-attention layer for each row $X^{(i,:)}$;

$$\boldsymbol{z}_i = (\boldsymbol{X} \boldsymbol{W}_V^{\mathsf{T}})^{\mathsf{T}} \beta_i = \boldsymbol{W}_V \boldsymbol{X}^{\mathsf{T}} \sigma_s \left(\frac{\boldsymbol{X} \boldsymbol{W}_K^{\mathsf{T}} \boldsymbol{W}_Q (\boldsymbol{X}^{(i,:)})^{\mathsf{T}}}{\sqrt{d_m}} \right)$$

Feed -forward ReLU layer

The layer with ReLU activation function is defined as follows;

$$A_2 \triangleq \sigma_r(A_1W_H)$$

where σ_r is the ReLU activation function. For ease of calculations, W_H is set as $W_H = I \in \mathbb{R}^{d_m \times d_m}$ Once again, define k_i as the final output of the Feed -forward ReLU layer for each row $X^{(i,:)}$;

$$\boldsymbol{k}_i = \sigma_r(\boldsymbol{z}_i) = \sigma_r \left(\boldsymbol{W}_V \boldsymbol{X}^{\text{T}} \sigma_s \left(\frac{\boldsymbol{X} \boldsymbol{W}_K^{\text{T}} \boldsymbol{W}_Q(\boldsymbol{X}^{(i,:)})^{\text{T}}}{\sqrt{d_{rn}}} \right) \right)$$

Average Pooling layer

The pooling is applied column-wise to reduce sequence length dimension from d_s to 1. This is done to ensure a scalar output from our transformer.

$$a_3 \triangleq \varphi(A_2)$$

where φ represents the column-wise average pooling. We can also define a_3 in terms of each k_i ;

$$oldsymbol{f}_{pre} = rac{1}{d_s} \sum_{i=1}^{d_s} oldsymbol{k}_i = rac{1}{d_s} \sum_{i=1}^{d_s} \sigma_r \left(oldsymbol{W}_V oldsymbol{X}^{\mathsf{T}} \sigma_s \left(rac{oldsymbol{X} oldsymbol{W}_K^{\mathsf{T}} oldsymbol{W}_Q (oldsymbol{X}^{(i,:)})^{\mathsf{T}}}{\sqrt{d_m}}
ight)
ight)$$

Output layer

The final output layer is defined as follows;

$$f(\boldsymbol{X}) \triangleq \boldsymbol{w}_O^{\mathrm{T}} \boldsymbol{f}_{pre}$$

where $w_O \in \mathbb{R}^{d_m}$ is the weight vector in the output layer. We can as well define the final model output f(X) in terms of each row $X^{(i,:)}$ of the input X;

$$f(\boldsymbol{X}) = \frac{1}{d_s} \boldsymbol{w}_O^\mathsf{T} \sum_{i=1}^{d_s} \sigma_r \left(\boldsymbol{W}_V \boldsymbol{X}^\mathsf{T} \sigma_s \left(\frac{\boldsymbol{X} \boldsymbol{W}_K^\mathsf{T} \boldsymbol{W}_Q (\boldsymbol{X}^{(i,:)})^\mathsf{T}}{\sqrt{d_m}} \right) \right)$$

Define θ as a vector representing the union of all parameters of the transformer model as shown below;

$$\boldsymbol{\theta} = \{\boldsymbol{W}_O, \boldsymbol{W}_K, \boldsymbol{W}_V, \boldsymbol{w}_O\}$$

When we pass a single input $\boldsymbol{X} \in \mathbb{R}^{d_s \times d}$ to the model, the output is given as $f(\boldsymbol{X}) \in \mathbb{R}$. When we give all inputs to the model as a batch $\{\boldsymbol{X}_n\}_{i=1}^N \in \mathbb{R}^{N \times d_s \times d}$, the output of the model will be $\boldsymbol{f} \triangleq \{f(\boldsymbol{X}_n)\}_{n=1}^N \in \mathbb{R}^N$ and output of the last hidden layer will be $\boldsymbol{F}_{pre} \triangleq \{\boldsymbol{f}_{pre}(\boldsymbol{X}_n)\}_{n=1}^N \in \mathbb{R}^{N \times d_m}$.

3.1.3 Initialization

Similar to Wu et al. (2024) we use the LeCun initialization described below. The parameters $\boldsymbol{W}_Q, \boldsymbol{W}_K, \boldsymbol{W}_V$ are initialized as $\boldsymbol{W}_Q^{(ij)} \sim \mathcal{N}(0, \frac{1}{d}), \ \boldsymbol{W}_K^{(ij)} \sim \mathcal{N}(0, \frac{1}{d}), \ \boldsymbol{W}_V^{(ij)} \sim \mathcal{N}(0, \frac{1}{d})$ for $i \in [d_m]$ and $j \in [d]$ while $\boldsymbol{w}_O^{(i)}$ is initialized as $\boldsymbol{w}_O^{(i)} \sim \mathcal{N}(0, \frac{1}{d_m})$ for $i \in [d_m]$.

3.1.4 Empirical Loss

We consider any loss function $\ell(f(X_n), y_n)$ which is 1-Lipschitz in the first argument;

$$\mathcal{L}_S(f) = \frac{1}{N} \sum_{n=1}^N \ell(f(\boldsymbol{X}_n), y_n)$$

This empirical loss is to be optimized using Gradient Descent algorithm shown below;

Input: data $(\boldsymbol{X}_n, y_n)_{n=1}^N$, step size γ Initialize weights as follows: $\boldsymbol{\theta}^0 := \{\boldsymbol{W}_Q^0, \boldsymbol{W}_K^0, \boldsymbol{W}_V^0, \boldsymbol{w}_O^0\}$ for t=0 to t'-1 do $\boldsymbol{W}_Q^{t+1} = \boldsymbol{W}_Q^t - \gamma \cdot \nabla_{\boldsymbol{W}_Q} \ell(\boldsymbol{\theta}^t)$ $\boldsymbol{W}_K^{t+1} = \boldsymbol{W}_K^t - \gamma \cdot \nabla_{\boldsymbol{W}_K} \ell(\boldsymbol{\theta}^t)$ $\boldsymbol{W}_V^{t+1} = \boldsymbol{W}_V^t - \gamma \cdot \nabla_{\boldsymbol{W}_V} \ell(\boldsymbol{\theta}^t)$ $\boldsymbol{W}_O^{t+1} = \boldsymbol{w}_O^t - \gamma \cdot \nabla_{\boldsymbol{W}_O} \ell(\boldsymbol{\theta}^t)$ end for Output: the model based on $\boldsymbol{\theta}^{t'}$.

3.1.5 True Loss

We are interested in upper bounding the true loss defined as follows;

$$\mathcal{L}_{\mathcal{D}}(f) = \mathbb{E}_{(\boldsymbol{X},y) \sim \mathcal{D}}[\ell(f(\boldsymbol{X}),y)]$$

3.2 Rademacher complexity

The theorem of Rademacher complexity is widely used to compute generalization bounds for machine learning models. As per Mohri et al. (2012) theorem 3.1 and Arora et al. (2019) theorem B.1, suppose that the loss function $\ell(\cdot, \cdot)$

is bounded in [0,c] and is ρ -Lipschitz in the first argument. Then with probability at least $1-\delta$ over the sample $S=\{(\boldsymbol{X}_n,y_n)\}_{n=1}^N$ of size N:

$$\sup_{f \in \mathcal{F}} \{ \mathcal{L}_{\mathcal{D}}(f) - \mathcal{L}_{S}(f) \} \le 2\rho \mathcal{R}_{S}(\mathcal{F}) + 3c\sqrt{\frac{\log(2/\delta)}{2N}}$$

where $\mathcal{L}_{\mathcal{D}}(f)$ is the true loss, $\mathcal{L}_{S}(f)$ is the empirical loss and $\mathcal{R}_{S}(\mathcal{F})$ is the empirical Rademacher complexity of a function class \mathcal{F} for samples $S = \{(\boldsymbol{X}_{n}, y_{n})\}_{n=1}^{N}$ of size N defined as follows;

$$\mathcal{R}_{S}(\mathcal{F}) = \frac{1}{N} \mathbb{E}_{\epsilon \sim \text{unif}(\{1, -1\})} \left[\sup_{f \in \mathcal{F}} \sum_{n=1}^{N} \epsilon_{n} f(\boldsymbol{X}_{n}) \right]$$

In order to construct our generalization bound, we shall upper bound both the Rademacher complexity $\mathcal{R}_S(\mathcal{F})$ and the training loss $\mathcal{L}_S(f)$ for all $f \in \mathcal{F}$.

3.3 Covering number bound

For a given class \mathcal{F} , the covering number $\mathcal{N}_{\infty}(\mathcal{F}; \epsilon; \{\boldsymbol{X}_n\}_{n=1}^N; \|\cdot\|_2)$ is the smallest size of a collection (a cover) $\mathcal{C} \subset \mathcal{F}$ such that $\forall f \in \mathcal{F}, \exists \hat{f} \in \mathcal{C}$ satisfying $\max_n \|f(\boldsymbol{X}_n) - \hat{f}(\boldsymbol{X}_n)\|_2 \leq \epsilon$.

The Rademacher complexity of the class \mathcal{F} with respect to samples $S = \{(\boldsymbol{X}_n, y_n)\}_{n=1}^N$ can be upper bounded using the covering number of \mathcal{F} (Edelman et al., 2021);

$$\mathcal{R}_{S}(\mathcal{F}) \leq c \cdot \inf_{\delta \geq 0} \left(\delta + \int_{\delta}^{A} \sqrt{\frac{\log \mathcal{N}_{\infty}(\mathcal{F}; \epsilon; \{\boldsymbol{X}_{n}\}_{n=1}^{N}; \|\cdot\|_{2})}{N}} d\epsilon \right)$$

for some constant c > 0 and $|f| \le A$ for all $f \in \mathcal{F}$.

