REALITY ONLY HAPPENS ONCE: SINGLE-PATH GENERALIZATION BOUNDS FOR TRANSFORMERS

Anonymous authors
Paper under double-blind review

ABSTRACT

One of the inherent challenges in deploying transformers on time series is that *reality only happens once*; namely, one typically only has access to a single trajectory of the data-generating process comprised of non-i.i.d. observations. We derive non-asymptotic statistical guarantees in this setting through bounds on the *generalization* of a transformer network at a future-time t, given that it has been trained using $N \leqslant t$ observations from a single perturbed trajectory of a bounded and exponentially ergodic Markov process. We obtain a generalization bound which effectively converges at the rate of $\mathcal{O}(1/\sqrt{N})$. Our bound depends explicitly on the activation function (Swish, GeLU, or $\tanh$ are considered), the number of self-attention heads, depth, width, and norm-bounds defining the transformer architecture. Our bound consists of three components: (I) The first quantifies the gap between the stationary distribution of the data-generating Markov process and its distribution at time t, this term converges exponentially to 0. (II) The next term encodes the complexity of the transformer model and, given enough time, eventually converges to 0 at the rate $\mathcal{O}(\log(N)^r/\sqrt{N})$ for any $r > 0$. (III) The third term guarantees that the bound holds with probability at least $1 - \delta$, and converges at a rate of $\mathcal{O}(\sqrt{\log(1/\delta)}/\sqrt{N})$. Example of (non i.i.d.) data-generating processes which we can treat are the projection of several SDEs onto a compact convex set C, and bounded Markov processes satisfying a log-Sobolev inequality.

1 INTRODUCTION

Transformers Vaswani et al. (2017) have become the main architectural building block in deep learning-based state-of-the-art foundation models Bommasani et al. (2021); Zhao et al. (2023); Wei et al. (2022). Transformers are primarily deployed on sequential learning tasks which have complex temporal relationships, and thus, transformers are trained on non-i.i.d. data. The i.i.d. assumption is typically made (e.g. Neyshabur et al. (2015); Bartlett et al. (2017); Zhang et al. (2024)) to derive theoretical statistical guarantees, but in practice, it is rarely satisfied; e.g. in natural language processing (NLP) (Zhou et al., 2021), physics Paul and Baschnagel (2013), medical research Beck and Pauker (1983), reinforcement learning Sutton and Barto (2018), optimal control Touzi (2013), and in finance Föllmer and Schied (2011). This creates a mismatch between available statistical guarantees in deep learning (which often rely on the i.i.d. assumption or they do not provide explicit constants for transformers trained on non-i.i.d. data) and how transformers are used in practice.

Thus, this paper fills this gap by guaranteeing that transformers trained on a single time-series trajectory can generalize at future moments in time, with explicit constants. We, therefore, consider the learning problem where the user is supplied with N paired samples $(X_1, Y_1), \ldots, (X_N, Y_N)$, where each input $Y_n = f^\star(X_n)$ for a smooth (unknown) *target function* $f^\star : \mathbb{R}^{d\times M} \to \mathbb{R}^D$ is to be learned, depending on a history length M, and where the inputs are generated by a time-homogeneous Markov process $X_\cdot \stackrel{\text{def.}}{=} (X_n)_{n=1}^\infty$. Note that the assumption $Y_n = f^\star(X_n)$ results in only a mild loss of generality since if $X_\cdot$ is a discretized solution to a stochastic differential equation then $Y_n \approx$ signal + additive noise due to stochastic calculus considerations (see Appendix G).

The performance of any transformer model $\mathcal{T} : \mathbb{R}^{d\times M} \to \mathbb{R}^D$ is quantified via a smooth loss function $\ell : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$. When $M = 1$, the generalization of such a $\mathcal{T}$ is measured by the gap between its *empirical risk* $\mathcal{R}^{(N)}$, computed from the single-path training data, and its *(true) t-future risk* $\mathcal{R}_t$ at a (possibly infinite) future time $N \leqslant t \leqslant \infty$ ($t \in \mathbb{N}_+$) defined by

$$\mathcal{R}_t(\mathcal{T}) \stackrel{\text{def.}}{=} \mathbb{E}\big[\ell(\mathcal{T}(X_t), f^\star(X_t))\big]$$

where $\mathcal{R}_t$ (resp. $\mathcal{R}_\infty$) is computed with respect to the distribution of X_t (resp. *stationary distribution* of $X_\cdot$). The time-t excess-risk $\mathcal{R}_t$, which is generally unobservable, is estimated by a single-path estimator known as the empirical risk computed using all the noisy samples observed thus far

$$\mathcal{R}^{(N)}(\mathcal{T}) \stackrel{\text{def.}}{=} \frac{1}{N}\sum_{n=1}^{N} \ell(\mathcal{T}(X_n), f^\star(X_n)).$$

Our objective is to obtain a statistical learning guarantee bounding the gap between the empirical risk and the t-future risk of transformer models trained on a single path.

Contribution. Our main result is a bound on the *future-generalization*, at any given time $t \geqslant N$, of a transformer trained from N samples collected from an unknown transformation ($f^\star$) of any suitable unknown Markov process ($X_\cdot$). For this, fix a class of transformers $\mathcal{TC}$ for respective input and output dimensions d and D, i.e. determine the number of transformer blocks, the number of attention heads, channel sizes, and specify a constraints on its weights. Then, the first takeaway of our main result (Theorem 1) is that with probability at least $1-\delta$

$$\sup_{\mathcal{T}\in\mathcal{TC}} \big|\mathcal{R}_t(\mathcal{T}) - \mathcal{R}^{(N)}(\mathcal{T})\big| \in \mathcal{O}\left(\frac{\log(1/\delta) + \log(N)^{1/s}}{\sqrt{N}}\right) \qquad \text{(FutureGen)}$$

where $s > 0$ can be made arbitrarily large and $\mathcal{O}$ hides a dimensional constant depending on s.

Our *primary contribution* is a full analysis of the constant under the big $\mathcal{O}$ in our future-generalization bound (Theorem 1) via a complete estimation of the higher order sensitivities/derivatives of the transformer network (Theorems 6 and 7). Our result provides the first generalization bound applicable to transformers trained on non-i.i.d. data with *explicit constants*; all other available statistical guarantees for models trained on non-i.i.d. data which we are aware of, e.g. Yu (1994); Mohri and Rostamizadeh (2008; 2010); Kuznetsov and Mohri (2017); Simchowitz et al. (2018); Foster et al. (2020); Ziemann and Tu (2022), do not yield explicit bounds for transformers since they alone do not yield explicit constants without appealing to our main technical results: Theorems 6 and 7.

Our *secondary contribution* is a detailed analysis of the effects of the number of attention heads, depth, and width of the transformed model, and weight and bias restriction, as well as on the activation functions used on the generalization of the transformer model. This is because the explicit constants our main results are clearly expressed in terms of these quantities. We also perform an in-depth analysis for the Swish Ramachandran et al. (2017), GeLU Hendrycks and Gimpel (2016), and the $\tanh$ activation functions. We validate the empirical evidence suggesting that the popular activation functions such as Swish provide superior performance than unconventional choices such as $\tanh$.

Benefit our Optimal Transport-Theoretic Approach. An important feature of our generalization bound is that it relies on a recently well-studied optimal transport-theoretic notion of exponential ergodicity, which is *easily verified, or already known,* for most data-generating processes. Indeed, there is a large and growing body of literature verifying that a broad range of standard processes verify this mixing condition (Assumption 2), from classical SDEs to McKean-Vlasov and reflected SDEs. Several examples are provided in Section 2.

Related Work. The mathematical foundations of transformer networks have recently come into focus in the deep learning theory community. Most of the available statistical guarantees for transformers either concern: in-context learning for linear transformers Zhang et al. (2024); Garg et al. (2022), transformers Von Oswald et al. (2023); Akyürek et al. (2023) trained with gradient descent, or instance-dependent bounds Trauger and Tewari (2023) for general transformers. These results, however, do not apply in time series analysis contexts where each training sample is not independent of the others but is rather generated by some recursive stochastic process, e.g. a Markov process.

Analytic counterparts to the statistical guarantees for transformers have also emerged. These include universal approximation theorems for transformer networks Yun et al. (2019; 2020); Fang et al. (2023) and contained universal approximation results for networks leveraging generalized attention mechanisms Kratsios and Papon (2022), and the identification of function classes which can be efficiently approximated by transformers special classes Likhosherstov et al. (2021); Frieder et al. (2024). From the computability standpoint, transformers are Turing complete Bhattamishra et al. (2020).

Generalization bounds for multilayer perceptrons (MLPs) have been actively studied for years. For classification problems, these generalization bounds often rely on bounding the VC-dimension of classes of MLPs, depending on their depth, width, norm bounds on their parameters and activation functions Bartlett et al. (1998; 2019), or similar quantities. In regression problems, one instead controls the Rademacher complexity of similar classes of MLPs Bartlett et al. (2017); Neyshabur et al. (2019); Yin et al. (2019), due to the results such as Koltchinskii (2001); Bartlett and Mendelson (2002), or turns to instance-dependent bounds which control the path-norm of the MLP Neyshabur et al. (2015); Golowich et al. (2020); Galanti et al. (2024) and local variants of these quantities; e.g. Bartlett et al. (2005) or Hou et al. (2023b). Our generalization bounds also partially borrow ideas from both of these directions, but instead, we use high-order sensitivities (partial derivatives) of our transformer networks to obtain tighter bounds for large enough N. This does not yield a faster rate, since the $\mathcal{O}(1/\sqrt{N})$ rate is generally optimal, by the central limit theorem, but it allows us to better control the constants in the generalization bound and thus yields more precise bounds. Thus, a key part of our *technical contributions* is the computation of these higher-order derivatives (C^s-norms, see Definition 3) both of the transformer and the MLP models using smooth activation functions.

These statistical learning results assume that the data samples are i.i.d. However, time-series data is rarely i.i.d, they are often generated by Markov process or at least embeddable into a Markovian setting Cuchiero and Teichmann (2019; 2020a). Though there are generalization bounds for non-i.i.d. relying on martingale arguments e.g. Kontorovich (2014) and concentration of measure phenomena for martingale sums e.g. Bercu et al. (2015); Boucheron et al. (2013) those results primarily focus on Lipschitz functions; thus, they do not consider higher-order derivatives. Our results add to this literature since we rely on the concentration of measure phenomena for Markov processes with respect to smooth counterparts of the 1-Wasserstein distance (a tool used in many martingale arguments, e.g. Kontorovich and Raginsky (2017), for Lipschitz classes).

There are several results in the literature addressing learning with non-i.i.d. data satisfying a mixing/ergodicity condition dating back, at least, to Yu (1994). However, none of these results provide explicit generalization bounds for transformer classes as they either rely on bounding the Rademacher complexity of the transformer class, e.g. in applying Mohri and Rostamizadeh (2008), or they rely on computing the cardinality of delta nets Ziemann and Tu (2022), both of which necessitate the computation of the worst-case Lipschitz (or C^s norm) of any transformer in the hypothesis class using (van der Vaart and Wellner, 2023, Theorem 2.7.4) and (Lorentz et al., 1996, Equation (15.1.8)). These highly technical computations of the worst-case C^s norm case of any transformer our hypothesis class was never computed before our Theorems 6 and 7. Alternatively, prior results impose strong assumptions on the data-generating process Simchowitz et al. (2018); Foster et al. (2020).

We require that the data-generating Markov process has an exponentially contracting Markov kernel Kloeckner (2020). For Markov chains, i.e. finite-state space Markov processes, this means that the generator (Q-matrix) of the Markov chain has a *spectral gap*. These spectral gaps are actively studied in the Markov chain literature Mufa (1996); Kontoyiannis and Meyn (2012); Atchadé (2021); Paulin (2015); Kloeckner (2019) since these have a finite mixing time, meaning that the distribution of such Markov chains approaches their stationary limit after a large finite time has elapsed; i.e. they have well-behaved (approximate) mixing times Montenegro et al. (2006); Hsu et al. (2015); Wolfer and Kontorovich (2019); Zamanlooy (2024). We rely on actively-studied optimal transport-theoretic notions of mixing since it is easily verified, or already known, for most data-generating processes than more classical notions; e.g. Kuznetsov and Mohri (2017); Mohri and Rostamizadeh (2010).

Our generalization bounds rely on concentration of measure arguments for the "smooth" integral probability metrics (IPMs) studied in Kloeckner (2020); Riekert (2022), by refining the arguments of Hou et al. (2023b); Benitez et al. (2023); Kratsios et al. (2024) to the non-i.i.d. and smooth setting. In the i.i.d. case, our computation of the maximum C^s-norm ($R \geqslant 0$) of the class $\mathcal{TC}$ (Theorem 6) can be used to relate the rate at which measure concentrates to other bounds based on classical quantities such as the Rademacher complexity of the class of C^s-functions on $\mathbb{R}^d$; which is bounded by R, see e.g. (Sriperumbudur et al., 2012, Theorem 3.3).

Further Applications of our Secondary Results. The upper bounds, which we compute for the C^s norms of the transformers models, can be used in conjunction with classical VC-dimension van der Vaart and Wellner (2023), Rademacher complexity Bartlett and Mendelson (2002), or optimal transport Hou et al. (2023b) type arguments to obtain generalization bounds in the simpler setting of i.i.d. data where there is *no notion of (future) time*, not considered here. This can be done using classical tools, e.g. entropy estimates in (van der Vaart and Wellner, 2023, Theorem 2.7.4) on compact domains due to the Sobolev embedding theorem, applied to the larger class of C^s on $\mathbb{R}^{d\times M}$ whose C^s-norms are almost equal to the one we have computed for $\mathcal{TC}$ in Theorems 6 and 7.

2 Background and Preliminaries

This section overviews the necessary background for a self-contained formulation of our main results. This includes the definition of transformers and examples of data-generating processes treatable within our framework.

2.1 Admissible Data-Generating Processes

Fix dimensions $d, D \in \mathbb{N}_+$, a finite memory $M \in \mathbb{N}_+$, and let $X_\cdot \stackrel{\text{def.}}{=} (X_n)_{n\in\mathbb{N}_0}$ be a stochastic process taking values in $\mathbb{R}^d$, such that the lifted/concatenated process $X_\cdot^M \stackrel{\text{def.}}{=} (X^M_{[0\vee(n-M),\dots,0\vee n]})_{n\in\mathbb{N}_0}$ is Markovian on $\mathbb{R}^{Md}$. Let P be a Markov kernel on a non-empty Borel $\mathcal{X}^M \subseteq \mathbb{R}^{Md}$ with initial distribution $X_0 \sim \mu_0 \in \mathcal{P}(\mathbb{R}^{Md})$ given by $X_n^M \sim \mu_n \stackrel{\text{def.}}{=} P^n\mu_0 \stackrel{\text{def.}}{=} \mathbb{P}(X_n^M \in \cdot)$ and for each $x \in \mathbb{R}^{Md}$ and $n \in \mathbb{N}_+$, set $P^n(x,\cdot) \stackrel{\text{def.}}{=} \mathbb{P}(X_n^M \in \cdot | X_0^M = x)$. The process $X_\cdot^M$ is called a *Markovian lift* of $X_\cdot$ in the literature; see e.g. Cuchiero and Teichmann (2020b).
Examples of processes with *finite-dimensional* Markovian lifts are ARIMA times-series models, see e.g. (Cryer and Kellet, 1991), or stochastic *delay* differential equations; see e.g. Buckwar (2000).

Assumption 1 (Bounded Trajectories)**.** *There is a $c > 0$ such that* $\mathbb{P}(\sup_{t\in\mathbb{N}} \|X_t\| \leqslant c) = 1$.

Assumption 2 (Exponential Ergodicity)**.** *There is a $\kappa \in (0,1)$ such that: for each $\mu, \nu \in \mathcal{P}(\mathbb{R}^{Md})$ and every $t \in \mathbb{N}_+$ one has $\mathcal{W}_1(P^t\mu, P^t\nu) \leqslant \kappa^t\, \mathcal{W}_1(\mu,\nu)$.*

2.1.1 Examples: Projected SDEs - From Langevin Dynamics to Martingales

A broad class of non-i.i.d. data-generating processes satisfying our assumptions is a broad generalization of any Markov processes obtained by "projecting" the strong solution to a stochastic differential equation (SDE) with overdampened drift onto a compact convex subset of $\mathbb{R}^d$. The processes which we can project are vast generalizations of the forward process used in *denoising diffusion models*; see e.g. Song et al. (2020) whose convergence is by now well-understood; see e.g. Chen et al. (2023).