4 Results

In this section, we develop a theoretical framework to analyze the generalization properties of Transformer models whose parameters remain close to their initialization during training. We begin by formally defining a class of models that satisfy this bounded-drift property, which corresponds to the *lazy training regime*. We then derive an upper bound on the Rademacher complexity of this class, followed by an upper bound on the empirical loss using convergence guarantees under gradient descent. Combining these results, we present our main theorem that establishes a high-probability bound on the true loss. Finally, we discuss the scope and limitations of our findings in light of existing results, and conclude with key insights and directions for future work.

For ease of proof, and without loss of generality, let us set the input feature dimension d to be equal to the model dimension d_m i.e., $d = d_m$.

4.1 Defining a class of Transformer models whose weights stay close to their initialization

To rigorously analyze the generalization behavior of Transformers, we first need to formalize the notion of models whose parameters remain close to their initialization throughout training. This assumption (often referred to as the bounded-drift assumption) characterizes the lazy training regime, where model updates are small, and the network operates in a nearly linear regime around initialization. In this subsection, we define the parameter space and construct a hypothesis class of Transformer models confined within a ball of radius R centered at the initialization point. This setup enables the derivation of subsequent complexity and loss bounds under analytically tractable conditions.

Recall that we defined θ as a vector representing the union of all parameters of the transformer model as shown below;

$$\boldsymbol{\theta} = \{ \boldsymbol{W}_Q, \boldsymbol{W}_K, \boldsymbol{W}_V, \boldsymbol{w}_O \}$$

The squared ℓ_2 -norm of the parameter vector can be expressed as the sum of the squared Frobenius norms (for matrices) and squared ℓ_2 -norms (for vectors);

$$\|m{\theta}\|_2^2 = \|m{W}_Q\|_F^2 + \|m{W}_K\|_F^2 + \|m{W}_V\|_F^2 + \|m{w}_O\|_2^2$$

We can therefore say that for all training steps t > 0;

$$\begin{split} \|\boldsymbol{\theta}^{t+1} - \boldsymbol{\theta}^{0}\|_{2}^{2} &= \|\boldsymbol{W}_{Q}^{t+1} - \boldsymbol{W}_{Q}^{0}\|_{F}^{2} + \|\boldsymbol{W}_{K}^{t+1} - \boldsymbol{W}_{K}^{0}\|_{F}^{2} \\ &+ \|\boldsymbol{W}_{V}^{t+1} - \boldsymbol{W}_{V}^{0}\|_{F}^{2} + \|\boldsymbol{w}_{O}^{t+1} - \boldsymbol{w}_{O}^{0}\|_{2}^{2} \\ &\leq R_{O}^{2} + R_{K}^{2} + R_{V}^{2} + R_{O}^{2} \end{split}$$

where $\| \boldsymbol{W}_{Q}^{t+1} - \boldsymbol{W}_{Q}^{0} \|_{F} \le R_{Q}, \| \boldsymbol{W}_{K}^{t+1} - \boldsymbol{W}_{K}^{0} \|_{F} \le R_{K}, \| \boldsymbol{W}_{V}^{t+1} - \boldsymbol{W}_{V}^{0} \|_{F} \le R_{V}, \| \boldsymbol{w}_{O}^{t+1} - \boldsymbol{w}_{O}^{0} \|_{2} \le R_{O}$ for some positive constants $R_{O}, R_{V}, R_{Q}, R_{K}$

Setting $R = \sqrt{R_Q^2 + R_K^2 + R_V^2 + R_O^2}$, we end up with;

$$\|\boldsymbol{\theta}^{t+1} - \boldsymbol{\theta}^0\|_2 < R$$

Let us now define our hypothesis class $\mathcal{F}_R^{\theta^0}$ comprised of the transformer models whose parameters θ stay in a ball close to θ^0 for all training steps t > 0;

$$\mathcal{F}_{R}^{\boldsymbol{\theta}^{0}} = \left\{ f_{\boldsymbol{\theta}}(\boldsymbol{X}_{n}) : \forall t > 0, \|\boldsymbol{\theta}^{t+1} - \boldsymbol{\theta}^{0}\|_{2} \leq R \right\}$$

4.2 Upper bounding the Rademacher complexity

To establish a generalization bound, we must first control the capacity of the hypothesis class of models under consideration. The Rademacher complexity provides a data-dependent measure of this capacity, quantifying how well the model class can fit random noise. In this subsection, we derive an upper bound on the Rademacher complexity of the bounded-drift Transformer class defined above. Our result shows that under reasonable assumptions on the input features and parameter norms, the Rademacher complexity scales as $\mathcal{O}\left(\sqrt{\frac{P}{N}}\log(A\sqrt{\frac{N}{P}})\right)$, indicating that generalization improves with an increasing number of samples and controlled parameter magnitudes. This bound parallels similar results for shallow transformer and provides the foundation for our overall generalization analysis.

The following lemma gives an upper bound on the Rademacher complexity of our class of transformer models i.e., an upper bound on $\mathcal{R}_S(\mathcal{F}_R^{\theta^0})$.

Lemma 1. Suppose that we have $\eta_V = \|\mathbf{W}_V^0\|_F + R_V$, $\eta_O = \|\mathbf{w}_O^0\|_2 + R_O$, $\eta_K = \|\mathbf{W}_K^0\|_F + R_K$, $\eta_Q = \|\mathbf{W}_Q^0\|_F + R_Q$ where R_O , R_V , R_K , R_Q remain as defined above. Also assume that the inputs have full rank and are bounded as $\|\mathbf{X}_n\|_F \leq \sqrt{d_s}R_X$ for all $n \in [N]$ where R_X is some positive constant. The empirical Rademacher complexity of the class of Transformer models $\mathcal{F}_R^{\boldsymbol{\theta}^0} = \{f_{\boldsymbol{\theta}}(\mathbf{X}_n) : \forall t > 0, \|\boldsymbol{\theta}^{t+1} - \boldsymbol{\theta}^0\|_2 \leq R\}$ given $\boldsymbol{\theta} = \{\mathbf{W}_Q, \mathbf{W}_K, \mathbf{W}_V, \mathbf{w}_O\}$ can be upper bounded as follows;

$$\mathcal{R}_S(\mathcal{F}_R^{\boldsymbol{\theta}^0}) \lesssim \mathcal{O}\left(\frac{1}{N}\sqrt{\frac{P}{N}}\left(1 + \log\left(A\sqrt{\frac{N}{P}}\right)\right)\right)$$

where \lesssim hides logarithmic dependencies on quantities besides N and d_s , $A = \eta_O \eta_V(\sqrt{d_s}R_X)$ and $P = (\sqrt{d_s}R_X)^2 \left(\left(\sqrt{d_m}\eta_V\right)^{\frac{2}{3}} + \left(\sqrt{d_m}\eta_K\eta_Q\eta_V\right)^{\frac{2}{3}}\right)^3 \log(Nd_s)$

Proof of lemma 1

Define the following quantities for simplicity $\eta_V = \| \boldsymbol{W}_V^0 \|_F + R_V, \eta_O = \| \boldsymbol{w}_O^0 \|_2 + R_O, \eta_K = \| \boldsymbol{W}_K^0 \|_F + R_K, \eta_Q = \| \boldsymbol{W}_Q^0 \|_F + R_Q$ where R_O, R_V, R_K, R_Q remain as defined above in section 4.1.

Our class of interest in section 4.1 was $\mathcal{F}_R^{\theta^0} = \{f_{\theta}(X_n) : \|\theta^{t+1} - \theta^0\|_2 \le R\}$ and we want to compute upper bound

on the empirical Rademacher complexity $\mathcal{R}_S(\mathcal{F}_R^{m{ heta}^0})$ which is given as follows;

$$\begin{split} \mathcal{R}_{S}(\mathcal{F}_{R}^{\boldsymbol{\theta}^{0}}) &= \frac{1}{N} \mathbb{E}_{\epsilon \sim \text{unif}(-1,1)} \left[\begin{array}{c} \sup_{\boldsymbol{w}_{O}, \boldsymbol{W}_{K}^{T} \boldsymbol{W}_{Q}, \boldsymbol{W}_{V}: \\ \|\boldsymbol{w}_{O}\|_{2} \leq \eta_{O} \\ \|\boldsymbol{W}_{V}\|_{F} \leq \eta_{V} \\ \|\boldsymbol{w}_{W}^{T}\|_{F} \leq \eta_{V} \end{array} \right] \\ &= \frac{1}{Nd_{s}} \mathbb{E}_{\epsilon \sim \text{unif}(-1,1)} \left[\begin{array}{c} \sup_{\boldsymbol{w}_{O}, \boldsymbol{W}_{K}^{T} \boldsymbol{W}_{Q}, \boldsymbol{W}_{V}: \\ \|\boldsymbol{w}_{V}^{T} \boldsymbol{w}_{Q} \\ \sqrt{d_{m}} \end{array} \right] \sum_{n=1}^{N} \epsilon_{n} \boldsymbol{w}_{O}^{T} \sum_{i=1}^{d_{s}} \sigma_{r} \left(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{T} \sigma_{s} \left(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{T} \boldsymbol{W}_{Q}(\boldsymbol{X}_{n}^{(i,:)})^{T}}{\sqrt{d_{m}}} \right) \right) \\ & \|\boldsymbol{w}_{O}\|_{2} \leq \eta_{O} \\ & \|\boldsymbol{w}_{V}\|_{F} \leq \eta_{V} \\ & \|\boldsymbol{w}_{V}^{T} \boldsymbol{w}_{Q} \right\|_{F} \leq \frac{\eta_{K} \eta_{Q}}{\sqrt{d_{m}}} \end{aligned}$$

Applying subadditivity of the supremum:

$$\begin{split} \mathcal{R}_{S}(\mathcal{F}_{R}^{\boldsymbol{\theta}^{0}}) &\leq \frac{1}{Nd_{s}} \sum_{i=1}^{d_{s}} \mathbb{E}_{\epsilon} \left[\begin{array}{c} \sup_{\|\boldsymbol{w}_{O}\|_{2} \leq \eta_{O}} \sum_{n=1}^{N} \epsilon_{n} \, \boldsymbol{w}_{O}^{\top} \, \sigma_{r} \bigg(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\top} \, \sigma_{s} \bigg(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\top} \boldsymbol{W}_{Q}(\boldsymbol{X}_{n}^{(i,:)})^{\top}}{\sqrt{d_{m}}} \bigg) \bigg) \right] \\ &= d_{s} \cdot \frac{1}{Nd_{s}} \, \mathbb{E}_{\epsilon} \left[\begin{array}{c} \sup_{\|\boldsymbol{w}_{O}\|_{2} \leq \eta_{O}} \sum_{n=1}^{N} \epsilon_{n} \, \boldsymbol{w}_{O}^{\top} \, \sigma_{r} \bigg(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\top} \, \sigma_{s} \bigg(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\top} \boldsymbol{W}_{Q}(\boldsymbol{X}_{n}^{(i,:)})^{\top}}{\sqrt{d_{m}}} \bigg) \bigg) \right] \\ &= \frac{1}{N} \, \mathbb{E}_{\epsilon} \left[\begin{array}{c} \sup_{\|\boldsymbol{w}_{O}\|_{2} \leq \eta_{O}} \sum_{n=1}^{N} \epsilon_{n} \, \boldsymbol{w}_{O}^{\top} \, \sigma_{r} \bigg(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\top} \, \sigma_{s} \bigg(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\top} \boldsymbol{W}_{Q}(\boldsymbol{X}_{n}^{(i,:)})^{\top}}{\sqrt{d_{m}}} \bigg) \right) \right] \\ &= \underbrace{\frac{1}{N} \, \mathbb{E}_{\epsilon} \left[\begin{array}{c} \sup_{\|\boldsymbol{w}_{O}\|_{2} \leq \eta_{O}} \sum_{n=1}^{N} \epsilon_{n} \, \boldsymbol{w}_{O}^{\top} \, \sigma_{r} \bigg(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\top} \, \sigma_{s} \bigg(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\top} \boldsymbol{W}_{Q}(\boldsymbol{X}_{n}^{(i,:)})^{\top}}{\sqrt{d_{m}}} \bigg) \right) \right]} \\ &= \mathcal{R}_{S}(\mathcal{G}_{R}^{\boldsymbol{\theta}^{0}}) \end{split}$$

for any fixed $i \in [d_s]$. Hence,

$$\left[\mathcal{R}_S(\mathcal{F}_R^{oldsymbol{ heta}^0}) \ \leq \ \mathcal{R}_S(\mathcal{G}_R^{oldsymbol{ heta}^0})
ight]$$

where $\mathcal{R}_S(\mathcal{G}_R^{oldsymbol{ heta}^0})$ is defined as follows

$$\mathcal{G}_R^{\boldsymbol{\theta}^0} := \left\{ (\boldsymbol{X}^{(i,:)})^\top \mapsto \boldsymbol{w}_O^\top \sigma_r \big(\boldsymbol{W}_V \boldsymbol{X}_n^\top \sigma_s \big(\frac{\boldsymbol{X}_n \boldsymbol{W}_K^\top \boldsymbol{W}_Q (\boldsymbol{X}_n^{(i,:)})^\top}{\sqrt{d_m}} \big) \big) : \ \| \boldsymbol{w}_O \|_2 \leq \eta_O, \ \| \boldsymbol{W}_V \|_F \leq \eta_V, \ \left\| \frac{\boldsymbol{W}_K^\top \boldsymbol{W}_Q}{\sqrt{d_m}} \right\|_F \leq \frac{\eta_K \eta_Q}{\sqrt{d_m}} \right\}.$$

The following lemma gives an upper bound on $\mathcal{R}_S(\mathcal{G}_R^{\theta^0})$. Its proof can be found in the appendix section;

Lemma 2. For any fixed $\epsilon > 0$ and $X_1, \ldots, X_N \in \mathbb{R}^{d_s \times d}$ such that $\|X_n\|_F \leq \sqrt{d_s} R_X$ for all $n \in [N]$, the Rademacher complexity of $\mathcal{G}_R^{\theta^0}$ satisfies the bound given below;

$$\mathcal{R}_S(\mathcal{G}_R^{\boldsymbol{\theta}^0}) \lesssim c\sqrt{\frac{P}{N}} \left(1 + \log\left(A\sqrt{\frac{N}{P}}\right)\right)$$

where \lesssim hides logarithmic dependencies on quantities besides N and d_s , $A = \eta_O \eta_V(\sqrt{d_s}R_X)$ and $P = (\sqrt{d_s}R_X)^2 \left(\left(\sqrt{d_m}\eta_V\right)^{\frac{2}{3}} + \left(\sqrt{d_m}\eta_K\eta_Q\eta_V\right)^{\frac{2}{3}}\right)^3 \log(Nd_s)$.

Finally, the upper bound on the Rademacher complexity $\mathcal{R}_S(\mathcal{F}_R^{\theta^0})$ can be given as;

$$\mathcal{R}_{S}(\mathcal{F}_{R}^{\boldsymbol{\theta}^{0}}) \leq \mathcal{R}_{S}(\mathcal{G}_{R}^{\boldsymbol{\theta}^{0}})$$

$$\lesssim \sqrt{\frac{P}{N}} \left(1 + \log \left(A \sqrt{\frac{N}{P}} \right) \right)$$

$$\lesssim \mathcal{O}\left(\sqrt{\frac{P}{N}} \left(1 + \log \left(A \sqrt{\frac{N}{P}} \right) \right) \right)$$

4.3 Upper bounding the empirical loss

Having bounded the complexity of our hypothesis class, we next analyze the empirical loss achieved by gradient descent under the bounded-drift condition. This subsection establishes that, given suitable conditions on model width, learning rate, and data structure, the empirical loss decays exponentially during training. Using results from convergence analyses of Transformers in the lazy regime, we derive an explicit upper bound on the empirical loss as a function of key quantities such as α , ρ , and η_O . This provides a quantitative connection between network conditioning, data complexity, and training behavior, ensuring that even under restricted parameter updates, the model achieves low empirical loss with high probability.

Define α as the minimum singular value of F_{pre}^0 , i.e., $\alpha \triangleq \sigma_{\min}(F_{\text{pre}}^0)$ and also define $\Phi(\theta)$ as follows;

$$\Phi(\boldsymbol{\theta}) = \frac{1}{2} \|\boldsymbol{f}(\boldsymbol{\theta}) - \boldsymbol{y}\|_2^2$$

We now state the following assumption about the input data matrix X;

Assumption 3. Assume that the input data has full row rank and is bounded as $||\mathbf{X}||_F \leq \sqrt{d_s} R_X$ with some positive constant R_X . Furthermore, For any data pair $(\mathbf{X}_n, \mathbf{X}_{n'})$, with $n \neq n'$ and $n, n' \in [N]$, then we assume that;

$$\mathbb{P}(|\langle \boldsymbol{X}_n^T \boldsymbol{X}_n, \boldsymbol{X}_{n'}^T \boldsymbol{X}_{n'} \rangle| \ge t) \le \exp(-t^{\hat{c}})$$

with some constant $\hat{c} > 0$

The lemma below gives an upper bound on the empirical loss for all training steps t > 0.

Lemma 4. Suppose that we have $\eta_V = \|\boldsymbol{W}_V^0\|_F + R_V$, $\eta_O = \|\boldsymbol{w}_O^0\|_2 + R_O$, $\eta_K = \|\boldsymbol{W}_K^0\|_F + R_K$, $\eta_Q = \|\boldsymbol{W}_Q^0\|_F + R_Q$, $\xi_Q = \|\boldsymbol{W}_Q^0\|_2 + R_Q$, $\xi_K = \|\boldsymbol{W}_K^0\|_2 + R_K$, $\xi_V = \|\boldsymbol{W}_V^0\|_2 + R_V$ where R_O , R_V , R_K , R_Q remain as defined earlier. Under assumption 3, if $d_m \geq \tilde{\Omega}(N^3)$, $\alpha^2 \geq 8\rho M \sqrt{2\Phi(\boldsymbol{\theta}^0)}$, $\alpha^3 \geq (32\rho^2z\sqrt{2\Phi(\boldsymbol{\theta}^0)})/\eta_O$ and $\ell(\boldsymbol{\theta})$ is any loss function which is 1-Lipschitz in the first argument, then with probability at least $1 - 8e^{-d_m/2} - \delta - \exp(-\Omega((N-1)^{-\hat{c}}d_s^{-1})))$, for proper δ , when training using GD with small step size $\gamma \leq 1/k$ where k is a constant depending on $(\xi_Q, \xi_K, \xi_V, \eta_O, \Phi(\boldsymbol{\theta}^0), \rho, d_m^{-1/2})$, the empirical loss can be bounded as follows for all t > 0;

$$\mathcal{L}_S(f_{\boldsymbol{\theta}^t}) \le \min\left(\frac{\alpha^2}{8\rho \hat{M}\sqrt{N}}, \frac{\alpha^3 \eta_O}{32\rho^2 \hat{z}\sqrt{N}}\right)$$

where $\widetilde{\Omega}$ omits the logarithmic factor and the other quantities are defined as follows; $\rho \triangleq N^{1/2} d_s^{3/2} R_X$, $z \triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \xi_V^2 (\xi_Q^2 + \xi_K^2))$, $\widehat{z} \triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \eta_V^2 (\eta_Q^2 + \eta_K^2))$, $M = \max(\xi_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \xi_K \xi_V \eta_O R_Q^{-1}, 2/\sqrt{d_m}) R_X^2 d_s \xi_Q \xi_V \eta_O R_K^{-1})$, $\widehat{M} = \max(\eta_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_K \eta_V \eta_O R_Q^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_Q \eta_V \eta_O R_K^{-1})$.