Example 1 (Projected SDEs with Overdampened Drift)*.* Consider a latent dimension $\bar{d} \in \mathbb{N}_+$, $\mu : \mathbb{R}^{\bar{d}} \to \mathbb{R}^{\bar{d}}$ be Lipschitz and the gradient of a strongly convex function; i.e. there is a $K > 0$ such that $(\mu(x) - \mu(y))^\top (x - y) \leqslant -K\|x - y\|^2$ for all $x, y \in \mathbb{R}^d$. For any $x \in \mathbb{R}^{\bar{d}}$ let $Z_\cdot^x \stackrel{\text{def.}}{=} (Z_t^x)_{t\geqslant 0}$ be the unique strong solution (which exists by (Da Prato, 2008, Theorem 8.2) since μ is Lipschitz)

$$Z_t^x = x + \int_0^t \mu(Z_s^x)\, ds + \int_0^t W_s \tag{1}$$

where $W_\cdot$ is a $\bar{d}$-dimensional Brownian motion. Let $f : \mathbb{R}^{\bar{d}} \to \mathbb{R}^d$ be a bounded 1-Lipschitz function and consider the discrete-time Markov process $X_\cdot \stackrel{\text{def.}}{=} (X_n)_{n=0}^\infty$ on $\mathbb{R}^d$ given by

$$X_n^x \stackrel{\text{def.}}{=} f(Z_n^x).$$

As shown in Proposition 2, $X_\cdot$ satisfies Assumptions 1 and 2. The standard example of SDEs (1) are *Langevin dynamics* for a strictly convex potential $U : \mathbb{R}^d \to \mathbb{R}$. As shown in Bolley et al. (2012)

$$\mu(x) = -\nabla U(x)/2. \quad \triangleleft$$

Example 2 (Projections of Diffusive Martingales)*.* Let $d \in \mathbb{N}_+$. Let $\sigma : \mathbb{R}^d \to P_d^+$ taking values in the cone P_d^+ of $d \times d$-dimensional positive definite matrices, be Lipschitz with the Fröbenius norm on $\mathbb{R}^{d\times d}$, and satisfy the uniform ellipticity condition: there exists a $\lambda > 0$ such that for every $x \in \mathbb{R}^d$ holds $s_{min}(\sigma(x)\sigma(x)^\top) \geqslant \lambda$, where $s_{min}(A)$ denotes the minimal singular values of a matrix A. Consider the martingale $Z_\cdot$ (see (Da Prato, 2008, Proposition 6.15) for a proof of martingality) defined for each $t \geqslant 0$ by $Z_t = \int_0^t \sigma(Z_s)\, dW_s$ where $W_\cdot \stackrel{\text{def.}}{=} (W_t)_{t\geqslant 0}$ is a d-dimensional

Brownian motion. Let $f : \mathbb{R}^d \to \mathbb{R}^d$ be any 1-Lipschitz bounded function. By Proposition 3, the data-generating Markov process $X_\cdot \overset{\text{def.}}{=} (X_n)_{n=0}^\infty$, defined for each $n \in \mathbb{N}_+$ by $X_n \overset{\text{def.}}{=} f(Z_n)$ satisfies both Assumptions 1 and 2. $\triangleleft$

We have presented the simplest cases here; which is readily generalizable. By Lemma 1 to any Markov process exponentially ergodic $Z_\cdot$, not necessarily solving the simple dynamics (1), automatically yields examples of data-generating processes satisfying both Assumptions 1 and 2. We list some examples of such processes here: McKean-Vlasov type with relatively general, i.e. it can have non-constant law-dependent drift and diffusion coefficients (Wang, 2023, Corollary 4.4) (possibly with reflections), several SDEs is driven by a pure-jump Lévy process (Luo and Wang, 2019, Theorem 3.1). Note when considering reflected SDEs (possibly of McKean-Vlasov type), where the reflections constrain the process to remain in a bounded convex domain, we do not need f to be bounded, as the processes themselves are already bounded. Further examples of such can be constructed using compact Riemannian sub-manifolds of $\mathbb{R}^d$ with suitable curvature bounds Ollivier (2009).

2.1.2 Examples: Markov Processes with Log-Sobolev-type Kernel

Our main result is equally valid under the assumption that the stationary distribution of the Markov chain and its kernels all satisfy a log-Sobolev inequality (LSI). Since their introduction, LSIs have been heavily studied Gross (1975); Ledoux et al. (2015); Zimmermann (2013); Inglis and Papageorgiou (2019); Chen et al. (2021) and have found numerous applications in differential privacy Minami et al. (2016); Ye and Shokri (2022), optimization Chaudhari et al. (2019), random matrix theory Wigner (1955; 1957), optimal transport Dolera and Mainini (2023), since they typically imply Gozlan (2010); Gozlan et al. (2015) and effectively characterizes Gozlan (2009) dimension-free rate for concentration of measure. We define the *entropy functional* $\mathcal{H}_\mu$ associated to any Borel probability measure μ on $\mathbb{R}^d$ acts on smooth functions $g : \mathbb{R}^d \to \mathbb{R}$ by

$$\mathbb{H}_\mu(g) \overset{\text{def.}}{=} \mathbb{E}_{X\sim\mu}\Big[g(X) \log\Big(\frac{g(X)}{\mathbb{E}_{Z\sim\mu}[g(Z)]}\Big)\Big].$$

The entropy functional can be used to express the log-Sobolev inequalities.

Definition 1 (Log-Sobolev Inequality). *A probability measure μ on $\mathbb{R}^d$ is said to satisfy a log-Sobolev inequality with constant $C > 0$ (LSI_C) if for every smooth function $g : \mathbb{R}^d \to \mathbb{R}$*

$$\mathbb{H}_\mu(g^2) \leqslant C\, \mathbb{E}_{X\sim\mu}[\|\nabla g(X)\|^2]$$

We require that the Markov process is time-homogeneous to admit a satisfactory measure. Further, we require that its Markov kernel and its stationary measure all satisfy LSI_C.

Assumption 3 (Satisfactions of the Log-Sobolev Inequality). *There exists a $C > 0$ such that $\bar{\mu}$, μ_0, and $P(x,\cdot)$ all satisfy LSI_C, for each $x \in \mathcal{X}$.*

Instead of the compact support Assumption 1 we may consider the following weaker condition.

Assumption 4 (Exponential Moments). *There exist $\lambda, \tilde{C} > 0$ and $\gamma \in (0,1)$ such that: for each $x \in \mathcal{X}$ we have $\mathbb{E}_{X\sim P(x,\cdot)}[e^{\lambda|X|}] \leqslant \gamma\, e^{\lambda|x|} + \tilde{C}$.*

Note that, Assumption 1 implies 4, but not conversely.

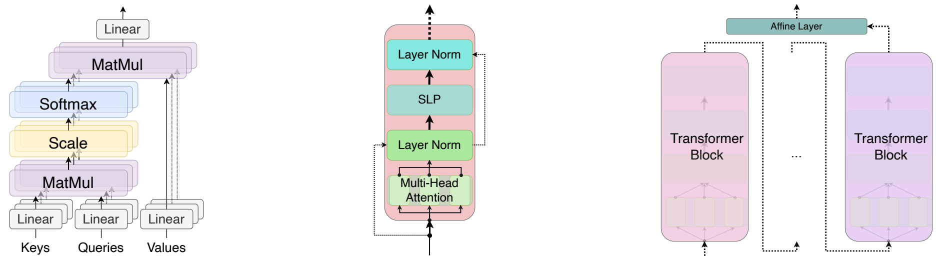
Several examples of Markov processes satisfying LSI inequalities are given in Ledoux (2006) and Gaussian processes satisfy the Exponential Moments Assumption. If one instead

Proposition 1 (Log-Sobolev Conditions and Exponential Moments Imply Assumption 2). *If Assumptions 4 and 3 hold then the process $X_\cdot$ satisfies Assumption 2.*

2.2 The Transformer Model

The overall structure of transformers is summarized in Figure 1, and we give an in-depth definition of all components with their respective dimensions in Appendix C, which is relevant for the details of the bound computation. On a high level, the most important aspects are:

Multi-Head Attention [$\mathcal{MH}$]. Consists of parallel application of the attention mechanism, described by the following steps. (i) Inputs are used three-fold, as keys, queries, and values, all are transformed by distinct linear transformations. (ii) Keys and queries are multiplied, scaled, and transformed by a softmax application. (iii) This output is combined in a matrix multiplication with the values.



(a) **Multi-Head Att. (Def. 4)** *(b)* **Transformer Block (Def. 5)** *(c)* **Transformer (Def. 6)**

Figure 1: The transformer architecture.

Transformer Block [$\mathcal{TB}$]. Here, (i) input features are mapped to contexts via *multi-head attention mechanism*, (ii) the output of the multi-head attention mechanism and the input features (via a skip connection) are normalized by a *layer-norm [$\mathcal{LN}$]* (see Appendix C), (iii) the normalized contextual features are transformed non-linearly by a *single-layer perceptron [$\mathcal{PL}$]*, and (iv) its outputs, together with the first set of normalized context (via another skip connection), are normalized by a final *layer-norm* and returned by the transformer block.

Transformer [$\mathcal{T}$]. Iteratively feed input features through a series of transformer blocks before processing their outputs with a (fully connected affine layer). We denote a class of transformers of a fixed architecture by $\mathcal{TC}$, with each parameter bounded to a predefined domain.

2.3 Setting

We consider smooth loss and target functions that are concentrated on a compact region, along with their derivatives. The growth rate of the C^s-norm (see Definition 3 in Appendix A) of the loss function and its derivatives quantifies the degree of concentration. One easily verifies that any function in the Schwartz class satisfies this former of the following conditions, cf. Treves (2016).

Definition 2 (Polynomial Growth of Derivatives)**.** *Let $d, D, M \in \mathbb{R}$. A smooth function $g : \mathbb{R}^{Md} \to \mathbb{R}^D$ is in the class $C^\infty_{poly:C,r}([0,1]^{Md}, \mathbb{R}^D)$ if $C, r \geqslant 0$ are such that $\|g\|_{C^s([0,1]^{Md})} \leqslant C\, s^r$ for each $s \in \mathbb{N}_+$. Here, $\|\cdot\|_{C^s}$ is the uniform Sobolev norm on the specified domain.*

In Appendix E.2 we show that, in one dimension, any real analytic function whose power series expansion at 0, has coefficients growing at an $\mathcal{O}((s+1)^r)$ rate belongs to $g \in C^\infty_{poly:C,r}([0,1], \mathbb{R})$. One can easily extend this argument to multiple dimensions to obtain further examples.

We consider an *realizable* PAC learning problem, determined by a smooth 1-Lipschitz *target function* $f^\star : \mathbb{R}^d \to \mathbb{R}^D$ which we would like to learn using a sequence of random observations $\big((X_t, Y_t)\big)_{t\in\mathbb{N}}$ as our training data. That is, for each $t \in \mathbb{N}_+$

$$Y_t \overset{\text{def.}}{=} f^\star(X_t)$$

We aim to learn f from a *single path*. The ability of a model to reliably recover the function $f : \mathbb{R}^d \to \mathbb{R}^D$ at time t, given the input X_t, is quantified by the *t-future risk*

$$\mathcal{R}_t(f) \overset{\text{def.}}{=} \mathbb{E}\big[\ell(f(X_t), f^\star(X_t))\big].$$

The time-t excess-risk $\mathcal{R}_t$, which is generally unobservable, is estimated by a single-path estimator known as the empirical risk computed using all the noisy samples to observed thus far

$$\mathcal{R}^{(N)}(f) \overset{\text{def.}}{=} \frac{1}{N} \sum_{n=1}^{N} \ell(f(X_t), f^\star(X_t)).$$

Our objective is to obtain a statistical learning guarantee on the quality of our estimate of the target function given by the *time t ($\in \mathbb{N}_+$) generalization gap* $\big|\mathcal{R}_t(f) - \mathcal{R}^{(N)}(f)\big|$.

We now summarize our setting and all parameters defining it, e.g. dimension, number of attention heads in the transformer, growth rate of the derivatives of the target and loss functions, etc.

Setting 2.1 (Standing Assumptions)**.** *Consider a hypothesis class $\mathcal{TC}$. Fix $r_f, r_\ell, C_f, C_\ell \geqslant 0$, as well as a target function f^* and loss function ℓ with*

$$f^\star \in C^\infty_{poly:C_f,r_f}(\mathbb{R}^{Md}, \mathbb{R}^D) \quad \text{and} \quad \ell \in C^\infty_{poly:C_\ell,r_\ell}(\mathbb{R}^{2D}, \mathbb{R});$$

and suppose that Assumption 1 and either of 2 or 3 hold.

3 Main Results

3.1 Future Generalization

Having formalized our setting, we may now state our first main result, which is a version of (FutureGen). This version provides insights on the future-generalization of transformers via: 1) explicit constants and 2) explicit *phase transition times* above which the convergence rate in (FutureGen) accelerates by a polylogarithmic factor. We express these times of convergence rate acceleration using the following *convergence rate function*

$$\mathrm{rate}_s(N) \overset{\text{def.}}{=} \begin{cases} \frac{\log(c\,N)^{d-2s+s/d}}{c_2\,N^{s/d}} & \text{if } Md > 2s \quad \textit{(initial phases)} \\ \frac{\log(c\,N)}{c\,N^{1/2}} & \text{if } Md = 2s \quad \textit{(critical phase)} \\ \frac{\log(c\,N)^{d/(2s+1)}}{c\,N^{1/2}} & \text{if } Md < 2s \quad \textit{(eventual phases)} \end{cases} \tag{rate}$$

where $c \overset{\text{def.}}{=} 1-\kappa$, $c_2 \overset{\text{def.}}{=} c^{s/d}$, and $0 < \kappa < 1$ are constants depending only on $X_\cdot$.

Theorem 1 (Pathwise Generalization Bounds for Transformers)**.** *In Setting 2.1, there exists* $\kappa \in (0,1)$*, depending only on* $X_\cdot$*, and* $t_0 \in \mathbb{N}_0$*; such that for each* $t_0 \leqslant N \leqslant t \leqslant \infty$ *and* $\delta \in (0,1]$ *the following holds with probability at-least* $1-\delta$

$$\sup_{\mathcal{T}\in\mathcal{TC}} \left|\mathcal{R}_{\max\{t,N\}}(\mathcal{T}) - \mathcal{R}^{(N)}(\mathcal{T})\right| \lesssim \sum_{s=0}^{\infty} I_{N\in[\tau_s,\tau_{s+1})}\, C_{\ell,\mathcal{TC},K,s}\Big(\underbrace{\kappa^t}_{\text{(I)}} + \underbrace{\mathrm{rate}_s(N)}_{\text{(II)}} + \underbrace{\frac{\sqrt{2\ln(1/\delta)}}{N^{1/2}}}_{\text{(III)}}\Big)$$

with $I_\cdot$ *as indicator function,* $\mathrm{rate}_s(N)$ *as in (rate), the constant* $C_{\ell,\mathcal{TC},K,s} \overset{\text{def.}}{=} \sup_{\mathcal{T}\in\mathcal{TC}} \|\ell(\mathcal{T}, f^*)\|_{C^s}$*, and the transition times* $(\tau_s)_{s=0}^{\infty}$ *are given iteratively by* $\tau_0 \overset{\text{def.}}{=} 0$ *and for each* $s \in \mathbb{N}_+$

$$\tau_s \overset{\text{def.}}{=} \inf\left\{ t \geqslant \tau_{s-1} : C_{\ell,\mathcal{TC},K,s}\Big(\kappa^t + \mathrm{rate}_s(N) + \frac{\sqrt{\log(1/\delta)}}{\sqrt{N}}\Big) \leqslant C_{\ell,\mathcal{TC},K,s-1}\Big(\kappa^t + \mathrm{rate}_{s-1}(N) + \frac{\sqrt{\log(1/\delta)}}{\sqrt{N}}\Big)\right\}.$$

Furthermore, $c \overset{\text{def.}}{=} 1-\kappa$*,* $c_2 \overset{\text{def.}}{=} c^{s/d}$*,* $\kappa^\infty \overset{\text{def.}}{=} \lim_{t\to\infty} \kappa^t = 0$*, and* $\lesssim$ *hides an absolute constant.*

Theorem 1 implies the order estimate in (FutureGen). This is because $C_{\ell,\mathcal{TC},K,s}$ is constant in N and $\mathrm{rate}_s(N) < \mathrm{rate}_{s-1}(N)$; thus, for every $s > 0$ the right-hand side our bound is eventually bounded by any $C_{\ell,\mathcal{TC},K,s}(\kappa^t + \sqrt{2\ln(1/\delta)}/N^{1/2} + \mathrm{rate}_s(N))$ for N large enough. However, unlike the order estimate (FutureGen), Theorem 1 provides an explicit description of the actual size of the future-generalization gap in terms of three factors which we now interpret.

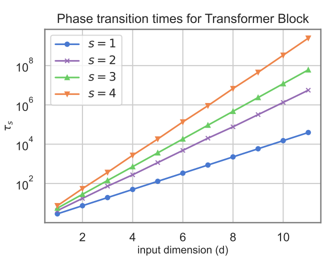


Figure 2: **Transition times:** (y-axis) when the future-generalization bound accelerates by a polylogarithmic factor (in N) for a single transformer block in terms of the input dimension d (x axis). See Section 3.2 for details on constants.

Non-Stationarity Term. Term (I) quantifies the rate at which the data-generating Markov process $X_\cdot$ becomes stationary. This term only depends on the time t and a constant $0 < \kappa < 1$ determined only by $X_\cdot$. We use the notational convention $\kappa^\infty \overset{\text{def.}}{=} \lim_{t\to\infty} \kappa^t = 0$ to describe the limiting case.