Proof of lemma 4

For the purpose of simplification, define the following quantities at initialization;

$$\xi_{Q} \triangleq \|\boldsymbol{W}_{Q}^{0}\|_{2} + R_{Q} \leq \|\boldsymbol{W}_{Q}^{0}\|_{F} + R_{Q} \triangleq \eta_{Q}$$

$$\xi_{K} \triangleq \|\boldsymbol{W}_{K}^{0}\|_{2} + R_{K} \leq \|\boldsymbol{W}_{K}^{0}\|_{F} + R_{K} \triangleq \eta_{K}$$

$$\xi_{V} \triangleq \|\boldsymbol{W}_{V}^{0}\|_{2} + R_{V} \leq \|\boldsymbol{W}_{V}^{0}\|_{F} + R_{V} \triangleq \eta_{V}$$

$$\eta_{O} \triangleq \|\boldsymbol{w}_{O}^{0}\|_{2} + R_{O}$$

where R_Q, R_K, R_V, R_O are as defined before. As mentioned earlier, α is the minimum singular value of \mathbf{F}_{pre}^0 , i.e., $\alpha \triangleq \sigma_{min}(\mathbf{F}_{pre}^0)$ and $\Phi(\boldsymbol{\theta})$ is given as $\Phi(\boldsymbol{\theta}) = \frac{1}{2}||\boldsymbol{f}(\boldsymbol{\theta}) - \boldsymbol{y}||_2^2$.

According to Wu et al. (2024) theorem 1, under assumption 3, if $d_m \geq \widetilde{\Omega}(N^3)$, $\alpha^2 \geq 8\rho M \sqrt{2\Phi(\pmb{\theta}^0)}$ and $\alpha^3 \geq (32\rho^2z\sqrt{2\Phi(\pmb{\theta}^0)})/\eta_O$, then with probability at least $1-8e^{-d_m/2}-\delta-\exp(-\Omega((N-1)^{-\hat{c}}d_s^{-1}))$ for proper δ , GD converges to a global minimum as follows for a sufficiently small step size $\gamma \leq 1/k$ with k as a constant depending on $(\xi_O, \xi_K, \xi_V, \eta_O, \Phi(\pmb{\theta}^0), \rho, d_m^{-1/2})$:

$$\Phi(\boldsymbol{\theta}^t) \le \left(1 - \gamma \frac{\alpha^2}{2}\right)^t \Phi(\boldsymbol{\theta}^0), \forall t \ge 0$$

where $M = \max(\xi_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \xi_K \xi_V \eta_O R_Q^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \xi_Q \xi_V \eta_O R_K^{-1})$ and $\rho \triangleq N^{1/2} d_s^{3/2} R_X, z \triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \xi_V^2 (\xi_Q^2 + \xi_K^2)).$

We can observe that $\Phi(\theta^t)$ decays exponentially as training proceeds. This implies the following bound;

$$\Phi(\boldsymbol{\theta}^t) \le \Phi(\boldsymbol{\theta}^0), \quad \forall t \ge 0$$

From the first condition i.e., $\alpha^2 \geq 8\rho M \sqrt{2\Phi(\theta^0)}$, we can say that $\Phi(\theta^0) \leq \alpha^4/(128\rho^2 M^2)$. We therefore end up with the bound below;

$$\Phi(\boldsymbol{\theta}^t) \le \frac{\alpha^4}{128\rho^2 M^2}, \quad \forall t \ge 0$$

From the second condition i.e., $\alpha^3 \geq (32\rho^2z\sqrt{2\Phi(\pmb{\theta}^0)})/\eta_O$, we can say that $\Phi(\pmb{\theta}^0) \leq (\alpha^6\eta_O^2)/(2048\rho^4z^2)$. We therefore end up with the bound below;

$$\Phi(\boldsymbol{\theta}^t) \le \frac{\alpha^6 \eta_O^2}{2048 \rho^4 z^2}, \quad \forall t \ge 0$$

Combining the two bounds on $\Phi(\theta^t)$, we obtain the final bound as;

$$\Phi(\boldsymbol{\theta}^t) \leq \min\left(\frac{\alpha^4}{128\rho^2 M^2}, \frac{\alpha^6\eta_O^2}{2048\rho^4 z^2}\right), \quad \forall t \geq 0$$

Our empirical loss i.e., $\mathcal{L}_S(f_{\theta^t}) = \frac{1}{N} \sum_{n=1}^N \ell(f_{\theta^t}(\boldsymbol{X}_n), y_n)$ for all t > 0 can be bounded as follows;

$$\begin{split} \mathcal{L}_{S}(f_{\pmb{\theta}^{t}}) &\leq \frac{1}{N} \sum_{n=1}^{N} \left(\ell(f_{\pmb{\theta}^{t}}(\pmb{X}_{n}), y_{n}) - \ell(y_{n}, y_{n}) \right) \\ &\leq \frac{1}{N} \sum_{n=1}^{N} |f_{\pmb{\theta}^{t}}(\pmb{X}_{n}) - y_{n}| \qquad \text{because } \ell(\cdot, \cdot) \text{ is 1-Lipschitz in the first argument} \\ &\leq \frac{1}{\sqrt{N}} \|\pmb{f}_{\pmb{\theta}^{t}} - \pmb{y}\|_{2} \\ &= \sqrt{\frac{2\Phi(\pmb{\theta}^{t})}{N}} \\ &\leq \min \left(\frac{\alpha^{2}}{8\rho M \sqrt{N}}, \frac{\alpha^{3}\eta_{O}}{32\rho^{2}z\sqrt{N}} \right) \end{split}$$

where $M = \max(\xi_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \xi_K \xi_V \eta_O R_Q^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \xi_Q \xi_V \eta_O R_K^{-1})$ and $\rho \triangleq N^{1/2} d_s^{3/2} R_X$, $z \triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \xi_V^2 (\xi_Q^2 + \xi_K^2))$.

Upper bounding $\xi_O, \xi_V, \xi_K, \xi_Q$ using $\eta_O, \eta_V, \eta_K, \eta_Q$, the upper bound on the empirical loss for all training steps can therefore be written as;

$$\mathcal{L}_S(f_{\boldsymbol{\theta}^t}) \le \min\left(\frac{\alpha^2}{8\rho \hat{M}\sqrt{N}}, \frac{\alpha^3 \eta_O}{32\rho^2 \hat{z}\sqrt{N}}\right)$$

where $\hat{M} = \max(\eta_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_K \eta_V \eta_O R_Q^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_Q \eta_V \eta_O R_K^{-1})$ and $\hat{z} \triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \eta_V^2 (\eta_O^2 + \eta_K^2))$

4.4 Main result

With both the Rademacher complexity and empirical loss bounds in place, we now combine these results to obtain our main theorem i.e., a high-probability upper bound on the true loss (expected generalization error) of shallow Transformer models under bounded parameter drift. The theorem demonstrates that the true loss decreases with the number of training samples N and depends explicitly on the initialization scale, data structure, and model dimension d_m . The bound captures the essence of lazy training: when model parameters remain near initialization, generalization behavior aligns with that of linearized models governed by the neural tangent kernel (NTK). While this result establishes a rigorous theoretical foundation for shallow Transformers, it also highlights the need for further analysis to extend such guarantees to deeper and more expressive models.

Theorem 5. Suppose that we have $\eta_V = \|\boldsymbol{W}_V^0\|_F + R_V$, $\eta_O = \|\boldsymbol{w}_O^0\|_2 + R_O$, $\eta_K = \|\boldsymbol{W}_K^0\|_F + R_K$, $\eta_Q = \|\boldsymbol{W}_Q^0\|_F + R_Q$, $\xi_Q = \|\boldsymbol{W}_Q^0\|_2 + R_Q$, $\xi_K = \|\boldsymbol{W}_K^0\|_2 + R_K$, $\xi_V = \|\boldsymbol{W}_V^0\|_2 + R_V$ where R_O , R_V , R_K , R_Q remain as defined earlier. Under assumption 3, if $d_m \geq \tilde{\Omega}(N^3)$, $\alpha^2 \geq 8\rho M \sqrt{2\Phi(\boldsymbol{\theta}^0)}$, $\alpha^3 \geq (32\rho^2z\sqrt{2\Phi(\boldsymbol{\theta}^0)})/\eta_O$ and $\ell(\boldsymbol{\theta})$ is any loss function which is 1-lipschitz in the first argument, then with probability at least $1 - 8e^{-d_m/2} - 2\delta - \exp(-\Omega((N-1)^{-\hat{c}}d_s^{-1}))$, if the transformer model is trained using Gradient Descent with small step size $\gamma \leq 1/k$ where k is a constant depending on $(\xi_Q, \xi_K, \xi_V, \eta_O, \ell(\boldsymbol{\theta}^0), \rho, d_m^{-1/2})$, the true loss $L_D(f)$ can be bounded as follows;

$$L_{\mathcal{D}}(f) \lesssim \min\left(\frac{\alpha^2}{8\rho \hat{M}\sqrt{N}}, \frac{\alpha^3 \eta_O}{32\rho^2 \hat{z}\sqrt{N}}\right) + \mathcal{O}\left(\sqrt{\frac{P}{N}}\left(1 + \log\left(A\sqrt{\frac{N}{P}}\right)\right) + \sqrt{\frac{\log\frac{R}{\delta}}{N}}\right)$$

where $\widetilde{\Omega}$ omits the logarithmic factor, \lesssim hides logarithmic dependencies on quantities besides N, d_s and δ and the other quantities are defined as follows; $\rho \triangleq N^{1/2} d_s^{3/2} R_X$,

$$\begin{split} z &\triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \xi_V^2 (\xi_Q^2 + \xi_K^2)), \, \hat{z} \triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \eta_V^2 (\eta_Q^2 + \eta_K^2)), \\ M &= \max(\xi_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \xi_K \xi_V \eta_O R_Q^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \xi_Q \xi_V \eta_O R_K^{-1}), \\ \hat{M} &= \max(\eta_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_K \eta_V \eta_O R_Q^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_Q \eta_V \eta_O R_K^{-1}), \\ A &= \eta_O \eta_V (\sqrt{d_s} R_X) \, \text{and} \, P = (\sqrt{d_s} R_X)^2 \left(\left(\sqrt{d_m} \eta_V \right)^{\frac{2}{3}} + \left(\sqrt{d_m} \eta_K \eta_Q \eta_V \right)^{\frac{2}{3}} \right)^3 \log(N d_s). \end{split}$$

Proof of Theorem 5

Recall that we defined our hypothesis class as follows;

$$\mathcal{F}_{R}^{\boldsymbol{\theta}^{0}} = \left\{ f_{\boldsymbol{\theta}}(\boldsymbol{X}_{n}) : \|\boldsymbol{\theta}^{t+1} - \boldsymbol{\theta}^{0}\|_{2} \leq R \right\}$$

Let us set $R_i = i$ for $i \in \{1, 2, ..., R\}$. This means that we can define a class of models whose parameter norm is bounded as $\|\boldsymbol{\theta}^{t+1} - \boldsymbol{\theta}^0\|_2 \le R_i$ for $i \in \{1, 2, ..., R\}$ as follows;

$$\mathcal{F}_{R_i}^{\boldsymbol{\theta}^0} = \left\{ f_{\boldsymbol{\theta}}(\boldsymbol{X}_n) : \|\boldsymbol{\theta}^{t+1} - \boldsymbol{\theta}^0\|_2 \le R_i \right\}$$

From Rademacher complexity and a union bound over a finite set of R_i 's, for any random initialization $(\boldsymbol{\theta}^0)$, with probability at least $1-\delta$ over the sample $S=\{(\boldsymbol{X}_n,y_n)\}_{n=1}^N$ of size N, we have that;

$$\sup_{f \in \mathcal{F}_{R_i}^{\boldsymbol{\theta}^0}} \{ L_{\mathcal{D}}(f) - L_S(f) \} \le 2\mathcal{R}_S(\mathcal{F}_{R_i}^{\boldsymbol{\theta}^0}) + \sqrt{\frac{\log \frac{2R}{\delta}}{2N}}$$

for all $i \in \{1, 2, 3, ..., R\}$. Note that $R_i \leq R$ for all $i \in \{1, 2, ..., R\}$ which implies that $\mathcal{R}_S(\mathcal{F}_{R_i}^{\boldsymbol{\theta}^0}) \leq \mathcal{R}_S(\mathcal{F}_R^{\boldsymbol{\theta}^0})$ for any $i \in \{1, 2, ..., R\}$. This gives us the following bound on $\mathcal{R}_S(\mathcal{F}_{R_i}^{\boldsymbol{\theta}^0})$ for all $i \in \{1, 2, ..., R\}$;

$$\mathcal{R}_S(\mathcal{F}_{R_i}^{\boldsymbol{\theta^0}}) \lesssim \mathcal{O}\left(\sqrt{\frac{P}{N}}\left(1 + \log\left(A\sqrt{\frac{N}{P}}\right)\right)\right)$$

where $P=(\sqrt{d_s}R_X)^2\left(\left(\sqrt{d_m}\eta_V\right)^{\frac{2}{3}}+\left(\sqrt{d_m}\eta_K\eta_Q\eta_V\right)^{\frac{2}{3}}\right)^3\log(Nd_s)$ and $A=\eta_O\eta_V(\sqrt{d_s}R_X)$. From lemma 4, with probability at least $1-8e^{-d_m/2}-\delta-\exp(-\Omega((N-1)^{-\hat{c}}d_s^{-1}))$, the training loss for our transformer model can be bounded as follows for all t>0;

$$\mathcal{L}_S(f_{\boldsymbol{\theta}^t}) \le \min\left(\frac{\alpha^2}{8\rho \hat{M}\sqrt{N}}, \frac{\alpha^3 \eta_O}{32\rho^2 \hat{z}\sqrt{N}}\right)$$

where $\rho \triangleq N^{1/2} d_s^{3/2} R_X$, $\hat{z} \triangleq \eta_O^2 (1 + (4/d_m) R_X^4 d_s^2 \eta_V^2 (\eta_Q^2 + \eta_K^2))$ and $\hat{M} = \max(\eta_V R_O^{-1}, \eta_O R_V^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_K \eta_V \eta_O R_Q^{-1}, (2/\sqrt{d_m}) R_X^2 d_s \eta_Q \eta_V \eta_O R_K^{-1})$. Putting everything together, with probability at east $1 - 8e^{-d_m/2} - 2\delta - \exp(-\Omega((N-1)^{-\hat{c}} d_s^{-1}))$, we have that;

$$L_{\mathcal{D}}(f) \lesssim \min\left(\frac{\alpha^2}{8\rho \hat{M}\sqrt{N}}, \frac{\alpha^3 \eta_O}{32\rho^2 \hat{z}\sqrt{N}}\right) + \mathcal{O}\left(\sqrt{\frac{P}{N}}\left(1 + \log\left(A\sqrt{\frac{N}{P}}\right)\right) + \sqrt{\frac{\log\frac{R}{\delta}}{N}}\right)$$

where \leq hides logarithmic dependencies on quantities besides N, d_s and δ .

4.5 Discussion

Our main theorem provides a generalization bound for a class of Transformer models whose weights remain close to their initialization during training. This bounded-drift assumption effectively constrains the training dynamics to what is commonly referred to as the *lazy training regime*. In this setting, the model behaves similarly to its linearized form around initialization, which has been extensively studied in the context of neural tangent kernels (NTK).

The implication of this assumption is that the results derived here apply most accurately to wide and shallow Transformers trained with sufficiently small learning rates that prevent the parameters from deviating significantly from their initial values. Such a setting captures the early or near-linear training phase of overparameterized models, where the NTK remains nearly constant and generalization can be controlled through classical complexity measures such as the Rademacher complexity.

Compared to prior results on generalization bounds for neural networks under the lazy regime (e.g., for two-layer networks and linearized models), our bound maintains a similar dependence on the sample size N and model width d_m .

Specifically, the $\mathcal{O}\left(\sqrt{\frac{P}{N}}\log(A\sqrt{\frac{N}{P}})\right)$ term scales analogously to existing NTK-based results, while the dependence on α and ρ in the empirical loss component reflects the conditioning of the pre-activation features and the interaction between model width and sequence length. However, unlike the more general results that extend to deep networks or non-lazy regimes through complex stability analyses or overparameterization assumptions, our result explicitly applies to single-layer (shallow) Transformer architectures only.

We also note that relaxing the bounded-drift assumption to capture non-lazy or feature-learning regimes remains an open problem. In such regimes, weights undergo significant changes during training, resulting in evolving representations and coupling across layers. Extending our analysis to this setting would require novel techniques to handle the dynamic evolution of the NTK or an equivalent representation matrix. Similarly, extending the bound to deeper multilayer architectures would require careful control of layerwise dependencies, possibly through hierarchical complexity bounds or layerwise Lipschitz control arguments.

Overall, our results contribute to the growing theoretical understanding of Transformers under simplified but analytically tractable conditions. They highlight the relationship between network width, data complexity, and generalization under bounded parameter drift, reinforcing the intuition that in the lazy regime, wide and shallow Transformers behave as near-linear models governed by their initialization structure.

Comparison with other norm-based Transformer bounds. Our result differs substantively from norm-based bounds tailored to Transformers. Edelman et al. (2021) obtain a gap bound that scales only *logarithmically* with sequence length by analyzing bounded-norm self-attention and the sparse variable creation inductive bias, while Trauger & Tewari (2024) strengthen this line by proving *sequence-length-independent* gap bounds via a covering-number analysis that upper-bounds the Rademacher complexity of Transformer classes and applies also to masked-token training objectives. In contrast, our theorem provides a *true-loss* bound that explicitly couples a data-dependent optimization guarantee (lazy-regime convergence for a shallow Transformer) with a capacity term. Practically, this means (i) norm-based results (Edelman et al., 2021; Trauger & Tewari, 2024) can be evaluated after training completes by plugging in norms to bound $|\mathcal{L}_{\mathcal{D}}(f) - \mathcal{L}_{S}(f)|$, and they cleanly characterize how sequence length enters (logarithmically or not at all), whereas (ii) our bound ties generalization to optimization-side quantities such as α , ρ , and $(\eta_{Q}, \eta_{K}, \eta_{V}, \eta_{O})$ under bounded drift and thus characterizes when low *true* risk is guaranteed without first computing $\mathcal{L}_{S}(f)$. Conceptually, the results are complementary: norm-based bounds offer architecture-wide, training-regime-agnostic control of the generalization gap (with refined sequence-length dependence), while our analysis isolates the lazy, shallow regime and provides optimization-aware control of the *level* of the true loss.