Model Complexity Term (Phase Transitions). Term (II) captures the complexity of the transformer network in terms of the number of self-attention heads, depth, width, and the activation function used to define the class $\mathcal{TC}$. Each constant $C_1 \leqslant \ldots \leqslant C_s \leqslant \ldots$ collects the higher-order sensitivities (s^{th} order partial derivatives; where $s \in \mathbb{N}_+$) of the transformer model. Each $0 = \tau_0 \leqslant \tau_1 \leqslant \ldots \leqslant \tau_s \leqslant$ indicates the times at which there is a phase-transition in the convergence rate of the generalization bound accelerates. Once $t \geqslant \tau_s$, then the convergence rate of Term (II) accelerates, roughly speaking, by a reciprocal log-factor of $1/\log(N)$. Observe that the rate function is asymptotically equal to the rate function from the central limit theorem, as s tends to infinity; that is, $\lim_{s\to\infty} \mathrm{rate}_s(N) = 1/(c\sqrt{N})$. The rate (rate) is the (optimal) rate at which the empirical measure generated by observations from a Markov process converges to its stationary distribution in 1-Wasserstein distance Kloeckner (2020); Riekert (2022). The polylogarithmic factor is removable if the data is i.i.d. Graf and Luschgy (2000); Dereich et al. (2013).

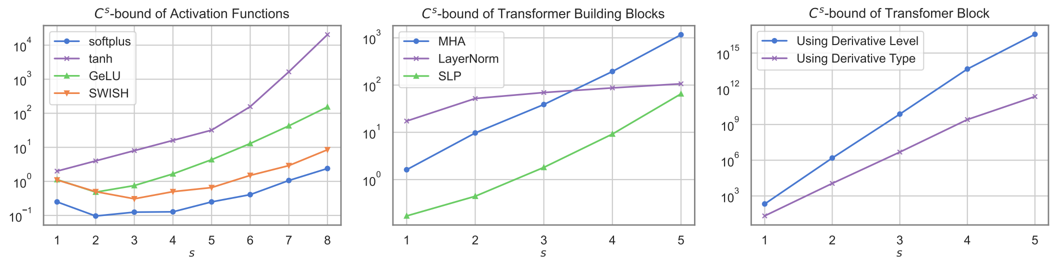


Figure 3: Effects of Transformer Components of FutureGen: (left to right.) The first figure shows the C^s bound of various activation functions according to results in Appendix F.3.3. The second illustrates C^s bounds for Multi-Head Attention (Definition 4), single-layer perceptrons, and the layer norm. The third shows the C^s-bound of a transformer block (Definition 5), distinguishing if the bound was computed level-specific (Corollary 1) or type specific (Theorem 5). The parameters used for the above plots are the base cases of Tables 1 to 5.

Probabilistic Validity Term. Term (III) captures the cost of the bound being valid with probability at least $1-\delta$. The convergence rate of this term cannot be improved due to the central limit theorem. It is responsible for the overall convergence rate of our generalization bound being "stuck" at the optimal rate of $\mathcal{O}(1/\sqrt{N})$ from the central limit theorem; as the other two terms converge exponentially to 0.

3.2 Bound of the C^s-Norm of Transformer Classes

Our second main result is the computation of $C_{\ell,\mathcal{TC},K,s}$, which encodes the maximal size of the first s partial derivatives of any transformer in the class $\mathcal{TC}$. Thus, it encodes the complexity of the class $\mathcal{TC}$ (e.g. int terms of number of attention heads, depth, width, etc...), the size of the compact set K, and the smoothness of the loss function and target functions.

We note that, any uniform generalization bound for smooth functions thus necessarily contains constants of the same order *hidden within the big* $\mathcal{O}$. See e.g. the entropy bound in (van der Vaart and Wellner, 2023, Theorem 2.71) which yields VC-dimension bounds via standard Dudley integral estimates in the i.i.d. case.

Critically, when the function class is defined by function composition, i.e. as in deep learning, then these maximal partial derivatives tend to grow factorially in s. This is a feature of the derivatives of composite functions in high dimensions as characterized by the multi-variate chain rule (i.e. the Faá di Bruno formula Faa di Bruno (1855); Constantine and Savits (1996)). The combinatorics of these partial derivatives is encoded by the coefficients in the well-studied bell-polynomials Bell (1934); Mihoubi (2008); Wang and Wang (2009) whose growth rate has been recently understood in Khorunzhiy (2022) and contains factors of the order of $\mathcal{O}\big(\big(\frac{2s}{e\ln s}(1+o(1))\big)^s\big)$.

Remark that, in the feedforward case, i.e. when no layernorms or multihead attention are used, then the $s=1$ case is bounded above by the well-studied path-norms; see e.g. Bartlett et al. (2017); Neyshabur et al. (2015), which are simply the product of the weight matrices of in the network and serve as a simple upper-bound for the largest Lipschitz constant (i.e. C^1 norm) of the class $\mathcal{TC}$. These constants are included as very specific cases of our constant bounds. This is why we present two versions: a weaker but simpler bound, as well as a more accurate but detailed bound.

Theorem 2 ($\mathcal{TC}$-bound in terms of $\mathcal{O}$)**.** *In the case of a single transformer block $C_{\ell,\mathcal{TC},K,s}$ is of the order of*

$$\mathcal{O}\Big(\underbrace{C^{\ell,f^\star}}_{\text{Loss \& Target}} \underbrace{C^{\mathcal{LN}}_{K^{(3)}}(\leqslant s)^s C^{\mathcal{LN}}_{K^{(1)}}(\leqslant s)^{s^3}}_{\text{Layernorms}} \underbrace{C^{\mathcal{PL}}_{K^{(2)}}(\leqslant s)^{s^2}}_{\text{Perceptron}} \underbrace{\Big(1+C^{\mathcal{MH}}_K(\leqslant s)\Big)^{s^4}}_{\text{Multihead Attention}} \underbrace{D^{s^2} d^{2s^3}}_{\text{dimensions}} \underbrace{c_s^{s^s+s^3+s^4}}_{\text{Generic: } s\text{-th order Derivative}} \Big)$$

where the "generic higher-order derivative constant" is $c_s \overset{\text{def.}}{=} \frac{2s}{e\ln s}(1+o(1))$. Further,

$$C^{\ell,f^\star} = \mathcal{O}\big(C_f^s\, s^{r_\ell+2s^2}\big), \qquad C^{\mathcal{PL}}_K(\leqslant s) = \mathcal{O}\big(c^{\mathcal{PL}} + d_{\text{ff}}\|\sigma\|_s \tilde{c}_s^s (c^{\mathcal{PL}})^{s+1}\big),$$
$$C^{\mathcal{LN}}_K(\leqslant s) = \mathcal{O}\big(s^{(1+s)/2} c_s^s\big), \qquad C^{\mathcal{MH}}_K(\leqslant s) = \mathcal{O}\big(e^{-2s} M^2 (2d_{\text{in}} d_K \cdot c_s)^s (s\cdot c^{\mathcal{MH}})^{2s+2}\big).$$

Here $\tilde{c}_s \overset{\text{def.}}{=} s^{1/2}(n/e)^s c_s^s$; d_{in} is the input-dimension and d_K is the key-dimension of the multi-head attention $\mathcal{MH}$ (see Definition 4 for details); d_{ff} is the width of the neural network $\mathcal{PL}$ (see Definition 5 for details); $c^{\mathcal{PL}}$ as well as $c^{\mathcal{MH}}$ are parameter bounds on $\mathcal{PL}$ as well as $\mathcal{MH}$, respectively (see

Theorem 7 for details); and $\|\sigma\|_s$ is the C^s-bound of the activation function used. If no layer norms, SLP, or multi head attention mechanisms are included in the class, then their respective terms in our order estimate should be taken to be 1.

Proof. The result is a direct consequence of Theorems 7 and 9. The order of the bounds $C_K^{\mathcal{LN}}$, $C_K^{\mathcal{PL}}$, and $C_K^{\mathcal{MH}}$ are given by Corollaries 4, 8 and 9. □

See Appendix F for a full version of this result for deep transformers (Theorem 7).

Explicit bound computation. We further refined this result by deriving formulae that enable the precise calculation of these bounds. In order to enhance the accuracy of these estimates, we distinguished not only between different levels of derivatives but also between various types of derivatives. An exemplary improvement of the bound by this distinction can be seen on the RHS of Figure 3. Since these results are fairly technical and verbose, we relegate them to Appendix F.3, see Theorem 6 for the analogue result to Theorem 7 and Lemmata 7, 12 and 13 for tighter bounds on $C_K^{\mathcal{LN}}$, $C_K^{\mathcal{PL}}$, and $C_K^{\mathcal{MH}}$. Additionally, we provide software tools to efficiently compute the bounds of a given transformer architecture.[1]

3.2.1 Implications of architecture choices.

Figure 3 illustrates the effect of various building blocks in the construction of a transformer (e.g. activation choice, multi-head attention (MHA), layernorms) through their effect on the constants in our generalization bounds. While Tables 1 to 5 contain more details, highlight here some key implications that architecture choices have on the bound:

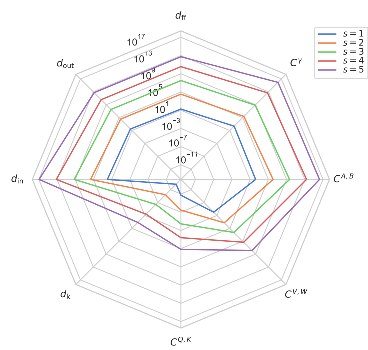


Figure 4: Absolute changes in C^s-bound for changes in architecture. Changes in dimensions ($d_\cdot$) are $\times 2$, while changes in parameter-bounds ($C^\cdot$) are $\times 10$, from the base parameters (see Tables 1 to 5).

I) Choice of Activation Function: We found (see Lemmata 8 to 11) that the C^s-bounds of activation function may vary substantially, framing `softplus` and `swish` as the more regular, and `tanh` resulting in the highest bound. Note that the activation bound impacts the $\mathcal{PL}$-bound linearly and therefore effects the transformer-block bound of order s^2.

II) Effects of Three Different Block-Types: Considering the three components – $\mathcal{MH}, \mathcal{LN}, \mathcal{PL}$ – that make up a transformer block, we observe that for low s the regularization by $\mathcal{LN}$ has the highest bound, but becomes less relevant with the exponential increase of the $\mathcal{MH}, \mathcal{PL}$-bounds for larger s.

III) Weight Size for MLP vs. Multi-Head Attention: As evident in Figure 4 (and Table 4), the parameter-bounds on $\mathcal{PL}$ (denoted by $C^{A,B}$) seem to have a more substantial impact on the bound than the parameter bounds of $\mathcal{MH}$. For the latter, bounds on key- and query-matrices ($C^{K,Q}$) seem to have bigger impacts for lower s than value- and aggregation-matrices ($C^{V,W}$) (see Definition 4 for details on notation), however show larger growth rates for larger s, as also shown in Table 5.

IV) Effect of Dimensions (Key, Input, etc...): Eventually, we can examine how various dimensions effect the bound. The input dimension (d_{in}) has a slightly higher impact than the output dimension (d_{out}). When it comes to choosing latent dimensions, scaling the hidden dimension of the $\mathcal{PL}$ (d_{ff}), has an effect similar to changes in the output dimension, and substantially higher comparing to the key-dimension d_K (see Definitions 4 and 5 in Appendix C for details and notation).

Consequentially, we show the effect on the phase-transition times $(\tau_t)_{t=0}^{\infty}$, defined in Theorem 1, dictating when the bound accelerates by a polylogarithmic factor in N.

3.3 Intuition Via Proof Sketch

The first step in deriving our generalization bounds is to quantify the regularity of the transformer model as a function of its depth, number of attention heads, and norm of its weight matrices. By

[1] The source code to compute derivative bounds is available at `https://anonymous.4open.science/r/transfomer-bounds-B476`.

regularity, we mean the number and size of the continuous partial derivatives admitted by the transformer. To quantify the size of the partial derivatives of the transformer we first remark that it is *smooth*; that is, it admits continuous partial derivatives of all orders (see Theorem 6).

We will uniformly bound the generalization capabilities of the class of transformers $\mathcal{T} \in \mathcal{TC}$ by instead uniformly bounding the generalization of any C^s functions on $\mathbb{R}^{Md}$ with C^s-norm at most equal to the largest C^s-norm in the class $\mathcal{TC}$. That is, we control the right-hand side of

$$\sup_{\mathcal{T}\in\mathcal{TC}} \left|\mathcal{R}_t(\mathcal{T}) - \mathcal{R}^{(N)}(\mathcal{T})\right| \leqslant \sup_{\hat{f}\in\mathcal{C}^s_R(\mathbb{R}^{Md})} \left|\mathcal{R}_t(\hat{f}) - \mathcal{R}^{(N)}(\hat{f})\right| \tag{2}$$

where $R = C_{\ell,\mathcal{TC},K,s}$ as defined in Theorem 1, describes the higher-order fluctuations of the "difference" between the target function $f^\star$ and any transformer $\mathcal{T} \in \mathcal{TC}$, as quantified by the loss function ℓ. Our first step is thus to bound R by upper-bounding maximal size of the s^{th} partial derivatives of all transformers $\mathcal{T} \in \mathcal{TC}$. Explicit bounds are computed in Theorem 6, and their order estimates (as a function of s) are given in Theorem 7. Combing these estimates with the maximal s^{th} partial derivatives of the loss and target function, via a Faá di Bruno-type formula (in Theorem 3 or Lemma 4), which is a multivariant higher-order chain rule, yields our estimate for R in (2).

Now that we have bounded R, appearing in the supremum term in (2), it remains to translate this into a generalization bound. We can do this by relating it to the so-called *smooth Wasserstein distance* d_s between the distribution of the Markov chain at time μ_t and its empirical distribution $\mu^{(N)} \overset{\text{def.}}{=} 1/N \sum_{n=1}^N \delta_{X_n}$ obtained by collecting samples up to time N. The *smooth Wasserstein distance* d_s, studied by Kloeckner (2020); Riekert (2022); Hou et al. (2023a), is the integral probability metric (IPM)-type distance quantifying the distance between any two Borel probability measures μ, ν on $\mathbb{R}^{Md}$ as the maximal distance which they can produced when tested on any function in $C^s_1(\mathbb{R}^{Md})$

$$d_s(\mu,\nu) \overset{\text{def.}}{=} \sup_{g\in\mathcal{C}^s_1(\mathbb{R}^{Md})} \mathbb{E}_{X\sim\mu}[g(X)] - \mathbb{E}_{Y\sim\nu}[g(Y)].$$

The right-hand side (RHS) of (2) can be expressed as R times the d_s distance between the (true) distribution μ_t of the process $X_\cdot$ at time t and the (empirical) distribution $\mu^{(N)}$ collected from samples

$$\text{RHS (2)} \leqslant \sup_{\hat{f}\in C^s_R(\mathbb{R}^{Md})} \|\ell(\hat{f}, f^\star)\|_{C^s}\, d_s(\mu_t, \mu^{(N)}). \tag{3}$$

The d_s distance between the process $X_\cdot$ at time t, i.e. μ_t, and the running empirical distribution $\mu^{(N)}$ can be accomplished in two steps. First, we *fast-forward time* and bound the d_s-distance between $\mu^{(N)}$ and the *stationary distribution* μ_∞ of the data-generating Markov chain $X_\cdot$ (at time $t = \infty$). We then *rewind time* and bound the d_s-distance between the stationary distribution μ_∞ and the distribution μ_t of the Markov process up to time t; by setting up the i.i.d. concentration of measure results of Kloeckner (2019); Riekert (2022). This last step is possible since our assumptions on $X_\cdot$ essentially guarantee that it has a finite (approximate) mixing time.

4 Conclusion, Limitations, and Future Work

We provided a theoretical foundation for the *future-generalization* of transformer trained on a single perturbed realization of a time-series trajectory (Theorem 1). Our results thus help provide insight on the reliability of LLMs outside the i.i.d. framework and their principled use in time-series analysis.

We obtain explicit estimates on the constants in these generalization bounds which relied on *explicitly* bounding all the higher-order derivatives of transformers; in terms of their number of attention heads, activation functions, depth, width, and weights constraints (Theorems 6 and 7). These bounds can equally be used in conjunction with classical tools, e.g. Rademacher or VC-type bounds in the i.i.d. setting, or other applications where one needs to understand the higher-order sensitivities of transformers to their inputs.

Several dynamical systems and financial markets have long-term memory and thus are non-Markovian. In future work, it would be interesting to extend our results to cover such settings as well. It would be interesting to extend our generalizations bounds to the fully non-Markovian setting, where every Markovian lift of $X_\cdot$ is infinite-dimensional. However, one would have to extend the concentration of measure result used in Benitez et al. (2024) to allow for non-i.i.d. data or use a local Glivenko-Cantelli theorem such as Cohen and Kontorovich (2023). One would only need more general concentration inequalities than Proposition 5, which is already extended well beyond the standard i.i.d. setting.

ETHICS STATEMENT

We believe that the potential societal consequences are minimal due to this research project being largely theoretical support of currently deployed deep learning technologies, and it does not deploy new deep learning models or learning algorithms.

REFERENCES

Ekin Akyürek, Dale Schuurmans, Jacob Andreas, Tengyu Ma, and Denny Zhou. What learning algorithm is in-context learning? investigations with linear models. In *The Eleventh International Conference on Learning Representations*, 2023. URL https://openreview.net/forum?id=0g0X4H8yN4I.

Ron Amit, Baruch Epstein, Shay Moran, and Ron Meir. Integral probability metrics pac-bayes bounds. *Advances in Neural Information Processing Systems*, 35:3123–3136, 2022.

Yves F Atchadé. Approximate spectral gaps for markov chain mixing times in high dimensions. *SIAM Journal on Mathematics of Data Science*, 3(3):854–872, 2021.

Kendall Atkinson and Weimin Han. *Spherical harmonics and approximations on the unit sphere: an introduction*, volume 2044 of *Lecture Notes in Mathematics*. Springer, Heidelberg, 2012. ISBN 978-3-642-25982-1. doi: 10.1007/978-3-642-25983-8. URL https://doi.org/10.1007/978-3-642-25983-8.

Jimmy Lei Ba, Jamie Ryan Kiros, and Geoffrey E Hinton. Layer normalization. *arXiv preprint arXiv:1607.06450*, 2016.

Peter Bartlett, Vitaly Maiorov, and Ron Meir. Almost linear vc dimension bounds for piecewise polynomial networks. In M. Kearns, S. Solla, and D. Cohn, editors, *Advances in Neural Information Processing Systems*, volume 11. MIT Press, 1998. URL https://proceedings.neurips.cc/paper_files/paper/1998/file/bc7316929fe1545bf0b98d114ee3ecb8-Paper.pdf.

Peter L Bartlett and Shahar Mendelson. Rademacher and gaussian complexities: Risk bounds and structural results. *Journal of Machine Learning Research*, 3(Nov):463–482, 2002.

Peter L. Bartlett, Olivier Bousquet, and Shahar Mendelson. Local Rademacher complexities. *Ann. Statist.*, 33(4):1497–1537, 2005. ISSN 0090-5364,2168-8966. doi: 10.1214/009053605000000282. URL https://doi.org/10.1214/009053605000000282.

Peter L Bartlett, Dylan J Foster, and Matus J Telgarsky. Spectrally-normalized margin bounds for neural networks. In I. Guyon, U. Von Luxburg, S. Bengio, H. Wallach, R. Fergus, S. Vishwanathan, and R. Garnett, editors, *Advances in Neural Information Processing Systems*, volume 30. Curran Associates, Inc., 2017. URL https://proceedings.neurips.cc/paper_files/paper/2017/file/b22b257ad0519d4500539da3c8bcf4dd-Paper.pdf.

Peter L. Bartlett, Nick Harvey, Christopher Liaw, and Abbas Mehrabian. Nearly-tight VC-dimension and pseudodimension bounds for piecewise linear neural networks. *J. Mach. Learn. Res.*, 20:Paper No. 63, 17, 2019. ISSN 1532-4435,1533-7928.

Daniel Barzilai and Ohad Shamir. Generalization in kernel regression under realistic assumptions, 2023.

J Robert Beck and Stephen G Pauker. The markov process in medical prognosis. *Medical decision making*, 3(4):419–458, 1983.

Eric Temple Bell. Exponential polynomials. *Annals of Mathematics*, pages 258–277, 1934.

J Benitez, Takashi Furuya, Florian Faucher, Anastasis Kratsios, Xavier Tricoche, and Maarten V de Hoop. Out-of-distributional risk bounds for neural operators with applications to the helmholtz equation. *arXiv preprint arXiv:2301.11509*, 2023.

Jose Antonio Lara Benitez, Takashi Furuya, Florian Faucher, Anastasis Kratsios, Xavier Tricoche, and Maarten V de Hoop. Out-of-distributional risk bounds for neural operators with applications to the helmholtz equation. *Journal of Computational Physics*, page 113168, 2024.

Bernard Bercu, Bernard Delyon, and Emmanuel Rio. *Concentration inequalities for sums and martingales*. SpringerBriefs in Mathematics. Springer, Cham, 2015. ISBN 978-3-319-22098-7; 978-3-319-22099-4. doi: 10.1007/978-3-319-22099-4. URL https://doi.org/10.1007/978-3-319-22099-4.

Satwik Bhattamishra, Arkil Patel, and Navin Goyal. On the computational power of transformers and its implications in sequence modeling. *arXiv preprint arXiv:2006.09286*, 2020.

S. G. Bobkov and F. Götze. Exponential integrability and transportation cost related to logarithmic Sobolev inequalities. *J. Funct. Anal.*, 163(1):1–28, 1999. ISSN 0022-1236,1096-0783. doi: 10.1006/jfan.1998.3326. URL https://doi.org/10.1006/jfan.1998.3326.

Fran¸cois Bolley, Ivan Gentil, and Arnaud Guillin. Convergence to equilibrium in Wasserstein distance for Fokker-Planck equations. *J. Funct. Anal.*, 263(8):2430–2457, 2012. ISSN 0022-1236,1096-0783. doi: 10.1016/j.jfa.2012.07.007. URL https://doi.org/10.1016/j.jfa.2012.07.007.

Rishi Bommasani, Drew A Hudson, Ehsan Adeli, Russ Altman, Simran Arora, Sydney von Arx, Michael S Bernstein, Jeannette Bohg, Antoine Bosselut, Emma Brunskill, et al. On the opportunities and risks of foundation models. *ArXiv preprint*, abs/2108.07258, 2021.

Stéphane Boucheron, Gábor Lugosi, and Pascal Massart. Concentration inequalities, 2013. URL https://doi.org/10.1093/acprof:oso/9780199535255.001.0001. A nonasymptotic theory of independence, With a foreword by Michel Ledoux.

Khristo N. Boyadzhiev. Derivative polynomials for tanh, tan, sech and sec in explicit form. *Fibonacci Quarterly*, 45(4):291–303, 2007.

Evelyn Buckwar. Introduction to the numerical analysis of stochastic delay differential equations. *Journal of computational and applied mathematics*, 125(1-2):297–307, 2000.

Pratik Chaudhari, Anna Choromanska, Stefano Soatto, Yann LeCun, Carlo Baldassi, Christian Borgs, Jennifer Chayes, Levent Sagun, and Riccardo Zecchina. Entropy-sgd: biasing gradient descent into wide valleys*. *Journal of Statistical Mechanics: Theory and Experiment*, 2019 (12):124018, dec 2019. doi: 10.1088/1742-5468/ab39d9. URL https://dx.doi.org/10.1088/1742-5468/ab39d9.

Hong-Bin Chen, Sinho Chewi, and Jonathan Niles-Weed. Dimension-free log-Sobolev inequalities for mixture distributions. *J. Funct. Anal.*, 281(11):Paper No. 109236, 17, 2021. ISSN 0022-1236,1096-0783. doi: 10.1016/j.jfa.2021.109236. URL https://doi.org/10.1016/j.jfa.2021.109236.

Sitan Chen, Sinho Chewi, Jerry Li, Yuanzhi Li, Adil Salim, and Anru Zhang. Sampling is as easy as learning the score: theory for diffusion models with minimal data assumptions. In *The Eleventh International Conference on Learning Representations*, 2023. URL https://openreview.net/forum?id=zyLVMgsZ0U_.

Tin Sum Cheng, Aurelien Lucchi, Anastasis Kratsios, and David Belius. Characterizing overfitting in kernel ridgeless regression through the eigenspectrum, 2024a.

Tin Sum Cheng, Aurelien Lucchi, Anastasis Kratsios, and David Belius. A comprehensive analysis on the learning curve in kernel ridge regression, 2024b.

Doron Cohen and Aryeh Kontorovich. Local glivenko-cantelli. 195:715–715, 12–15 Jul 2023. URL https://proceedings.mlr.press/v195/cohen23a.html.

Samuel N. Cohen and Robert J. Elliott. *Stochastic calculus and applications*. Probability and its Applications. Springer, Cham, second edition, 2015. ISBN 978-1-4939-2866-8; 978-1-4939-2867-5. doi: 10.1007/978-1-4939-2867-5. URL https://doi.org/10.1007/978-1-4939-2867-5.

G. M. Constantine and T. H. Savits. A multivariate Faà di Bruno formula with applications. *Trans. Amer. Math. Soc.*, 348(2):503–520, 1996. ISSN 0002-9947. doi: 10.1090/S0002-9947-96-01501-2. URL https://doi.org/10.1090/S0002-9947-96-01501-2.

Jonathan D Cryer and Natalie Kellet. *Time series analysis*. Springer, 1991.

Christa Cuchiero and Josef Teichmann. Markovian lifts of positive semidefinite affine volterra-type processes. *Decisions in Economics and Finance*, 42:407–448, 2019.

Christa Cuchiero and Josef Teichmann. Generalized Feller processes and Markovian lifts of stochastic Volterra processes: the affine case. *J. Evol. Equ.*, 20(4):1301–1348, 2020a. ISSN 1424-3199,1424-3202. doi: 10.1007/s00028-020-00557-2. URL https://doi.org/10.1007/s00028-020-00557-2.

Christa Cuchiero and Josef Teichmann. Generalized feller processes and markovian lifts of stochastic volterra processes: the affine case. *Journal of evolution equations*, 20(4):1301–1348, 2020b.

Giuseppe Da Prato. *Introduction to stochastic analysis and Malliavin calculus*, volume 7. Edizioni della Normale, Pisa, second edition, 2008.

Mauri Aparecido de Oliveira and Ricardo Hirata Ikeda. Representation of the n-th derivative of the normal pdf using bernoulli numbers and gamma function. *Applied Mathematical Sciences*, 6(74): 3661–3673, 2012.

Steffen Dereich, Michael Scheutzow, and Reik Schottstedt. Constructive quantization: approximation by empirical measures. *Ann. Inst. Henri Poincaré Probab. Stat.*, 49(4):1183–1203, 2013. ISSN 0246-0203,1778-7017. doi: 10.1214/12-AIHP489. URL https://doi.org/10.1214/12-AIHP489.

E. Dolera and E. Mainini. Lipschitz continuity of probability kernels in the optimal transport framework. *Ann. Inst. Henri Poincaré Probab. Stat.*, 59(4):1778–1812, 2023. ISSN 0246-0203,1778-7017. doi: 10.1214/23-aihp1389. URL https://doi.org/10.1214/23-aihp1389.

Lawrence C Evans. *Partial differential equations*, volume 19. American Mathematical Society, 2022.

Francesco Faa di Bruno. Sullo sviluppo delle funzioni. *Annali di scienze matematiche e fisiche*, 6(1): 479–480, 1855.

Zhiying Fang, Yidong Ouyang, Ding-Xuan Zhou, and Guang Cheng. Attention enables zero approximation error, 2023. URL https://openreview.net/forum?id=AV_bv4Ydcr9.

Charles L. Fefferman. A sharp form of Whitney's extension theorem. *Ann. of Math. (2)*, 161 (1):509–577, 2005. ISSN 0003-486X,1939-8980. doi: 10.4007/annals.2005.161.509. URL https://doi.org/10.4007/annals.2005.161.509.

Hans Föllmer and Alexander Schied. *Stochastic finance*. Walter de Gruyter & Co., Berlin, extended edition, 2011. ISBN 978-3-11-021804-6. doi: 10.1515/9783110218053. URL https://doi.org/10.1515/9783110218053. An introduction in discrete time.

Dylan Foster, Tuhin Sarkar, and Alexander Rakhlin. Learning nonlinear dynamical systems from a single trajectory. In *Learning for Dynamics and Control*, pages 851–861. PMLR, 2020.

Simon Frieder, Luca Pinchetti, Ryan-Rhys Griffiths, Tommaso Salvatori, Thomas Lukasiewicz, Philipp Petersen, and Julius Berner. Mathematical capabilities of chatgpt. *Advances in Neural Information Processing Systems*, 36, 2024.

Tomer Galanti, Mengjia Xu, Liane Galanti, and Tomaso Poggio. Norm-based generalization bounds for sparse neural networks. *Advances in Neural Information Processing Systems*, 36, 2024.

Shivam Garg, Dimitris Tsipras, Percy S Liang, and Gregory Valiant. What can transformers learn in-context? a case study of simple function classes. *Advances in Neural Information Processing Systems*, 35:30583–30598, 2022.

Noah Golowich, Alexander Rakhlin, and Ohad Shamir. Size-independent sample complexity of neural networks. *Information and Inference: A Journal of the IMA*, 2020.

Nathael Gozlan. A characterization of dimension free concentration in terms of transportation inequalities. *Ann. Probab.*, 37(6):2480–2498, 2009. ISSN 0091-1798,2168-894X. doi: 10.1214/09-AOP470. URL https://doi.org/10.1214/09-AOP470.

Nathael Gozlan. Poincaré inequalities and dimension free concentration of measure. *Ann. Inst. Henri Poincaré Probab. Stat.*, 46(3):708–739, 2010. ISSN 0246-0203,1778-7017. doi: 10.1214/09-AIHP209. URL https://doi.org/10.1214/09-AIHP209.

Nathael Gozlan, Cyril Roberto, and Paul-Marie Samson. From dimension free concentration to the Poincaré inequality. *Calc. Var. Partial Differential Equations*, 52(3-4):899–925, 2015. ISSN 0944-2669,1432-0835. doi: 10.1007/s00526-014-0737-6. URL https://doi.org/10.1007/s00526-014-0737-6.

Siegfried Graf and Harald Luschgy. *Foundations of quantization for probability distributions*, volume 1730 of *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 2000. ISBN 3-540-67394-6. doi: 10.1007/BFb0103945. URL https://doi.org/10.1007/BFb0103945.

Leonard Gross. Logarithmic Sobolev inequalities. *Amer. J. Math.*, 97(4):1061–1083, 1975. ISSN 0002-9327,1080-6377. doi: 10.2307/2373688. URL https://doi.org/10.2307/2373688.

Michael Hardy. Combinatorics of partial derivatives. *Electron. J. Combin.*, 13(1):Research Paper 1, 13, 2006. doi: 10.37236/1027. URL https://doi.org/10.37236/1027.

Dan Hendrycks and Kevin Gimpel. Gaussian error linear units (GeLUs). *arXiv preprint arXiv:1606.08415*, 2016.

Songyan Hou, Parnian Kassraie, Anastasis Kratsios, Andreas Krause, and Jonas Rothfuss. Instance-dependent generalization bounds via optimal transport. *J. Mach. Learn. Res.*, 24:Paper No. [349], 51, 2023a. ISSN 1532-4435,1533-7928.

Songyan Hou, Parnian Kassraie, Anastasis Kratsios, Andreas Krause, and Jonas Rothfuss. Instance-dependent generalization bounds via optimal transport. *Journal of Machine Learning Research*, 24:1–50, 2023b.

Daniel J Hsu, Aryeh Kontorovich, and Csaba Szepesvári. Mixing time estimation in reversible markov chains from a single sample path. *Advances in neural information processing systems*, 28, 2015.

James Inglis and Ioannis Papageorgiou. Log-Sobolev inequalities for infinite-dimensional Gibbs measures with non-quadratic interactions. *Markov Process. Related Fields*, 25(5):879–897, 2019. ISSN 1024-2953.

Oleksiy Khorunzhiy. On asymptotic properties of bell polynomials and concentration of vertex degree of large random graphs. *Journal of Theoretical Probability*, 35:1–32, 03 2022. doi: 10.1007/s10959-020-01025-w.

Benoît Kloeckner. Effective berry–esseen and concentration bounds for markov chains with a spectral gap. *The Annals of Applied Probability*, 29(3):1778–1807, 2019.

Benoît R. Kloeckner. Empirical measures: regularity is a counter-curse to dimensionality. *ESAIM Probab. Stat.*, 24:408–434, 2020. ISSN 1292-8100,1262-3318. doi: 10.1051/ps/2019025. URL https://doi.org/10.1051/ps/2019025.

Vladimir Koltchinskii. Rademacher penalties and structural risk minimization. *IEEE Transactions on Information Theory*, 2001.

Aryeh Kontorovich. Concentration in unbounded metric spaces and algorithmic stability. In Eric P. Xing and Tony Jebara, editors, *Proceedings of the 31st International Conference on Machine Learning*, volume 32 of *Proceedings of Machine Learning Research*, pages 28–36, Bejing, China, 22–24 Jun 2014. PMLR. URL https://proceedings.mlr.press/v32/kontorovicha14.html.

Aryeh Kontorovich and Maxim Raginsky. Concentration of measure without independence: a unified approach via the martingale method. In *Convexity and Concentration*, pages 183–210. Springer, 2017.

Ioannis Kontoyiannis and Sean P Meyn. Geometric ergodicity and the spectral gap of non-reversible markov chains. *Probability Theory and Related Fields*, 154(1):327–339, 2012.