Relation to PAC-Bayes and stability-based bounds. Compared to PAC-Bayes/compression bounds for LLMs (Lotfi et al., 2023; Zhou et al., 2018b), our result targets a different regime and objective: we operate under a bounded-drift (lazy) assumption and obtain a *true-loss* bound for a *single-layer* Transformer trained by gradient descent, with explicit dependence on quantities like α , ρ , and $(\eta_Q, \eta_K, \eta_V, \eta_O)$. PAC-Bayes bounds, in contrast, typically control $|\mathcal{L}_{\mathcal{D}}(f) - \mathcal{L}_{S}(f)|$ via a data-informed posterior and compression, and have been instantiated for large, deep, pretrained language models without requiring lazy dynamics. Stability-based results for Transformers (e.g., in-context learning) quantify sensitivity to sample perturbations through stability coefficients (Li et al., 2023), again bounding the generalization gap rather than the true loss. Thus, our contribution is complementary: it connects *optimization-driven* lazy training (bounded drift + shallow width assumptions) to generalization, while PAC-Bayes and stability provide depth-agnostic, training-regime-agnostic controls on the gap. Extending our approach to remove the lazy assumption or to handle deeper stacks could help bridge these viewpoints, potentially yielding hybrid bounds that combine optimization-aware true-loss control with posterior- or stability-based gap terms (cf. Yao et al., 2025; Deora, 2024).

5 Conclusion

In summary, we established a generalization bound for shallow Transformer models trained in the bounded-drift (lazy) regime, where the model parameters remain close to their initialization throughout training. By combining Rademacher complexity analysis with an upper bound on the empirical loss, we obtained a probabilistic bound on the true loss that decreases with the number of samples N and depends explicitly on model and data parameters.

Our theoretical results align with existing findings for wide, overparameterized models analyzed under the NTK framework, but they are specific to single-layer Transformers. This limitation ensures that our claims remain within the the-

oretical scope supported by the bounded-drift assumption. Extending the analysis to deeper architectures or non-lazy training regimes (where substantial feature learning occurs) remains an important direction for future research.

Through this work, we provide a rigorous foundation for understanding how bounded-drift dynamics influence generalization in Transformer models and set the stage for future extensions that aim to capture the richer behavior of modern, deeper architectures trained beyond the lazy regime.

References

- Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical report. arXiv preprint arXiv:2303.08774, 2023.
- Sanjeev Arora, Rong Ge, Behnam Neyshabur, and Yi Zhang. Stronger generalization bounds for deep nets via a compression approach. *CoRR*, abs/1802.05296, 2018. URL http://arxiv.org/abs/1802.05296.
- Sanjeev Arora, Simon S. Du, Wei Hu, Zhiyuan Li, and Ruosong Wang. Fine-grained analysis of optimization and generalization for overparameterized two-layer neural networks. *CoRR*, abs/1901.08584, 2019. URL http://arxiv.org/abs/1901.08584.
- Peter L. Bartlett, Dylan J. Foster, and Matus Telgarsky. Spectrally-normalized margin bounds for neural networks. *CoRR*, abs/1706.08498, 2017. URL http://arxiv.org/abs/1706.08498.
- Yuan Cao and Quanquan Gu. Generalization bounds of stochastic gradient descent for wide and deep neural networks. *CoRR*, abs/1905.13210, 2019. URL http://arxiv.org/abs/1905.13210.
- Minshuo Chen, Xingguo Li, and Tuo Zhao. On generalization bounds of a family of recurrent neural networks. *CoRR*, abs/1910.12947, 2019. URL http://arxiv.org/abs/1910.12947.
- Puneesh Deora. On the optimization and generalization of self-attention models: a stability and implicit bias perspective. PhD thesis, University of British Columbia, 2024. URL https://open.library.ubc.ca/collections/ubctheses/24/items/1.0445320.
- Puneesh Deora, Rouzbeh Ghaderi, Hossein Taheri, and Christos Thrampoulidis. On the optimization and generalization of multi-head attention. *ArXiv*, abs/2310.12680, 2023. URL https://api.semanticscholar.org/CorpusID:264306388.
- Alexey Dosovitskiy, Lucas Beyer, Alexander Kolesnikov, Dirk Weissenborn, Xiaohua Zhai, Thomas Unterthiner, Mostafa Dehghani, Matthias Minderer, Georg Heigold, Sylvain Gelly, Jakob Uszkoreit, and Neil Houlsby. An image is worth 16x16 words: Transformers for image recognition at scale. *CoRR*, abs/2010.11929, 2020. URL https://arxiv.org/abs/2010.11929.
- Gintare Karolina Dziugaite and Daniel M. Roy. Computing nonvacuous generalization bounds for deep (stochastic) neural networks with many more parameters than training data. *CoRR*, abs/1703.11008, 2017. URL https://arxiv.org/abs/1703.11008.
- Benjamin L. Edelman, Surbhi Goel, Sham M. Kakade, and Cyril Zhang. Inductive biases and variable creation in self-attention mechanisms. *CoRR*, abs/2110.10090, 2021. URL https://arxiv.org/abs/2110.10090.
- Hengyu Fu, Tianyu Guo, Yu Bai, and Song Mei. What can a single attention layer learn? a study through the random features lens. *Advances in Neural Information Processing Systems*, 36, 2024.
- Noah Golowich, Alexander Rakhlin, and Ohad Shamir. Size-independent sample complexity of neural networks. *CoRR*, abs/1712.06541, 2017. URL http://arxiv.org/abs/1712.06541.
- Iryna Gurevych, Michael Kohler, and Gözde Gül Şahin. On the rate of convergence of a classifier based on a transformer encoder. *IEEE Transactions on Information Theory*, 68(12):8139–8155, 2022.

- Ruiquan Huang, Yingbin Liang, and Jing Yang. Non-asymptotic convergence of training transformers for next-token prediction. *ArXiv*, abs/2409.17335, 2024. URL https://api.semanticscholar.org/CorpusID: 272910946.
- Michael Kohler and Adam Krzyzak. On the rate of convergence of an over-parametrized transformer classifier learned by gradient descent. *arXiv preprint arXiv:2312.17007*, 2023.
- Xingguo Li, Junwei Lu, Zhaoran Wang, Jarvis D. Haupt, and Tuo Zhao. On tighter generalization bound for deep neural networks: Cnns, resnets, and beyond. *CoRR*, abs/1806.05159, 2018. URL http://arxiv.org/abs/1806.05159.
- Yingcong Li, Muhammed Emrullah Ildiz, Dimitris Papailiopoulos, and Samet Oymak. Transformers as algorithms: Generalization and stability in in-context learning. In *International Conference on Machine Learning*, 2023. URL https://api.semanticscholar.org/CorpusID:256616253.
- Philip M. Long and Hanie Sedghi. Size-free generalization bounds for convolutional neural networks. *CoRR*, abs/1905.12600, 2019. URL http://arxiv.org/abs/1905.12600.
- Sanae Lotfi, Marc Finzi, Yilun Kuang, Tim G. J. Rudner, Micah Goldblum, and Andrew Gordon Wilson. Non-vacuous generalization bounds for large language models. *ArXiv*, abs/2312.17173, 2023. URL https://api.semanticscholar.org/CorpusID:266573256.
- Mehryar Mohri, Afshin Rostamizadeh, and Ameet Talwalkar. *Foundations of Machine Learning*. The MIT Press, 2012. ISBN 026201825X.
- Behnam Neyshabur, Ryota Tomioka, and Nathan Srebro. Norm-based capacity control in neural networks. *CoRR*, abs/1503.00036, 2015. URL http://arxiv.org/abs/1503.00036.
- Behnam Neyshabur, Srinadh Bhojanapalli, David McAllester, and Nathan Srebro. A pac-bayesian approach to spectrally-normalized margin bounds for neural networks. *CoRR*, abs/1707.09564, 2017. URL http://arxiv.org/abs/1707.09564.
- Behnam Neyshabur, Zhiyuan Li, Srinadh Bhojanapalli, Yann LeCun, and Nathan Srebro. Towards understanding the role of over-parametrization in generalization of neural networks. *CoRR*, abs/1805.12076, 2018. URL http://arxiv.org/abs/1805.12076.
- Konstantinos Pitas, Mike E. Davies, and Pierre Vandergheynst. Pac-bayesian margin bounds for convolutional neural networks technical report. *CoRR*, abs/1801.00171, 2018. URL http://arxiv.org/abs/1801.00171.
- Wei Shen, Ruida Zhou, Jing Yang, and Cong Shen. On the training convergence of transformers for in-context classification. *arXiv preprint arXiv:2410.11778*, 2024.
- Gemini Team, Rohan Anil, Sebastian Borgeaud, Jean-Baptiste Alayrac, Jiahui Yu, Radu Soricut, Johan Schalkwyk, Andrew M Dai, Anja Hauth, Katie Millican, et al. Gemini: a family of highly capable multimodal models. *arXiv* preprint arXiv:2312.11805, 2023.
- Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. Llama: Open and efficient foundation language models. *arXiv preprint arXiv:2302.13971*, 2023.
- Jacob Trauger and Ambuj Tewari. Sequence length independent norm-based generalization bounds for transformers. In *International Conference on Artificial Intelligence and Statistics*, pp. 1405–1413. PMLR, 2024.
- Yongtao Wu, Fanghui Liu, Grigorios Chrysos, and Volkan Cevher. On the convergence of encoder-only shallow transformers. *Advances in Neural Information Processing Systems*, 36, 2024.
- Xinhao Yao, Hongjin Qian, Xiaolin Hu, Gengze Xu, Wei Liu, Jian Luan, Bin Wang, and Yong Liu. Theoretical insights into fine-tuning attention mechanism: Generalization and optimization. In *Proceedings of the Thirty-Fourth International Joint Conference on Artificial Intelligence, IJCAI 2025, Montreal, Canada, August 16-22, 2025*, pp. 6830–6838. ijcai.org, 2025. doi: 10.24963/IJCAI.2025/760. URL https://doi.org/10.24963/ijcai. 2025/760.

Wenda Zhou, Victor Veitch, Morgane Austern, Ryan P Adams, and Peter Orbanz. Non-vacuous generalization bounds at the imagenet scale: a pac-bayesian compression approach. *arXiv preprint arXiv:1804.05862*, 2018a.

Wenda Zhou, Victor Veitch, Morgane Austern, Ryan P. Adams, and Peter Orbanz. Non-vacuous generalization bounds at the imagenet scale: a pac-bayesian compression approach. In *International Conference on Learning Representations*, 2018b. URL https://api.semanticscholar.org/CorpusID:67855429.

A Proof of lemma 2

We want to obtain an upper bound on $\mathcal{R}_S(\mathcal{G}_R^{\theta^0})$ where $\mathcal{G}_R^{\theta^0}$ is defined as follows;

$$\mathcal{G}_R^{\boldsymbol{\theta}^0} := \left\{ (\boldsymbol{X}^{(i,:)})^{\mathrm{T}} \longrightarrow \boldsymbol{w}_O^{\mathrm{T}} \sigma_r \left(\boldsymbol{W}_V \boldsymbol{X}_n^{\mathrm{T}} \sigma_s \left(\frac{\boldsymbol{X}_n \boldsymbol{W}_K^{\mathrm{T}} \boldsymbol{W}_Q (\boldsymbol{X}_n^{(i,:)})^{\mathrm{T}}}{\sqrt{d_m}} \right) \right) : \left\| \frac{\|\boldsymbol{w}_O\|_2 \leq \eta_O}{\|\boldsymbol{W}_V\|_F \leq \eta_V} \right\|_F \leq \frac{\eta_K \eta_Q}{\sqrt{d_m}} \right\}$$

Let's begin by defining the following bounds on the matrices;

$$\|\boldsymbol{W}_{V}\|_{2} \leq \|\boldsymbol{W}_{V}^{0}\|_{2} + b_{V} \leq \eta_{V}$$

$$\|\boldsymbol{W}_{V}\|_{2,1} \leq \|\boldsymbol{W}_{V}^{0}\|_{2,1} + B_{V} \leq \sqrt{d_{m}}\eta_{V}$$

$$\|\frac{\boldsymbol{W}_{K}^{\mathsf{T}}\boldsymbol{W}_{Q}}{\sqrt{d_{m}}}\|_{2,1} \leq \frac{\left(\|(\boldsymbol{W}_{K}^{0})^{\mathsf{T}}\|_{1,2} + B_{K}\right)\left(\|\boldsymbol{W}_{Q}^{0}\|_{2,1} + B_{Q}\right)}{\sqrt{d_{m}}} \leq \frac{d_{m}\eta_{K}\eta_{Q}}{\sqrt{d_{m}}} = \sqrt{d_{m}}\eta_{K}\eta_{Q}$$

$$\|\boldsymbol{X}_{n}^{\mathsf{T}}\|_{2,\infty} \leq B_{X} \leq \|\boldsymbol{X}_{n}\|_{F} \leq \sqrt{d_{s}}R_{X} \quad \forall n \in [N]$$

where b_V, B_V, B_K, B_Q, B_X are some positive constants and R_O, R_V, R_K, R_Q, R_X remain as defined earlier. The norm $\|\cdot\|_{2,1}$ interpreted as first taking the ℓ_2 -norm for each column of a matrix and then summing these column norms. Define another class $\mathcal{G}_B^{\theta^0}$ as shown below;

$$\mathcal{G}_{B}^{\boldsymbol{\theta}^{0}} := \left\{ (\boldsymbol{X}^{(i,:)})^{\mathrm{T}} \longrightarrow \boldsymbol{w}_{O}^{\mathrm{T}} \sigma_{r} \left(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\mathrm{T}} \sigma_{s} \left(\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\mathrm{T}} \boldsymbol{W}_{Q} (\boldsymbol{X}_{n}^{(i,:)})^{\mathrm{T}} \right) \right) : \frac{\|\boldsymbol{w}_{O}\|_{2} \leq \eta_{O}}{\|\boldsymbol{W}_{V}\|_{2} \leq \|\boldsymbol{W}_{V}^{0}\|_{2} + b_{V}} \\ \left\| \frac{\boldsymbol{w}_{V}^{\mathrm{T}} \boldsymbol{w}_{Q}}{\sqrt{d_{m}}} \right\|_{2,1} \leq \frac{\|\boldsymbol{w}_{O}\|_{2} + B_{V}}{\sqrt{d_{m}}} \left(\|\boldsymbol{w}_{O}^{0}\|_{2,1} + B_{V}} \right) \right\}$$

The following lemma gives an upper bound on the log covering number of the class $\mathcal{G}_B^{\pmb{\theta^0}}$;

Lemma 6. ((Edelman et al., 2021) Corollary 4.5). For any fixed $\epsilon > 0$ and $X_1, \ldots, X_N \in \mathbb{R}^{d_s \times d}$ such that $\|X_n^T\|_{2,\infty} \leq B_X$ for all $n \in [N]$, the covering number of $\mathcal{G}_B^{\theta^0}$ satisfies the bound given below;

$$\log \mathcal{N}_{\infty}(\mathcal{G}_{B}^{\theta^{0}}; \epsilon; \{\boldsymbol{X}_{n}\}_{n=1}^{N}, \|\cdot\|_{2})$$

$$\lesssim B_{X}^{2} \cdot \frac{\left(\left(\|\boldsymbol{W}_{V}^{0}\|_{2,1} + B_{V}\right)^{\frac{2}{3}} + \left(\left(\frac{\left(\|(\boldsymbol{W}_{K}^{0})^{T}\|_{1,2} + B_{K}\right)\left(\|\boldsymbol{W}_{Q}^{0}\|_{2,1} + B_{Q}\right)}{\sqrt{d_{m}}}\right)\left(\|\boldsymbol{W}_{V}^{0}\|_{2} + b_{V}\right)\right)^{\frac{2}{3}}\right)^{3}}{\epsilon^{2}} \cdot \log(Nd_{s})$$

where \leq hides logarithmic dependencies on quantities besides N and d_s .

Upper bounding the norms $\|\cdot\|_{2,1}$ and $\|\cdot\|_{2,\infty}$ using the Frobenius norm, $\|\cdot\|_F$, we end up with;

$$\log \mathcal{N}_{\infty}(\mathcal{G}_{R}^{\boldsymbol{\theta}^{0}}; \epsilon; \{\boldsymbol{X}_{n}\}_{n=1}^{N}, \|\cdot\|_{2}) \lesssim (\sqrt{d_{s}}R_{X})^{2} \cdot \frac{\left(\left(\sqrt{d_{m}}\eta_{V}\right)^{\frac{2}{3}} + \left(\sqrt{d_{m}}\eta_{K}\eta_{Q}\eta_{V}\right)^{\frac{2}{3}}\right)^{3}}{\epsilon^{2}} \cdot \log(Nd_{s})$$

This can also be written as;

$$\log \mathcal{N}_{\infty}(\mathcal{G}_{R}^{\boldsymbol{\theta}^{0}}; \epsilon; \{\boldsymbol{X}_{n}\}_{n=1}^{N}, \|\cdot\|_{2}) \lesssim \frac{P}{\epsilon^{2}}$$

where
$$P = (\sqrt{d_s}R_X)^2 \left(\left(\sqrt{d_m}\eta_V\right)^{\frac{2}{3}} + \left(\sqrt{d_m}\eta_K\eta_Q\eta_V\right)^{\frac{2}{3}}\right)^3 \log(Nd_s)$$
.

We can now write the bound on the Rademacher complexity $\mathcal{R}_S(\mathcal{G}_R^{\pmb{\theta}^0})$ as follows for some constant c>0 and $|f|\leq A$ for all $f\in\mathcal{G}_R^{\pmb{\theta}^0}$;

$$\mathcal{R}_{S}(\mathcal{G}_{R}^{\boldsymbol{\theta}^{0}}) \leq c \cdot \inf_{\delta \geq 0} \left(\delta + \int_{\delta}^{A} \sqrt{\frac{\log \mathcal{N}_{\infty}(\mathcal{G}_{R}^{\boldsymbol{\theta}^{0}}; \epsilon; \{\boldsymbol{X}_{n}\}_{n=1}^{N}; \| \cdot \|_{2})}{N}} d\epsilon \right)$$

$$\lesssim c \cdot \inf_{\delta \geq 0} \left(\delta + \int_{\delta}^{A} \sqrt{\frac{P}{\epsilon^{2} N}} d\epsilon \right)$$

$$= c \cdot \inf_{\delta \geq 0} \left(\delta + \sqrt{\frac{P}{N}} \int_{\delta}^{A} \frac{1}{\epsilon} d\epsilon \right)$$

$$= c \cdot \inf_{\delta \geq 0} \left(\delta + \sqrt{\frac{P}{N}} \log \left(\frac{A}{\delta} \right) \right)$$

$$= c \sqrt{\frac{P}{N}} \left(1 + \log \left(A \sqrt{\frac{N}{P}} \right) \right)$$