Anastasis Kratsios and Leonie Papon. Universal approximation theorems for differentiable geometric deep learning. *Journal of Machine Learning Research*, 23(196):1–73, 2022.

Anastasis Kratsios, A. Martina Neuman, and Gudmund Pammer. Tighter generalization bounds on digital computers via discrete optimal transport, 2024.

Vitaly Kuznetsov and Mehryar Mohri. Generalization bounds for non-stationary mixing processes. *Machine Learning*, 106(1):93–117, 2017.

Michel Ledoux. Concentration of measure and logarithmic sobolev inequalities. In *Seminaire de probabilites XXXIII*, pages 120–216. Springer, 2006.

Michel Ledoux, Ivan Nourdin, and Giovanni Peccati. Stein's method, logarithmic Sobolev and transport inequalities. *Geom. Funct. Anal.*, 25(1):256–306, 2015. ISSN 1016-443X,1420-8970. doi: 10.1007/s00039-015-0312-0. URL https://doi.org/10.1007/s00039-015-0312-0.

Valerii Likhosherstov, Krzysztof Choromanski, and Adrian Weller. On the expressive power of self-attention matrices. *arXiv preprint arXiv:2106.03764*, 2021.

George G. Lorentz, Manfred v. Golitschek, and Yuly Makovoz. *Constructive approximation*, volume 304 of *Grundlehren der mathematischen Wissenschaften [Fundamental Principles of Mathematical Sciences]*. Springer-Verlag, Berlin, 1996. ISBN 3-540-57028-4. doi: 10.1007/978-3-642-60932-9. URL https://doi.org/10.1007/978-3-642-60932-9. Advanced problems.

Dejun Luo and Jian Wang. Exponential convergence in lp-Wasserstein distance for diffusion processes without uniformly dissipative drift. *Math. Nachr.*, 289(14-15):1909–1926, 2016. ISSN 0025-584X,1522-2616. doi: 10.1002/mana.201500351. URL https://doi.org/10.1002/mana.201500351.

Dejun Luo and Jian Wang. Refined basic couplings and Wasserstein-type distances for SDEs with Lévy noises. *Stochastic Process. Appl.*, 129(9):3129–3173, 2019. ISSN 0304-4149,1879-209X. doi: 10.1016/j.spa.2018.09.003. URL https://doi.org/10.1016/j.spa.2018.09.003.

Miloud Mihoubi. Bell polynomials and binomial type sequences. *Discrete Mathematics*, 308(12): 2450–2459, 2008.

Ali A. Minai and Ronald D. Williams. On the derivatives of the sigmoid. *Neural Networks*, 6(6):845–853, 1993. ISSN 0893-6080. doi: https://doi.org/10.1016/S0893-6080(05)80129-7. URL https://www.sciencedirect.com/science/article/pii/S0893608005801297.

Kentaro Minami, HItomi Arai, Issei Sato, and Hiroshi Nakagawa. Differential privacy without sensitivity. *Advances in Neural Information Processing Systems*, 29, 2016.

Mehryar Mohri and Afshin Rostamizadeh. Rademacher complexity bounds for non-iid processes. *Advances in neural information processing systems*, 21, 2008.

Mehryar Mohri and Afshin Rostamizadeh. Stability bounds for stationary φ-mixing and β-mixing processes. *Journal of Machine Learning Research*, 11(2), 2010.

Ravi Montenegro, Prasad Tetali, et al. Mathematical aspects of mixing times in markov chains. *Foundations and Trends® in Theoretical Computer Science*, 1(3):237–354, 2006.

Chen Mufa. Estimation of spectral gap for markov chains. *Acta Mathematica Sinica*, 12(4):337–360, 1996.

Behnam Neyshabur, Ryota Tomioka, and Nathan Srebro. Norm-based capacity control in neural networks. In Peter Grünwald, Elad Hazan, and Satyen Kale, editors, *Proceedings of The 28th Conference on Learning Theory*, volume 40 of *Proceedings of Machine Learning Research*, pages 1376–1401, Paris, France, 03–06 Jul 2015. PMLR. URL https://proceedings.mlr.press/v40/Neyshabur15.html.

Behnam Neyshabur, Zhiyuan Li, Srinadh Bhojanapalli, Yann LeCun, and Nathan Srebro. The role of over-parametrization in generalization of neural networks. In *International Conference on Learning Representations*, 2019. URL https://openreview.net/forum?id=BygfghAcYX.

Christian Olivera and Ciprian Tudor. Density for solutions to stochastic differential equations with unbounded drift. *Brazilian Journal of Probability and Statistics*, 33(3):520–531, 2019.

Yann Ollivier. Ricci curvature of Markov chains on metric spaces. *J. Funct. Anal.*, 256(3):810–864, 2009. ISSN 0022-1236,1096-0783. doi: 10.1016/j.jfa.2008.11.001. URL https://doi.org/10.1016/j.jfa.2008.11.001.

Wolfgang Paul and Jörg Baschnagel. *Stochastic processes: From physics to finance*. Springer, Heidelberg, second edition, 2013. ISBN 978-3-319-00326-9; 978-3-319-00327-6. doi: 10.1007/978-3-319-00327-6. URL https://doi.org/10.1007/978-3-319-00327-6.

Daniel Paulin. Concentration inequalities for Markov chains by Marton couplings and spectral methods. *Electron. J. Probab.*, 20:no. 79, 32, 2015. ISSN 1083-6489. doi: 10.1214/EJP.v20-4039. URL https://doi.org/10.1214/EJP.v20-4039.

Prajit Ramachandran, Barret Zoph, and Quoc V Le. Searching for activation functions. *arXiv preprint arXiv:1710.05941*, 2017.

Adrian Riekert. Convergence rates for empirical measures of Markov chains in dual and Wasserstein distances. *Statist. Probab. Lett.*, 189:Paper No. 109605, 8, 2022. ISSN 0167-7152,1879-2103. doi: 10.1016/j.spl.2022.109605. URL https://doi.org/10.1016/j.spl.2022.109605.

Walter Rudin. *Principles of mathematical analysis*. International Series in Pure and Applied Mathematics. McGraw-Hill Book Co., New York-Auckland-Düsseldorf, third edition, 1976.

Max Simchowitz, Horia Mania, Stephen Tu, Michael I Jordan, and Benjamin Recht. Learning without mixing: Towards a sharp analysis of linear system identification. In *Conference On Learning Theory*, pages 439–473. PMLR, 2018.

James B Simon, Madeline Dickens, Dhruva Karkada, and Michael Deweese. The eigenlearning framework: A conservation law perspective on kernel ridge regression and wide neural networks. *Transactions on Machine Learning Research*, 2023.

Yang Song, Jascha Sohl-Dickstein, Diederik P Kingma, Abhishek Kumar, Stefano Ermon, and Ben Poole. Score-based generative modeling through stochastic differential equations. *arXiv preprint arXiv:2011.13456*, 2020.

Bharath K. Sriperumbudur, Kenji Fukumizu, Arthur Gretton, Bernhard Schölkopf, and Gert R. G. Lanckriet. On the empirical estimation of integral probability metrics. *Electron. J. Stat.*, 6:1550–1599, 2012. ISSN 1935-7524. doi: 10.1214/12-EJS722. URL https://doi.org/10.1214/12-EJS722.

Richard S. Sutton and Andrew G. Barto. *Reinforcement learning: an introduction*. Adaptive Computation and Machine Learning. MIT Press, Cambridge, MA, second edition, 2018. ISBN 978-0-262-03924-6.

Nizar Touzi. *Optimal stochastic control, stochastic target problems, and backward SDE*, volume 29 of *Fields Institute Monographs*. Springer, New York; Fields Institute for Research in Mathematical Sciences, Toronto, ON, 2013. ISBN 978-1-4614-4285-1; 978-1-4614-4286-8. doi: 10.1007/978-1-4614-4286-8. URL https://doi.org/10.1007/978-1-4614-4286-8. With Chapter 13 by Angès Tourin.

Jacob Trauger and Ambuj Tewari. Sequence length independent norm-based generalization bounds for transformers. *arXiv preprint arXiv:2310.13088*, 2023.

François Treves. *Topological Vector Spaces, Distributions and Kernels: Pure and Applied Mathematics, Vol. 25*, volume 25. Elsevier, 2016.

Alexander Tsigler and Peter L Bartlett. Benign overfitting in ridge regression. *J. Mach. Learn. Res.*, 24:123–1, 2023.

A. W. van der Vaart and Jon A. Wellner. *Weak convergence and empirical processes—with applications to statistics*. Springer Series in Statistics. Springer, Cham, second edition, 2023. ISBN 978-3-031-29038-1; 978-3-031-29040-4. doi: 10.1007/978-3-031-29040-4. URL https://doi.org/10.1007/978-3-031-29040-4.

Ashish Vaswani, Noam Shazeer, Niki Parmar, Jakob Uszkoreit, Llion Jones, Aidan N. Gomez, Lukasz Kaiser, and Illia Polosukhin. Attention is all you need. In Isabelle Guyon, Ulrike von Luxburg, Samy Bengio, Hanna M. Wallach, Rob Fergus, S. V. N. Vishwanathan, and Roman Garnett, editors, *Advances in Neural Information Processing Systems 30: Annual Conference on Neural Information Processing Systems 2017, December 4-9, 2017, Long Beach, CA, USA*, pages 5998–6008, 2017.

Cédric Villani. *Optimal transport*, volume 338 of *Grundlehren der mathematischen Wissenschaften*. Springer-Verlag, Berlin, 2009. ISBN 978-3-540-71049-3. doi: 10.1007/978-3-540-71050-9. URL https://doi.org/10.1007/978-3-540-71050-9. Old and new.

Johannes Von Oswald, Eyvind Niklasson, Ettore Randazzo, João Sacramento, Alexander Mordvintsev, Andrey Zhmoginov, and Max Vladymyrov. Transformers learn in-context by gradient descent. In *International Conference on Machine Learning*, pages 35151–35174. PMLR, 2023.

Feng-Yu Wang. Exponential ergodicity for singular reflecting McKean-Vlasov SDEs. *Stochastic Process. Appl.*, 160:265–293, 2023. ISSN 0304-4149,1879-209X. doi: 10.1016/j.spa.2023.03.009. URL https://doi.org/10.1016/j.spa.2023.03.009.

Weiping Wang and Tianming Wang. General identities on bell polynomials. *Computers & Mathematics with Applications*, 58(1):104–118, 2009.

Jason Wei, Yi Tay, Rishi Bommasani, Colin Raffel, Barret Zoph, Sebastian Borgeaud, Dani Yogatama, Maarten Bosma, Denny Zhou, Donald Metzler, et al. Emergent abilities of large language models. *ArXiv preprint*, abs/2206.07682, 2022.

Eugene P. Wigner. Characteristic vectors of bordered matrices with infinite dimensions. *Ann. of Math. (2)*, 62:548–564, 1955. ISSN 0003-486X. doi: 10.2307/1970079. URL https://doi.org/10.2307/1970079.

Eugene P. Wigner. Characteristic vectors of bordered matrices with infinite dimensions. II. *Ann. of Math. (2)*, 65:203–207, 1957. ISSN 0003-486X. doi: 10.2307/1969956. URL https://doi.org/10.2307/1969956.

Geoffrey Wolfer and Aryeh Kontorovich. Estimating the mixing time of ergodic markov chains. In *Conference on Learning Theory*, pages 3120–3159. PMLR, 2019.

Jiayuan Ye and Reza Shokri. Differentially private learning needs hidden state (or much faster convergence). *Advances in Neural Information Processing Systems*, 35:703–715, 2022.

Dong Yin, Ramchandran Kannan, and Peter Bartlett. Rademacher complexity for adversarially robust generalization. In Kamalika Chaudhuri and Ruslan Salakhutdinov, editors, *Proceedings of the 36th International Conference on Machine Learning*, volume 97 of *Proceedings of Machine Learning Research*, pages 7085–7094. PMLR, 09–15 Jun 2019. URL https://proceedings.mlr.press/v97/yin19b.html.

Bin Yu. Rates of convergence for empirical processes of stationary mixing sequences. *The Annals of Probability*, pages 94–116, 1994.

Chulhee Yun, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank J Reddi, and Sanjiv Kumar. Are transformers universal approximators of sequence-to-sequence functions? *arXiv preprint arXiv:1912.10077*, 2019.

Chulhee Yun, Yin-Wen Chang, Srinadh Bhojanapalli, Ankit Singh Rawat, Sashank Reddi, and Sanjiv Kumar. O (n) connections are expressive enough: Universal approximability of sparse transformers. *Advances in Neural Information Processing Systems*, 33:13783–13794, 2020.

Behnoosh Zamanlooy. On the mixing times of contractive markov kernels. *ArXiV*, 2024.

Ruiqi Zhang, Spencer Frei, and Peter L Bartlett. Trained transformers learn linear models in-context. *Journal of Machine Learning Research*, 25(49):1–55, 2024.

Wayne Xin Zhao, Kun Zhou, Junyi Li, Tianyi Tang, Xiaolei Wang, Yupeng Hou, Yingqian Min, Beichen Zhang, Junjie Zhang, Zican Dong, et al. A survey of large language models. *ArXiv preprint*, abs/2303.18223, 2023.

Haoyi Zhou, Shanghang Zhang, Jieqi Peng, Shuai Zhang, Jianxin Li, Hui Xiong, and Wancai Zhang. Informer: Beyond efficient transformer for long sequence time-series forecasting. In *Proceedings of the AAAI conference on artificial intelligence*, volume 35, pages 11106–11115, 2021.

Ingvar Ziemann and Stephen Tu. Learning with little mixing. *Advances in Neural Information Processing Systems*, 35:4626–4637, 2022.

David Zimmermann. Logarithmic Sobolev inequalities for mollified compactly supported measures. *J. Funct. Anal.*, 265(6):1064–1083, 2013. ISSN 0022-1236,1096-0783. doi: 10.1016/j.jfa.2013.05.029. URL https://doi.org/10.1016/j.jfa.2013.05.029.

Appendix Contents

A Notation

In this section, we present the notation that will be employed throughout the appendix. This notation builds upon the framework established in the main body of the text, while incorporating additional levels of specificity. Given the technical nature of certain results discussed herein, a more detailed and precise formulation of the notation is necessary to ensure clarity and rigor in the statements that follow.

Notation 1 (Multi-index Notation). *We will fix the following multivariate notation.*

- *Multi-indices* $\alpha \overset{\text{def.}}{=} (\alpha_1, \dots, \alpha_k) \in \mathbb{N}^k$, $k \in \mathbb{N}$ *are denoted by Greek letters.*
- *The sum of entries is given by* $|\alpha| \overset{\text{def.}}{=} \sum_{i=1}^k \alpha_k$.

- *Its faculty is defined by* $\alpha! \stackrel{\text{def.}}{=} \prod_{i=1}^k \alpha_k!$,
- *We denote the derivative w.r.t.* α *by* $D^\alpha \stackrel{\text{def.}}{=} \partial^{|\alpha|}/\partial x_1^{\alpha_1} \cdots \partial x_k^{\alpha_k}$ *if* $|\alpha| > 0$ *else* D^α *is the identity operator.*
- *For a vector* $x \in \mathbb{R}^k$, *we write* $x^\alpha \stackrel{\text{def.}}{=} \prod_{i=1}^k x_k^{\alpha_k}$.
- *We define the relation* $\alpha \prec \beta$ *for* $\beta \in \mathbb{N}^k$ *if one of the three following holds*
  (i) $|\alpha| < |\beta|$;
  (ii) $|\alpha| = |\beta|$, *and* $\alpha_1 < \beta_1$; *or*
  (iii) $|\alpha| = |\beta|$, *and* $\alpha_i = \beta_i$ *for* $i \in \{1, \dots, j-1\}$ *and* $\alpha_j < \beta_j$ *for* $j \in \{2, \dots, k\}$.
- *Unit vectors* $e_i \in \{0,1\}^k$ *are defined by* $(e_i)_j = 0$ *for* $i \neq j$ *and* $(e_i)_i = 1$.

Definition 3 (C^s-norm)**.** *For any* $s > 0$, *the norm* $\|\cdot\|_{C^s}$ *of a smooth function* $f : \mathbb{R}^d \to \mathbb{R}$ *is defined by*

$$\|f\|_{C^s} \stackrel{\text{def.}}{=} \max_{k=1,\dots,s-1} \max_{\alpha\in\{1,\dots,d\}^d} \Big\| \frac{\partial^k f}{\partial x_{\alpha_1} \dots \partial x_{\alpha_k}} \Big\|_\infty + \max_{\alpha\in\{1,\dots,d\}^{s-1}} \operatorname{Lip}\big(\frac{\partial^{s-1} f}{\partial x_{\alpha_1} \dots \partial x_{\alpha_{s-1}}}\big).$$

We use the following notation to streamline the analytic challenges the tacking of C^s-norms.