Note that $|f| \leq A$ for all $f \in \mathcal{G}_R^{\theta^0}$. A can be obtained as follows;

$$\begin{split} & \left\| \boldsymbol{w}_{O}^{\mathsf{T}} \sigma_{r} \left(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\mathsf{T}} \sigma_{s} \left(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\mathsf{T}} \boldsymbol{W}_{Q} (\boldsymbol{X}_{n}^{(i,:)})^{\mathsf{T}}}{\sqrt{d_{m}}} \right) \right) \right\| \\ & \leq \| \boldsymbol{w}_{O} \|_{2} \left\| \sigma_{r} \left(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\mathsf{T}} \sigma_{s} \left(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\mathsf{T}} \boldsymbol{W}_{Q} (\boldsymbol{X}_{n}^{(i,:)})^{\mathsf{T}}}{\sqrt{d_{m}}} \right) \right) \right\|_{2} \\ & = \| \boldsymbol{w}_{O} \|_{2} \left\| \sigma_{r} \left(\boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\mathsf{T}} \sigma_{s} \left(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\mathsf{T}} \boldsymbol{W}_{Q} (\boldsymbol{X}_{n}^{(i,:)})^{\mathsf{T}}}{\sqrt{d_{m}}} \right) \right) \right\|_{2} \\ & \leq \| \boldsymbol{w}_{O} \|_{2} \left\| \boldsymbol{W}_{V} \boldsymbol{X}_{n}^{\mathsf{T}} \sigma_{s} \left(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\mathsf{T}} \boldsymbol{W}_{Q} (\boldsymbol{X}_{n}^{(i,:)})^{\mathsf{T}}}{\sqrt{d_{m}}} \right) \right\|_{2} \\ & \leq \| \boldsymbol{w}_{O} \|_{2} \left\| \boldsymbol{W}_{V} \right\|_{2} \left\| \boldsymbol{X}_{n}^{\mathsf{T}} \sigma_{s} \left(\frac{\boldsymbol{X}_{n} \boldsymbol{W}_{K}^{\mathsf{T}} \boldsymbol{W}_{Q} (\boldsymbol{X}_{n}^{(i,:)})^{\mathsf{T}}}{\sqrt{d_{m}}} \right) \right\|_{2} \\ & \leq \| \boldsymbol{w}_{O} \|_{2} \left\| \boldsymbol{W}_{V} \right\|_{2} \left\| \boldsymbol{X}_{n} \right\|_{2} \quad \left(\text{because } \| \sigma_{s} (\boldsymbol{z}) \|_{2} \leq \| \sigma_{s} (\boldsymbol{z}) \|_{1} = 1 \right) \\ & \leq \| \boldsymbol{w}_{O} \|_{2} \left\| \boldsymbol{W}_{V} \right\|_{2} \left\| \boldsymbol{X}_{n} \right\|_{2} \quad \left(\text{because } \| \sigma_{s} (\boldsymbol{z}) \|_{2} \leq \| \sigma_{s} (\boldsymbol{z}) \|_{1} = 1 \right) \\ & \leq \| \boldsymbol{w}_{O} \|_{2} \left\| \boldsymbol{W}_{V} \right\|_{F} \left\| \boldsymbol{X}_{n} \right\|_{F} \\ & \leq \left(\| \boldsymbol{w}_{O}^{0} \|_{2} + R_{O} \right) \left(\| \boldsymbol{W}_{V}^{0} \|_{F} + R_{V} \right) \left(\sqrt{d_{s}} R_{X} \right) \\ & = \eta_{O} \eta_{V} \left(\sqrt{d_{s}} R_{X} \right) \end{split}$$

This means that $A = \eta_O \eta_V(\sqrt{d_s} R_X)$.

B Experiments

B.1 Image Classification

We use the transformer model defined in section 3.1.2 to perform classification of images. From MNIST dataset, we extract the images belonging to classes 0 and 1 and create our new dataset. Each image of size 28×28 is broken into

tokens each of dimension d=64. The main goal of the experiments is to demonstrate that the test loss of the trained transformer model decreases with increasing number of of samples i.e., N=400, N=1200 and N=10000. This trend holds for all the values of model dimension which we tested i.e., $d_m=64$, $d_m=1024$ and $d_m=4096$. The learning rate used is 0.1, the optimization algorithm is batch gradient descent and the loss function is the cross-entropy loss. The results for the experiments are presented below. Each figure 1-3 shows the training loss and test loss of the transformer model as training proceeds.

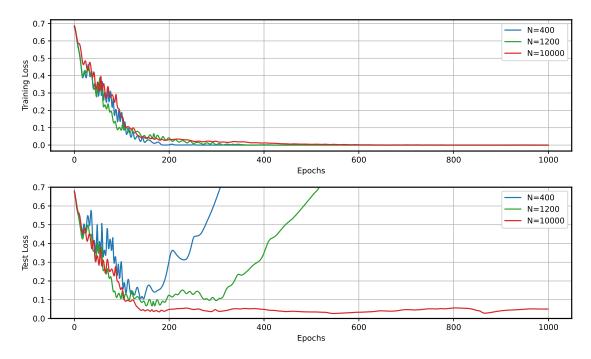


Figure 1: Evolution of training loss (top) and test loss(bottom) for each epoch of training for model dimension $d_m = 64$.

Table 1: Lowest test loss and the epoch at which it was achieved for different values of d_m and N.

d_m	N	Lowest Test Loss	Epoch
64	400	0.1048	147
64	1200	0.0668	165
64	10000	0.0263	546
1024	400	0.1839	95
1024	1200	0.0760	271
1024	10000	0.0045	251
4096	400	0.1269	139
4096	1200	0.0899	169
4096	10000	0.0123	312

B.2 Text Classification

We also perform similar experiments for text classification using the 20 Newsgroups dataset restricted to the categories sci.med and sci.space. Each text document is represented as a sequence of 40 tokens ($d_s=40$), where each token corresponds to a 50-dimensional GloVe embedding (d=50). This forms the input sequence for our shallow Transformer model. The main goal of these experiments is to demonstrate that the test loss of the trained Transformer model decreases as the number of training samples increases, i.e., for N=400, N=1200, and N=10000. This decreasing trend in test loss is observed consistently across all model dimensions tested, namely $d_m=64$, $d_m=1024$, and $d_m=4096$. The learning rate used in the experiments is 0.01, the optimization algorithm is batch gradient descent,

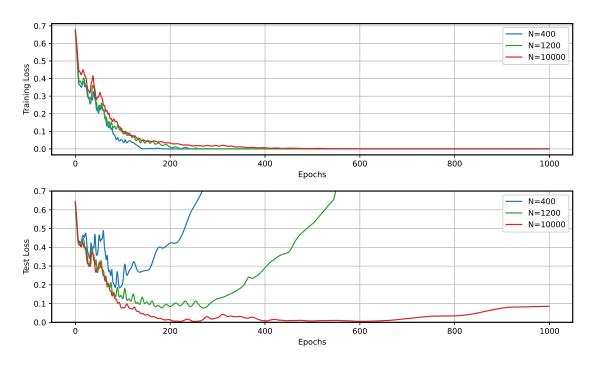


Figure 2: Evolution of training loss (top) and test loss(bottom) for each epoch of training for model dimension $d_m = 1024$.

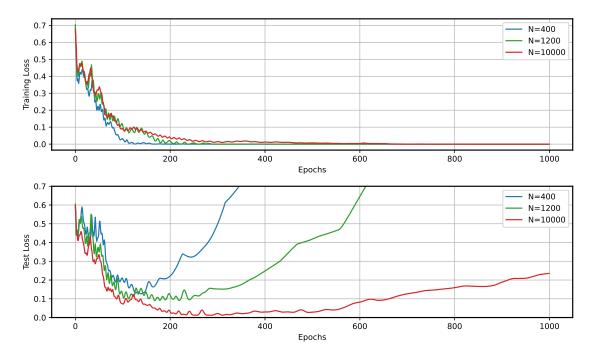


Figure 3: Evolution of training loss (top) and test loss(bottom) for each epoch of training for model dimension $d_m = 4096$.

and the loss function employed is the mean squared error (MSE) loss. The results are presented below, where each figure 4-6 shows the training loss and test loss trajectories of the Transformer model as training progresses over 2000 epochs.

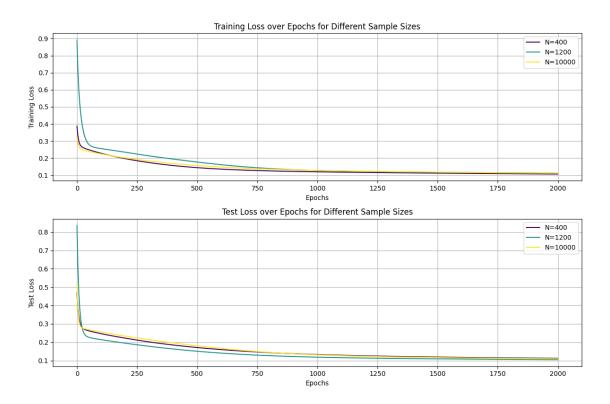


Figure 4: Evolution of training loss (top) and test loss(bottom) for each epoch of training for model dimension $d_m = 64$.

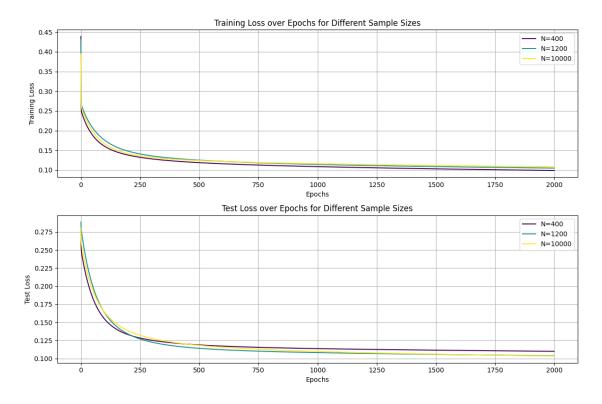


Figure 5: Evolution of training loss (top) and test loss(bottom) for each epoch of training for model dimension $d_m = 1024$.

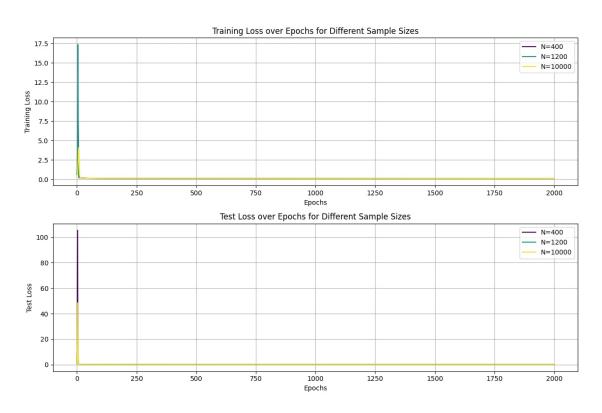


Figure 6: Evolution of training loss (top) and test loss(bottom) for each epoch of training for model dimension $d_m = 4096$.