Notation 2 (Order operator for multi-indeces)**.** *Define the order operator* $\mathfrak{o}$ *for multi-indeces by*

$$\mathfrak{o} : \mathbb{N}^k \longrightarrow \mathbb{N}^k, \quad \alpha_1, \dots, \alpha_k \longmapsto \alpha_{\tau_\alpha(1)}, \dots, \alpha_{\tau_\alpha(k)},$$

where $\tau_\alpha : \{1, \dots, k\} \to \{1, \dots, k\}$ *s.t.* $\alpha_{\tau_\alpha(1)} \geqslant \dots \geqslant \alpha_{\tau_\alpha(k)}$. *We write* $\alpha \sim \beta$ *if* $\mathfrak{o}(\alpha) = \mathfrak{o}(\beta)$ *for* $\alpha, \beta \in \mathbb{N}^k$. *Further, denote by* $\mathfrak{O}_n^k$ *the set* $\{\mathfrak{o}(\alpha) : \alpha \in \mathbb{N}^k, |\alpha| = n\}$ *and write* $\mathfrak{O}_{\leqslant n}^k \stackrel{\text{def.}}{=} \{\mathfrak{o}(\alpha) : \alpha \in \mathbb{N}^k, |\alpha| \leqslant n\}$. *Eventually, define* $N(\alpha) \stackrel{\text{def.}}{=} \#|\{\alpha' \in \mathbb{N}^k : \mathfrak{o}(\alpha') = \alpha\}|$.

We will use the following notation to tabulate the sizes of a C^s-norm.

Notation 3 (Derivatives)**.** *Let* $k \in \mathbb{N}$, $K \in \mathbb{R}^k$ *be a set,* $f : K \to \mathbb{R}^m$ *a function and* $\alpha \in \mathfrak{O}_n^k$ *an ordered multi-index. Then,*

- *the uniform bound of* α*-like derivatives on* K *is given by*

$$C_K^f(\alpha) \stackrel{\text{def.}}{=} \max_{i\in\{1,\dots,m\}} \max_{\gamma\sim\alpha} \|D^\gamma f_i\|_K,$$

- *we define the bound at / up to derivative level* n *by*

$$C_K^f(n) \stackrel{\text{def.}}{=} \max_{\alpha\in\mathfrak{O}_n^k} C_K^f(\alpha), \qquad C_K^f(\leqslant n) \stackrel{\text{def.}}{=} \max_{\alpha\in\mathfrak{O}_{\leqslant n}^k} C_K^f(\alpha),$$

- *we write* $\|K\| \stackrel{\text{def.}}{=} \sup_{x\in K} \|x\|$, *and*
- *the* ℓ^∞*-matrix norm of any* $n \times m$ *matrix* $A \in \mathbb{R}^{n\times m}$ *is abbreviated as*

$$C^A \stackrel{\text{def.}}{=} \max_{i\in\{1,\dots,n\}, j\in\{1,\dots,m\}} |A_{i,j}|.$$

When segmenting, truncating, or manipulating time series we will using the following notation.

Notation 4 (Time Series Notation)**.** *The following notation is when indexing paths of any time series.*

- Realized Path up to time t *is denoted by* $x_{\leqslant t} \stackrel{\text{def.}}{=} (x_s)_{s\in\mathbb{Z},\, s\leqslant t}$.
- Segment of a Path *Given a sequence* $x \in \mathbb{R}^\mathbb{Z}$ *and integers* $s \leqslant t$, *we denote* $x_{[s:t]} \stackrel{\text{def.}}{=} (x_i)_{i=s}^t$.

Lastly, we recorded some additional notations that were required throughout our manuscript.

Notation 5 (Miscellaneous)**.** *We define:*

- N-Simplex. *For* $N \in \mathbb{N}$ *we write*

$$\Delta_N \stackrel{\text{def.}}{=} \{u \in [0,1]^N : \sum_{i=1}^N u_i = 1\}.$$

- Infinite powers*: For* $c \in (0,1)$, *we define*

$$c^\infty \stackrel{\text{def.}}{=} \lim_{t\to\infty} c^t = 0.$$

- Reshape operator*: For any $F_1, F_2 \in \mathbb{N}_+$, the operator is given by* $\operatorname{reshape}_{F_1\times F_2}$, *mapping any vector $u \in \mathbb{R}^{F_1F_2}$ to the $F_1 \times F_2$ matrix*

$$\operatorname{reshape}_{F_1\times F_2}(x)_{i,j} \stackrel{\text{def.}}{=} x_{(i-1)F_2+j}.$$

We denote the inverse of the map $\operatorname{reshape}_{F_1\times F_2}$ *by* $\operatorname{vec}_{F_1,F_2} : \mathbb{R}^{F_1\times F_2} \to \mathbb{R}^{F_1F_2}$.

- Softmax operator*: For each $F \in \mathbb{N}_+$ and each $x \in \mathbb{R}^F$,*

$$\operatorname{softmax}(x) \stackrel{\text{def.}}{=} \operatorname{smax}(x) \stackrel{\text{def.}}{=} \big(\exp(x_i)/\textstyle\sum_{j=0}^{F-1}\exp(x_j)\big)_{i=0}^{F-1}.$$

B Examples of Data-Generating Processes Satisfying Assumptions 1 and 2

This section provides several examples of stochastic (data-generating) processes which satisfy our assumptions and are outside the i.i.d. restrictions.

B.1 Projected Exponentially Ergodic Latent Processes

Proposition 2 (Lipschitz-Transformed SDEs with Overdampened Drift)**.** *In the setting of Example 1, $\{(P^n(x,\cdot))_{n=0}^\infty\}_{x\in[0,1]^d}$ satisfies both Assumptions 1 and 2.*

The proof of Proposition 2 uses the following lemma.

Lemma 1 (Enforcing Boundedness via 1-Lipschitz Maps Preserves Exponential Ergodicity)**.** *Let $\tilde{d}, d \in \mathbb{N}_+$ and $Z_\cdot$ be a Markov process on $\mathbb{R}^{\tilde{d}}$ satisfying Assumption 2. Given any bounded Lipschitz function $f : \mathbb{R}^{\tilde{d}} \to \mathbb{R}^d$ the Markov process $X_\cdot \stackrel{\text{def.}}{=} (X_n)_{n=0}^\infty$ in $\mathbb{R}^d$, defined for each n by $X_n \stackrel{\text{def.}}{=} f(Z_n)$, satisfies both Assumption 1 and 2.*

Proof of Lemma 1. Since f is bounded, then there exists some $r > 0$ such that $f(\mathbb{R}^d) \subset B_r^d \stackrel{\text{def.}}{=} \{u \in \mathbb{R}^d : \|u\| \leqslant\}$. For each $x \in \mathbb{N}_+$, let $P^n(x,\cdot) \stackrel{\text{def.}}{=} \mathbb{P}(X_t \in \cdot | X_0 = x) = \mathbb{P}(f(Z_t) \in \cdot | f(Z_0) = f(x)) = f_\# P^n(x,\cdot)$ then the Kantorovich duality, see e.g. (Villani, 2009, Theorem 5.10), implies that $f_\# : \mathcal{P}_1(\mathbb{R}^d) \to \mathcal{P}_1(B_r^d)$ is 1-Lipschitz; whence (4) imples that: for each $x \in [0,1]^d$ and every $n \in \mathbb{N}$ we have

$$\mathcal{W}_1\big(P^n(x,\cdot), P^n(y,\cdot)\big) \leqslant \operatorname{Lip}(f)\mathcal{W}_1\big(\tilde{P}^n(x,\cdot), \tilde{P}^n(y,\cdot)\big) \leqslant \kappa\,\|x-y\|. \tag{4}$$

Thus, Assumption 2 holds. Finally, we note that Assumption 1 holds since each $P^n(x,\cdot) \in \mathcal{P}_1(B_r^d)$. ☐

Proof of Proposition 2. For any $\mu \in \mathcal{P}_1(\mathbb{R}^D)$ consider the unique strong solution (which exists by our Lipschitz assumption) For the following SDE (which is a Markov process)

$$Z_t^\mu = Z_0^\mu + \int_0^t \mu(Z_s^\mu)\,ds + \int_0^t W_s$$

where $W_\cdot \stackrel{\text{def.}}{=} (W_n)_{n=0}^\infty$ is a d-dimensional Brownian motion and Z_0^μ is distributed according to μ. For every $n \in \mathbb{N}_+$ let $\tilde{P}^n\mu \stackrel{\text{def.}}{=} \mathbb{P}(Z_n^\mu \in \cdot)$ and, for each $x \in \mathbb{R}^d$, let $\tilde{P}^n(x,\cdot) \stackrel{\text{def.}}{=} \tilde{P}^n\delta_x$. Then (Luo and Wang, 2016, Theorem 1.1) implies that: for all $n \in \mathbb{N}$ and each $\mu, \nu \in \mathcal{P}_1(\mathbb{R}^d)$ we have

$$\mathcal{W}_1\big(\tilde{P}^n\mu, \tilde{P}^n\nu\big) \leqslant \kappa\,\mathcal{W}_1(\mu,\nu) \tag{5}$$

where $\kappa = \exp(-K)$; note that $\kappa \in (0,1)$ since $K > 0$. That is, $(\tilde{P}^n)_{n=0}^\infty$ satisfies Assumption 2 upon taking $\mu = \delta_x$ and $\nu = \delta_y$, for any given $x, y \in \mathbb{R}^d$, since $\mathcal{W}_1(\delta_x,\delta_y) = \|x-y\|$, see e.g. (Villani, 2009, page 99 point 5) or note that the only coupling between δ_x and δ_y is the product measure $\delta_x \otimes \delta_y$).

$$\mathcal{W}_1\big(\tilde{P}^n(x,\cdot), \tilde{P}^n(x,\cdot)\big) \leqslant \kappa\,\|x-y\|.$$

Applying Lemma 1 yields the conclusion. ☐

Proposition 3. *Consider the setting of Example 2. Then, the process $X_\cdot$ satisfies both Assumptions 1 and 2.*

Proof of Proposition 3. Under our assumptions σ satisfies (Wang, 2023, Assumption (A8) (1) and (A8) (3)). Therefore, the stochastic process $Z_{\cdot} \overset{\text{def.}}{=} (Z_t)_{t\geqslant 0}$ defined by

$$Z_t \overset{\text{def.}}{=} \int_0^t \sigma(Z_s)\, dW_s \tag{6}$$

where $W_{\cdot}$ is a d-dimensional Brownian motion, satisfies the conditions of (Wang, 2023, Corollary 4.4) from which we deduce that $Z_{\cdot}$ satisfies Assumption 2. Applying Lemma 1 yields the conclusion. □

B.2 Markov Processes Satisfying a Log-Sobolev Inequalities

Proof of Proposition 1. Under the log-Sobolev Assumption 3, (Bobkov and Götze, 1999, Theorem 1.3) can be applied to $\bar{\mu}$ and $P(x,\cdot)$ for each $x \in \mathcal{X}$, implying that the transport inequalities hold: for each $\nu \in \mathcal{P}(\mathcal{X})$ and each $\tilde{\mu} \in \{\bar{\mu}, \mu_0\} \cup \{P(x,\cdot)\}_{x\in\mathcal{X}}$

$$\mathcal{W}_1(\tilde{\mu}, \nu)^2 \leqslant 2C^2 \ \mathrm{KL}(\nu|\tilde{\mu}) \tag{7}$$

where we recall the definition of the Kullback–Leibler divergence $\mathrm{KL}(\nu|\mu) \overset{\text{def.}}{=} \mathbb{E}_{X\sim\nu}[\log(\frac{d\nu}{d\mu}(X))]$. Thus, (7) implies that the following exponential contractility property of the Markov kernel: there exists some $\kappa \in (0,1)$ such that for each $x, \tilde{x} \in \mathcal{X}$ and every $t \in \mathbb{N}_+$

$$\mathcal{W}_1\big(P^t(x,\cdot), P^t(\tilde{x},\cdot)\big) \leqslant \kappa^t\, \|x - \tilde{x}\|. \tag{8}$$

This completes the proof. □

C Transformer Definition Details

For any $F \in \mathbb{N}_+$, we will consider a weighted (parametric) variant of the *layer normalization* function of Ba et al. (2016), which permits a variable level of regularization. Our weighted *layer normalization* is defined by $\mathrm{LayerNorm} : \mathbb{R}^F \to \mathbb{R}^F$ defined for any $u \in \mathbb{R}^F$ by

$$\mathcal{LN}(u; \gamma, \beta, w) \overset{\text{def.}}{=} \gamma \, \frac{(u - \mu_u^w)}{\sqrt{1 + (\sigma_u^w)^2}} + \beta$$

where $\mu_u^w \overset{\text{def.}}{=} \sum_{i=1}^F \frac{w}{F} u_i$ and $(\sigma_u^w)^2 \overset{\text{def.}}{=} \sum_{i=1}^F \frac{w}{F}\, \|u_i - \mu_u\|^2$, splus $\overset{\text{def.}}{=} \ln(1 + \exp(\cdot))$, parameters $\beta \in \mathbb{R}^F$ and $\gamma \in \mathbb{R}$, and the normalization strength parameter $w \in [0,1]$ with $w = 1$ being the default choice. Here, we prohibit the layer norm from magnifying the size of its outputs when the layer-wise weighted variance σ_u^w is small.[2]

Definition 4 (Multi-Head Self-Attention)**.** *Fix $d_{\text{in}} \in \mathbb{N}$. For $x \in \mathbb{R}^{M\times d_{\text{in}}}$, $Q, K \in \mathbb{R}^{d_K\times d_{\text{in}}}$, and $V \in \mathbb{R}^{d_V\times d_{\text{in}}}$, where we have key-dimension $d_K \in \mathbb{N}$ and value-dimension $d_V \in \mathbb{N}$; we define*

$$\mathrm{Att}(x; Q, K, V) \overset{\text{def.}}{=} \left(\sum_{j=0}^M \mathrm{softmax}\left(\left(\frac{\langle Qx_m, Kx_i\rangle}{\sqrt{d_k}}\right)_{i=0}^M\right)_j V x_j\right)_{m=1}^M \in \mathbb{R}^{M\times d_V}.$$

For $H \in \mathbb{N}$, set $Q \overset{\text{def.}}{=} (Q^{(h)})_{h=1}^H, K \overset{\text{def.}}{=} (K^{(h)})_{h=1}^H \subseteq \mathbb{R}^{d_K\times d_{\text{in}}}$, $V \overset{\text{def.}}{=} (V^{(h)})_{h=1}^H \subseteq \mathbb{R}^{d_V\times d_{\text{in}}}$, and $W \overset{\text{def.}}{=} (W^{(h)})_{h=1}^H \subseteq \mathbb{R}^{d_{\text{in}}\times d_V}$. For $x \in \mathbb{R}^{M\times d_{\text{in}}}$, we define

$$\mathcal{MH}(x; Q, K, V, W) \overset{\text{def.}}{=} \left(\sum_{h=1}^H W^{(h)}\, \mathrm{Att}(x; Q^{(h)}, K^{(h)}, V^{(h)})_m\right)_{m=1}^M \in \mathbb{R}^{M\times d_{\text{in}}}.$$

Each transformer block takes a set of inputs and intersperses normalization via layer norms, contextual comparisons via multi-head attention mechanisms, and non-linear transformations via a single layer perceptron (SLP). We also allow the transformer block to extend or contract the length of the generated sequence.

Definition 5 (Transformer Block)**.** *Fix a non-affine activation function $\sigma \in C^\infty(\mathbb{R})$. Fix a dimensional multi-index $d = (d_{\text{in}}, d_K, d_V, d_{\text{ff}}, d_{\text{out}}) \in \mathbb{N}^5$, a sequence length $M \in \mathbb{N}_+$, and a*

[2] Note that this formulation of the layer norm avoids division by 0 when the entries of u are identical.

number of self-attention heads $H \in \mathbb{N}_+$. A transformer block is a permutation equivariant map $\mathcal{TB} : \mathbb{R}^{M\times d_{\text{in}}} \to \mathbb{R}^{M\times d_{\text{out}}}$ represented for each $x \in \mathbb{R}^{M\times d_{\text{in}}}$

$$\begin{aligned}\mathcal{TB}(x) &\overset{\text{def.}}{=} \Big(\mathcal{LN}\left(B^{(1)}x'_m + B^{(2)}(\sigma \bullet (A\,x'_m + a));\, \gamma_2, \beta_2, w_2\right)\Big)_{m=1}^{M} \\ x' &\overset{\text{def.}}{=} \Big(\mathcal{LN}\left(x_m + \mathcal{MH}(x; Q, K, V, W)_m;\, \gamma_1, \beta_1, w_1\right)\Big)_{m=1}^{M}\end{aligned} \tag{9}$$

for $\gamma_1, \gamma_2 \in \mathbb{R}$, $w_1, w_2 \in [0,1]$, $\beta_1 \in \mathbb{R}^{d_{\text{in}}}$, $\beta_2 \in \mathbb{R}^{d_{\text{out}}}$, $A \in \mathbb{R}^{d_{\text{ff}}\times d_{\text{in}}}$, $a \in \mathbb{R}^{d_{\text{ff}}}$, $B^{(1)} \in \mathbb{R}^{d_{\text{out}}\times d_{\text{in}}}$, $B^{(2)} \in \mathbb{R}^{d_{\text{out}}\times d_{\text{ff}}}$, and Q, K, V, W as in Definition 4. Above, we write $\bullet$ for a pointwise application.

The class of transformer blocks with representation (9) and bounds on $\gamma_1, \gamma_2, \beta_1, \beta_2, a, A, B^{(1)}, B^{(2)}, Q, K, V, W$ is denoted by $\mathcal{TBC}$.

A transformer concatenates several transformer blocks before passing their outputs to an affine layer and ultimately outputting its prediction.

Definition 6 (Transformers)**.** *Fix depth $L \in \mathbb{N}_+$, memory $M \in \mathbb{N}$, width $W \in \mathbb{N}_+^5$, number of heads $H \in \mathbb{N}_+$, and input-output dimensions $D, d \in \mathbb{N}_+$. A transformer (network) is a map $\mathcal{T} : \mathbb{R}^{M\times D} \to \mathbb{R}^d$ with representation*

$$\mathcal{T}(x) = A\big(\operatorname{vec}_{1+M,d^L_{\text{out}}} \circ \mathcal{TB}_L \circ \cdots \circ \mathcal{TB}_1(x)\big) + b \tag{10}$$

where multi-indices $d^l = (d^l_{\text{in}}, d^l_K, d^l_V, d^l_{\text{ff}}, d^l_{\text{out}}) \leqslant W$ are such that $d^1_{\text{in}} = D$, $d^{l+1}_{\text{in}} = d^l_{\text{out}}$ for each $l = 1, \ldots, L-1$, and where $H \overset{\text{def.}}{=} (H^l)_{l=1}^L$ are the number of self-attention heads, $C' \overset{\text{def.}}{=} (C^l)_{l=1}^L$ the parameter bounds, and for $l = 1, \ldots, L$ we have $\mathcal{TB}_l \in \mathcal{TBC}_l$, where $\mathcal{TBC}_l$ is a transformer block class with $d_{\text{in}} = d^l$, $M = M$, and $H = H^l$. Furthermore, $A \in \mathbb{R}^{d\times M d^L_{\text{out}}}$ and $b \in \mathbb{R}^d$.

The set of transformer networks with representation (10) and bounds on A, b is denoted by $\mathcal{TC}$.

D Elucidation of Constants in Theorem 1

The aim of this section is to elucidate the magnitude of the constants appearing in Theorem 1. We aim of to make each of these concrete by numerically estimating them, which we report in a series of tables. Importantly, we see how subtle choices of the activation function used to define the transformer model can have dramatic consequences on the size of these constants, which could otherwise be hidden in big $\mathcal{O}$ notation.

Interestingly, in Tables 1 and 2, we see that the $\mathrm{softplus}$ activation function produces significantly tighter bounds than the $\tanh$ activation function through much smaller constants, and the GeLU and SWISH activation functions are a relatively comparable second-place.

The bounds depicted in Table 2 exhibits a notable trait of independence from both input dimension and the compactum they are defined on. Notably, the selection of latent dimensionality demonstrates a relatively minor influence in contrast to the pronounced impact of parameter bounds. This suggests that while adjusting the latent dimension may have some effect, the primary driver of the derivative bound lies within the constraints imposed on the parameters. Despite the seemingly conservative nature of the chosen parameter-bounds, it is important to acknowledge their alignment with the parameter ranges observed in trained transformer-models.

Note that the latter can be observed as well for Multi-Head attention (Table 5), however, we see that here the input dimension (composed of d_{in} and M) is of greater importance with respect to the derivative bound.

Table 1: C^s-bounds of activation functions based on numerical maximization of analytic derivatives in Appendix F.3.3.

Bound	softplus	GeLU	tanh	Swish
C^1	0.25	1.12	4.00	1.10
C^2	0.10	0.48	8.00	0.50
C^3	0.12	0.75	16.00	0.31
C^4	0.13	1.66	32.00	0.50
C^5	0.25	4.34	156.65	0.66
C^6	0.41	12.95	1651.32	1.50
C^7	1.06	42.77	20405.43	2.91
C^8	2.39	153.76	292561.95	8.50
C^9	7.75	594.17	4769038.09	21.76
C^{10}	22.25	2445.69	87148321.71	77.50

The bound of the layer-norm (see Table 3) seems to be particularly effected by the domain it is defined on, which can be problematic if it appears in later layers. An immediate solution is the usage of its parameter γ, a more drastic approach would be applications in combination with an upstream sigmoid activation.

Eventually, as also shown in Figure 3, we included in Tables 4 and 5 a comparison of using type-specific bounds (see Theorem 5) or level-specific bounds (Theorem 4) in the computation of the constants. This effect seems to become more evident with higher number of function compositions.

Table 2: Derivative Bounds of the Perceptron Layer by derivative level according to Lemma 13.

Parameters			Derivative Level				
σ	d_{ff}	$C^{\{A,B^{(1)},B^{(2)}\}}$	1	2	3	4	5
softmax	64	1.0	17.00	50.47	236.94	1.34E+03	1.33E+04
tanh			129.00	1.02E+03	8.96E+03	9.83E+04	1.34E+06
GeLU			73.25	237.41	1.25E+03	1.16E+04	1.81E+05
SWISH			71.39	236.78	870.75	5.33E+03	4.13E+04
	16		5.00	12.62	59.23	334.15	3.31E+03
	32		9.00	25.24	118.47	668.30	6.63E+03
	128		33.00	100.95	473.87	2.67E+03	2.65E+04
	256		65.00	201.90	947.75	5.35E+03	5.30E+04
		0.01	17.00	44.32	180.94	919.87	6.52E+03
		0.1	17.00	44.38	181.00	919.92	6.52E+03
		10.0	17.00	660.15	5.62E+04	4.17E+06	6.73E+08
		100.0	17.00	6.16E+04	5.60E+07	4.17E+10	6.73E+13

Table 3: Layer Norm

Parameters			Derivative Level				
k	$\|K\|$	γ	1	2	3	4	5
5	10.0	0.1	18.67	28.56	104.49	1.49E+03	4.93E+03
3			18.67	28.56	104.49	945.21	4.93E+03
10			18.67	28.56	104.49	1.49E+03	4.93E+03
20			18.67	28.56	104.49	1.49E+03	4.93E+03
	0.1		0.17	3.61	5.37	7.05	8.87
	1.0		1.73	5.20	6.95	8.71	10.64
	100.0		321.71	7.68E+03	7.88E+05	1.42E+08	4.39E+09
	1000.0		321.71	7.68E+03	7.88E+05	1.42E+08	4.39E+09
		0.01	1.73	2.07	2.24	2.42	2.59
		1.0	321.71	7.75E+03	7.91E+05	1.42E+08	4.44E+09

Table 4: Derivative Bounds of Transformer Block by derivative level according to Theorem 7.

Parameters				Derivative Level				
d_{in}	$C^{\{K,Q,V,W\}}$	$C^{\{A,B^{(1,2)}\}}$	γ	1	2	3	4	5
5	0.01	0.001	0.01	21.15	1.13E+04	4.81E+06	2.59E+09	2.22E+11
— using derivative level —				212.70	1.53E+06	7.47E+09	4.55E+13	3.75E+16
10				111.32	4.51E+05	1.71E+09	1.45E+13	8.70E+16
20				1.29E+03	1.25E+08	3.47E+13	1.85E+19	2.20E+24
	0.001			21.15	1.13E+04	4.81E+06	2.59E+09	2.22E+11
	0.1			21.16	1.13E+04	4.83E+06	2.61E+09	2.32E+11
	1.0			22.30	4.64E+04	6.96E+08	1.70E+13	1.95E+17
		0.0001		5.05	126.27	1.12E+04	4.94E+06	6.87E+08
		0.01		182.17	1.12E+06	4.66E+09	2.43E+13	1.71E+16
		0.1		1.79E+03	1.12E+08	4.65E+12	2.42E+17	1.70E+21
			0.0001	0.21	108.21	4.44E+04	2.27E+07	1.58E+09
			0.001	2.09	1.09E+03	4.46E+05	2.29E+08	1.60E+10
			0.1	240.09	2.45E+05	7.31E+08	4.96E+12	8.79E+15

Table 5: Derivative Bounds of Multi-Head Attention by derivative level according to Corollary 4.

Parameters								Derivative Level				
d_{in}	M	d_K	C^K	C^Q	C^V	C^W	$\|K\|$	1	2	3	4	5
5	1	3	0.1	0.1	0.1	0.1	1.0	7.67	46.08	184.82	931.81	5.73E+03
— using derivative level —								7.67	46.15	186.90	1.01E+03	7.84E+03
10								7.82E+03	4.87E+04	8.14E+05	2.95E+08	2.38E+11
20								1.57E+04	1.09E+05	1.03E+07	9.25E+09	1.50E+13
	5							3.90E+03	2.37E+04	1.34E+05	9.96E+06	3.83E+09
	20							4.71E+06	2.85E+07	7.11E+08	2.66E+12	1.40E+16
		3						7.67	45.99	183.98	920.53	5.53E+03
		10						7.70	46.41	190.35	1.07E+03	1.03E+04
		20						7.75	47.52	226.02	2.87E+03	1.23E+05
			0.01					7.65	45.91	183.61	918.01	5.51E+03
			1.0					7.90	54.45	740.55	6.51E+04	9.33E+06
				0.01				7.65	45.91	183.61	918.01	5.51E+03
				1.0				7.90	54.45	740.55	6.51E+04	9.33E+06
					0.01			0.77	4.61	18.48	93.18	573.32
					1.0			76.75	460.80	1.85E+03	9.32E+03	5.73E+04
						0.01		0.77	4.61	18.48	93.18	573.32
						1.0		76.75	460.80	1.85E+03	9.32E+03	5.73E+04
			0.001	0.001	0.001	0.001		0.00	0.00	0.02	0.09	0.55
			0.01	0.01	0.01	0.01		0.08	0.46	1.84	9.18	55.08
			1.0	1.0	1.0	1.0		1.02E+03	8.06E+04	4.95E+07	5.70E+10	8.04E+13
							0.1	0.77	32.14	142.34	752.79	4.68E+03
							10.0	79.00	259.65	5.54E+03	5.73E+05	8.04E+07
							100.0	1.02E+03	7.66E+04	4.88E+07	5.63E+10	7.90E+13

E SUPPORTING TECHNICAL RESULTS ON THE C^s-NORMS OF SMOOTH FUNCTIONS

This section contains many of the technical tools on which we build our analysis. Most results concern smooth functions, especially their derivatives and those of compositions thereof. However, the first set of results concerns the integral probability metric d_s.

E.1 INTEGRAL PROBABILITY METRICS AND RESTRICTION TO COMPACT SETS

Fix $d \in \mathbb{N}_+$ and a non-empty compact subset $K \subseteq \mathbb{R}^d$. Observe that any Borel probability measure μ on K can be canonically extended to a compactly supported Borel probability measure μ^+ on all of $\mathbb{R}^d$ via

$$\mu^+(B) \stackrel{\text{def.}}{=} \mu(B \cap K),$$

for any Borel subset B of $\mathbb{R}^d$; noting only that $B \cap K$ is Borel.

Let $\mathcal{P}(K)$ denote the set of Borel probability measures on K. Suppose that K is a regular compact set, i.e. the closure of its interior is itself. As usual, see Evans (2022), for any $s \in \mathbb{N}_+$, we denote the set of functions from the interior of K to $\mathbb{R}$ with s continuous partial derivatives thereon and with a continuous extension to K by $C^s(K)$. This space, is a Banach space when equipped with the (semi-)norm

$$\|f\|_{s:K} \stackrel{\text{def.}}{=} \max_{k=1,\dots,s-1} \max_{\alpha\in\{1,\dots,d\}^k} \sup_{u\in K} \left\| \frac{\partial^k f}{\partial x_{\alpha_1}\dots\partial x_{\alpha_k}}(u) \right\| + \max_{\alpha\in\{1,\dots,d\}^{s-1}} \operatorname{Lip}\left(\frac{\partial^{s-1} f}{\partial x_{\alpha_1}\dots\partial x_{\alpha_{s-1}}} \right).$$

We may define an associated integral probability metric $d_{s:K}$ on $\mathcal{P}(K)$ via

$$d_{s:K}(\mu, \nu) \stackrel{\text{def.}}{=} \sup_{f\in C^s(K)} \|\mathbb{E}_{X\sim\mu}[f(X)] - \mathbb{E}_{X\sim\nu}[f(X)]\|$$

for any $\mu, \nu \in \mathcal{P}(K)$. The main purpose of this technical subsection is simply to reassure ourselves, and the reader, that quantities $d_{s:K}(\mu, \nu)$ and $d_s(\mu^+, \nu^+)$ are equal for any $\mu, \nu \in \mathcal{P}(K)$. Therefore, we may use them interchangeably.

Lemma 2 (Consistency of Smooth IMP Extension - Beyond Regular Compact Sets)**.** *Fix $d, s \in \mathbb{N}_+$ and let K be a non-empty regular compact subset of $\mathbb{R}^d$. For any $\mu, \nu \in \mathcal{P}(K)$ the following holds*

$$d_{s:K}(\mu, \nu) = d_s(\mu^+, \nu^+).$$

Proof. Let $\operatorname{int}(K)$ denote the interior of K, By the Whitney extension theorem, as formulated in (Fefferman, 2005, Theorem A), for any $f \in C^s(K)$ there exists a C^s-extension $F : \mathbb{R}^d \to \mathbb{R}$ of $f|_{\operatorname{int}(K)}$ to all of $\mathbb{R}^d$; i.e. $F|_{\operatorname{int}(K)} = f$ and $\in C^s(\mathbb{R}^d)$. Since any continuous function is uniformly continuous on a compact set, $\operatorname{int}(K)$ is dense in K, and since uniformly continuous functions are uniquely determined by their values on compact sets, then f coincides with F on all of K (not only on $\operatorname{int}(K)$).

For any $\mu \in \mathcal{P}(K)$, by definition of μ^+ we have that

$$\mathbb{E}_{X\sim\mu^+}[F(X)] = \mathbb{E}_{X\sim\mu^+}[F(X)I_{X\in K}] = \mathbb{E}_{X\sim\mu^+}[f(X)I_{X\in K}] = \mathbb{E}_{X\sim\mu}[f(X)].$$

Therefore, for any $\mu, \nu \in \mathcal{P}(K)$ we conclude that and each $f \in C^s(K)$ there exists some $F \in C^s(\mathbb{R}^d)$ such that

$$\mathbb{E}_{Y\sim\mu}[f(Y)] - \mathbb{E}_{Y\sim\nu}[f(Y)] = \mathbb{E}_{X\sim\mu^+}[F(X)] - \mathbb{E}_{X\sim\nu^+}[F(X)].$$

Consequentially, $d_{s:K}(\mu, \nu) \leqslant d_s(\mu^+, \nu^+)$. Conversely, since the restriction of any $g \in C^s(\mathbb{R}^d)$ to K belongs to $C^s(K)$ then the reverse inequality holds; namely, $d_{s:K}(\mu, \nu) \geqslant d_s(\mu^+, \nu^+)$. □

By Lemma 2 we henceforth may interpret any such μ as its extension μ^+, without loss of generality.

E.2 EXAMPLES OF FUNCTIONS IN THE CLASSES $C^s_{poly:C,r}([0,1]^d, \mathbb{R})$ AND $C^s_{exp:C,r}([0,1]^d, \mathbb{R})$

In several learning theory papers, especially in the kernel ridge regression literature e.g. Simon et al. (2023); Barzilai and Shamir (2023); Tsigler and Bartlett (2023); Simon et al. (2023); Cheng et al. (2024a;b), one often quantifies the *learnability* of a target function in terms of some sort of decay/growth rates of its coefficients in an appropriate expansion; e.g. the decay of its coefficients in an eigenbasis associated to a kernel. These decay/growth rates are often equivalent to the smoothness of a function[3]. Therefore, in a like spirit, we unpack the meaning of the smoothness condition in

[3] See e.g. (Atkinson and Han, 2012, page 120-121) for an example between the decay rate of the Laplacian eigenspectrum characterize the smoothness of the functions in the RKHS of radially symmetric kernels.

Assumption 2 which impacts the learning rates in Theorem 1 by giving examples of functions in the classes $C^s_{poly:C,r}([0,1]^d,\mathbb{R})$ and $C^s_{exp:C,r}([0,1]^d,\mathbb{R})$.

For brevity and transparency in our illustration, we consider the one-dimensional case. In particular, this shows that the class is far from being void.

Proposition 4 (Functions with Polynomially/Exponentially Growing C^s-Norms on $[0,1]$)**.** *Fix $d \in \mathbb{N}_+$ and let K be a non-empty regular compact subset of $\mathbb{R}^d$. If $f:\mathbb{R}\to\mathbb{R}$ is real-analytic with power-series expansion at 0 given by*

$$f(x) = \sum_{i=0}^{\infty} \frac{\beta_i\, x^i}{i!},$$

and if there are $C, r > 0$ such that

(i) ***Polynomial Growth:*** $|\beta_i| \leqslant C e^{i\,r}$ $(\forall i \in \mathbb{N})$*, then* $f \in C^{\infty}_{poly:C,r}([0,1],\mathbb{R})$*; or*

(ii) ***Exponential Growth:*** $|\beta_i| \leqslant C(1+i)^r$ $(\forall i \in \mathbb{N})$*, then* $f \in C^{\infty}_{poly:C,r}([0,1],\mathbb{R})$*.*

Proof. Since f is real-analytic we may consider its Maclaurin-Taylor series expansion which, coincides with $\sum_{i=0}^{\infty} \frac{\beta_i\, x^i}{i!}$; meaning that for each $i \in \mathbb{N}$ we have $\beta_i = \partial^i f(0)$. Therefore, standard analytic estimates and manipulations of the Maclaurin-Taylor series—see e.g. (Rudin, 1976, page 173)—yield

$$\begin{aligned}\max_{0\leqslant x\leqslant 1} \Big|\sum_{i=0}^{\infty} \frac{\beta_i\, x^i}{i!} - f(x)\Big| \leqslant & \frac{1}{(s+1)!} \sup_{0\leqslant x\leqslant 1} \Big|\Big(\sum_{i=0}^{\infty} \frac{\beta_i\, x^i}{i!}\Big)^{s+1} - \partial f^{s+1}(x)\Big| \\ \leqslant & \frac{1}{(s+1)!}\, \beta_s (s+1)!. \end{aligned} \tag{11}$$

If (i) holds, then the right-hand side of (11) is bounded from above by $C\,(s+1)^r$ and $f \in C^{\infty}_{poly:C,r}([0,1],\mathbb{R})$. If instead (ii) holds, then the right-hand side of (11) is bounded from above by $C\, e^{s\,r}$ implying $f \in C^{\infty}_{exp:C,r}([0,1],\mathbb{R})$. □

F PROOF OF THEOREM 1

Section 3.3, the proof will be largely broken down into two steps. First, we derive our concentration of measure result for the empirical mean compared to the true mean general of an arbitrary C^s function applied to a random input, where the C^s-norm of the C^s function is at most $R \geqslant 0$ (in Subsection F.2).

Next, (in Subsection F.2), we use the Faà di Bruno-type results in Section F.1 to bound the maximal C^s norm over the relevant class of transformer networks. We do this by first individually bounding each of the C^s-norms of its constituent pieces, namely the multi-head attention layers, the SLP blocks with smooth activation functions, and then ultimately, we bound the C^s-norms of the composition of transformer blocks using the earlier Faà di Bruno-type results.

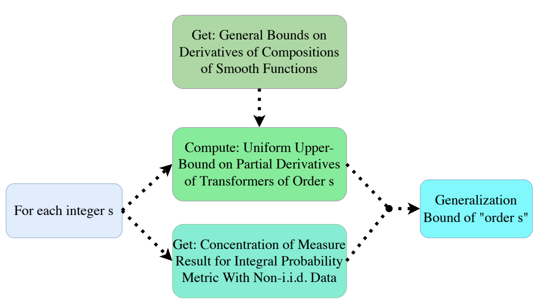


Figure 5: Workflow of the proof technique used to derive Theorem 1.

Our main result (Theorem 1) is then then obtained upon merging these two sets of estimates. The workflow which we use can be applied to derive generalization bounds for other machine learning, and is summarized in Figure 5.

F.1 Step 0 - Bounds on the C^s Regularity of Multivariate Composite Functions

In this section, we will derive a bound for the Sobolev norm of multivariate composite functions.

F.1.1 Multivariate Faà di Bruno formula revisited

We begin by establishing notation and stating the multivariate Faà di Bruno formula from Constantine and Savits (1996).

Theorem 3 (Multivariate Faà di Bruno Formula, Constantine and Savits (1996))**.** *Let $n, m, k \in \mathbb{N}$, $\alpha \in \mathbb{N}^k$ with $|\alpha| = n$, and define*

$$h(x_1, \ldots, x_k) \overset{\text{def.}}{=} f^{(1)}(g^{(1)}(x_1, \ldots, x_k), \ldots, g^{(m)}(x_1, \ldots, x_k)).$$

Then, using the multivariate notation from Notation 1,

$$D^\alpha h(x) = \sum_{1 \leqslant |\beta| \leqslant n} (D^\beta f)(g(x)) \sum_{\eta, \zeta \in \mathcal{P}(\alpha, \beta)} \alpha! \prod_{j=1}^n \frac{[D^{\zeta^{(j)}} g(x)]^{\eta^{(j)}}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}.$$

where

$$\begin{aligned}\mathcal{P}(\alpha, \beta) = \Big\{ &\eta \overset{\text{def.}}{=} (\eta^{(1)}, \ldots, \eta^{(n)}) \in (\mathbb{N}^m)^n, \zeta \overset{\text{def.}}{=} (\zeta^{(1)}, \ldots, \zeta^{(n)}) \in (\mathbb{N}^k)^n : \\ &\exists j \leqslant m : \eta^{(i)} = 0, \zeta^{(i)} = 0 \text{ for } i < j, |\eta^{(i)}| > 0 \text{ for } i \geqslant j, \\ &0 \prec \zeta^{(j)} \prec \ldots \prec \zeta^{(n)}, \textstyle\sum_{i=1}^n \eta^{(i)} = \beta \text{ and } \sum_{i=1}^n |\eta^{(i)}| \zeta^{(i)} = \alpha \Big\}.\end{aligned}$$

Proof. See Constantine and Savits (1996). □

F.1.2 Universal Bounds

Theorem 4. *In the notation of Theorem 3, we have for a compact set $K \subseteq \mathbb{R}^k$ and an multi-index $\alpha \in \mathbb{N}^k$, $|\alpha| = n$,*

$$C_K^h(\alpha) \leqslant \max_{n' \in \{1, \ldots, n\}} C_{g[K]}^g(n') C_K^f(\leqslant n)^{n'} \sum_{1 \leqslant |\beta| \leqslant n} \sum_{\eta, \zeta \in \mathcal{P}(\alpha, \beta)} \alpha! \prod_{j=1}^n \frac{1}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}$$

where $C_K^h(\cdot)$, $C_{g[K]}^f(\cdot)$, $C_K^g(\cdot)$ are defined as in Notation 3.

Proof. Using Theorem 3,

$$\begin{aligned} C_K^h(\alpha) &\leqslant \sum_{1 \leqslant |\beta| \leqslant n} \|D^\beta f\|_{g[K]} \sum_{\eta, \zeta \in \mathcal{P}(\alpha, \beta)} \alpha! \prod_{j=1}^n \frac{\prod_{i=1}^m \|(D^{\zeta^{(j)}} g)_i\|_K^{\eta_i^{(j)}}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} \\ &\leqslant \sum_{1 \leqslant |\beta| \leqslant n} C_{g[K]}^g(|\beta|) \sum_{\eta, \zeta \in \mathcal{P}(\alpha, \beta)} \alpha! \prod_{j=1}^n \frac{\prod_{i=1}^m C_K^f(\leqslant n)^{\eta_i^{(j)}}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} \\ &\leqslant \sum_{1 \leqslant |\beta| \leqslant n} C_{g[K]}^g(|\beta|) C_K^f(\leqslant n)^{|\beta|} \sum_{\eta, \zeta \in \mathcal{P}(\alpha, \beta)} \alpha! \prod_{j=1}^n \frac{1}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} \\ &\leqslant \max_{n' \in \{1, \ldots, n\}} C_{g[K]}^g(n') C_K^f(\leqslant n)^{n'} \sum_{1 \leqslant |\beta| \leqslant n} \sum_{\eta, \zeta \in \mathcal{P}(\alpha, \beta)} \alpha! \prod_{j=1}^n \frac{1}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}. \end{aligned}$$

□

Next, we refine the strategy used in Hou et al. (2023b) to convert our uniform risk-bound to a concentration of measure problem. Once done, the remainder of the proof will be to obtain bounds on the rate at which this measure concentrates.

Lemma 3. *For $\alpha \in \{1, \cdots, k\}^n$, it satisfies that*

$$\sum_{1 \leqslant |\beta| \leqslant n} \sum_{\eta, \zeta \in \mathcal{P}(\alpha,\beta)} \alpha! \prod_{j=1}^{n} \frac{1}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} = \Big[\frac{2m|\alpha|}{e \ln |\alpha|}(1+o(1))\Big]^{|\alpha|}$$

where $\mathcal{P}(\alpha, \beta)$ is as defined in Theorem 3.

Proof. Consider functions

$$g^{(i)}(x) = g^{(i)}(x_1, \cdots, x_d) \overset{\text{def.}}{=} \exp\Big(\sum_{j=1}^{d} x_j\Big) : \mathbb{R}^d \to \mathbb{R}, \quad i = 1, ..., 2m,$$

$$f(g^{(1)}, \cdots, g^{(2m)}) \overset{\text{def.}}{=} \exp\Big(\sum_{i=1}^{2m} g^{(i)}\Big) : \mathbb{R}^{2m} \to \mathbb{R},$$

Since

$$\frac{\partial}{\partial g^{(i)}} f(g^{(1)}, \cdots, g^{(2m)}) = f(g^{(1)}, \cdots, g^{(2m)}),$$

it follows that

$$(D^\beta f)(g^{(1)}(x), \cdots, g^{(2m)}(x)) = f(g^{(1)}(x), \cdots, g^{(2m)}(x)), \quad \forall \beta \in \{1, \cdots, 2m\}^n.$$

Since

$$\begin{aligned}
&\frac{\partial}{\partial x^j} f(g^{(1)}(x_1, \cdots, x_k), \cdots, g^{(2m)}(x_1, \cdots, x_k)) \\
=&\sum_{i=1}^{2m} \frac{\partial}{\partial g^{(i)}} f(g^{(1)}(x_1, \cdots, x_k), \cdots, g^{(2m)}(x_1, \cdots, x_k)) \frac{\partial g^{(i)}(x_1, \cdots, x_k)}{\partial x_j} \\
=&\sum_{i=1}^{2m} f(g^{(1)}(x_1, \cdots, x_k), \cdots, g^{(2m)}(x_1, \cdots, x_k)) g^{(i)}(x_1, \cdots, x_k) \\
=&\sum_{i=1}^{2m} \frac{\partial}{\partial g^{(i)}} f(g^{(1)}(x), \cdots, g^{(2m)}(x)) \frac{\partial g^{(i)}(x)}{\partial x_j} \\
=&f(g^{(1)}(x), \cdots, g^{(2m)}(x)) \sum_{i=1}^{2m} g^{(i)}(x)
\end{aligned}$$

and

$$\frac{\partial g^{(i)}(x_1, \cdots, x_k)}{\partial x_j} = g^{(i)}(x_1, \cdots, x_k),$$

we can show by the Faà di Bruno formula that

$$\begin{aligned}
&D^\alpha f(g^{(1)}(x), \cdots, g^{(2m)}(x)) \\
&= D^\alpha \exp\Big(\sum_{i=1}^{2m} g^{(i)}(x)\Big) \\
&= \sum \frac{|\alpha|!}{\gamma_1!(1!)^{\gamma_1} \cdots \gamma_{|\alpha|}!(|\alpha|!)^{\gamma_{|\alpha|}}} \big(D^{\gamma_1 + \cdots + \gamma_{|\alpha|}} \exp\big)\Big(\sum_{i=1}^{2m} g^{(i)}(x)\Big) \prod_{j=1}^{|\alpha|} \Big[m^j \Big(\sum_{i=1}^{2m} g^{(i)}(x)\Big)\Big]^{\gamma_j},
\end{aligned}$$

where the summation on the right side of the last equality is over all $|\alpha|$-tuples $(\gamma_1, \cdots, \gamma_{|\alpha|}) \geqslant 0$ such that $1 \cdot \gamma_1 + 2 \cdot \gamma_2 + \cdots + |\alpha| \cdot \gamma_{|\alpha|} = |\alpha|$.

By the multivariate Faà di Bruno formula. For each $n = 1, ..., s-1$ fixed, and for each $\alpha \in \{1, \cdots, k\}^n$, we have

$$D^\alpha f(g^{(1)}(x), \cdots, g^{(2m)}(x)) = \sum_{1 \leqslant |\beta| \leqslant n} (D^\beta f)(g^{(1)}(x), \cdots, g^{(2m)}(x)) \sum_{\eta,\zeta \in \mathcal{P}(\alpha,\beta)} \alpha! \prod_{j=1}^{n} \frac{[D^{\zeta^{(j)}}(g^{(1)}(x), \cdots, g^{(2m)}(x))]^{\eta^{(j)}}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}.$$

Taking $x = (x_1, \cdots, x_k) = 0$, we have

$$D^\alpha f(g^{(1)}(0), \cdots, g^{(2m)}(0)) = \sum \frac{|\alpha|!}{\gamma_1!(1!)^{\gamma_1} \cdots \gamma_{|\alpha|}!(|\alpha|!)^{\gamma_{|\alpha|}}} \exp(2m) \prod_{j=1}^{|\alpha|} (2m)^{\gamma_j}$$
$$(m^\beta f)(g^{(1)}(0), \cdots, g^{(2m)}(0)) = f(g^{(1)}(0), \cdots, g^{(2m)}(0)) = \exp(2m),$$
$$D^{\zeta^{(j)}}(g^{(1)}(x), \cdots, g^{(2m)}(x)) = (1, \cdots, 1).$$

Substituting the above derivatives into the Faà di Bruno formula, we obtain

$$\begin{aligned}\sum_{1 \leqslant |\beta| \leqslant n} \sum_{\eta,\zeta \in \mathcal{P}(\alpha,\beta)} \alpha! \prod_{j=1}^{k} \frac{1}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} =& \sum \frac{|\alpha|!}{\gamma_1!(1!)^{\gamma_1} \cdots \gamma_{|\alpha|}!(|\alpha|!)^{\gamma_{|\alpha|}}} \prod_{j=1}^{|\alpha|} (2m)^{\gamma_j} \\ \leqslant& (2m)^{|\alpha|} \sum \frac{|\alpha|!}{\gamma_1!(1!)^{\gamma_1} \cdots \gamma_{|\alpha|}!(|\alpha|!)^{\gamma_{|\alpha|}}} \\ =& (2m)^{|\alpha|} \Big(\frac{|\alpha|}{e \ln |\alpha|}\Big)^{|\alpha|} (1 + o(1))^{|\alpha|},\end{aligned}$$

where the last equality follows from (Khorunzhiy, 2022, Theorem 2.1),

$$\sum \frac{|\alpha|!}{\gamma_1!(1!)^{\gamma_1} \cdots \gamma_{|\alpha|}!(|\alpha|!)^{\gamma_{|\alpha|}}} = \Big(\frac{|\alpha|}{e \ln |\alpha|}\Big)^{|\alpha|} (1 + o(1))^{|\alpha|}.$$

□

Corollary 1 (Level Specific C^s-Norm Bounds for Transformer Blocks)**.** *In the notation of Theorem 4, it holds for $n \in \mathbb{N}, n > 1$ that*

$$C_K^h(\leqslant n) \leqslant \max_{n' \in \{1,\dots,n\}} C_{g[K]}^g(n') C_K^f(\leqslant n)^{n'} \Big[\frac{2mn}{e \ln n}(1 + o(1))\Big]^n.$$

and if $C_K^f(\leqslant n) \geqslant 1$,

$$C_K^h(\leqslant n) \leqslant C_{g[K]}^g(\leqslant n) C_K^f(\leqslant n)^n \Big[\frac{2mn}{e \ln n}(1 + o(1))\Big]^n.$$

Proof. Follows directly from Theorem 4 and Lemma 3. □

F.1.3 Bounds in Derivative Type

The goal of this section is to bound the derivative of composite functions by grouping with respect to $\sim$, defined in Notation 2.

Theorem 5. *In the notation of Theorem 3, we have for a compact set $K \subseteq \mathbb{R}^k$ and an ordered multi-index $\alpha \in \mathfrak{O}_n^k$*

$$C_K^h(\alpha) \leqslant \alpha! \sum_{\beta \in \mathfrak{O}_{\leqslant n}^m} N(\beta) C_{g[K]}^f(\beta) \sum_{\eta,\zeta \in \mathcal{P}'(\alpha,\beta)} \prod_{j=1}^{n} \frac{C_K^g(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}},$$

where $C_K^h(\cdot)$, $C_{g[K]}^f(\cdot)$, $C_K^g(\cdot)$ are defined as in Notation 3; and

$$\begin{aligned}\mathcal{P}'(\alpha,\beta) = \Big\{&\eta \stackrel{\text{def.}}{=} (\eta^{(1)}, \dots, \eta^{(n)}) \in (\mathbb{N}^m)^n, \zeta \stackrel{\text{def.}}{=} (\zeta^{(1)}, \dots, \zeta^{(n)}) \in (\mathbb{N}^k)^n : \\ &\exists j \leqslant m : \eta^{(i)} = 0, \zeta^{(i)} = 0 \text{ for } i < j, |\eta^{(i)}| > 0 \text{ for } i \geqslant j, \\ &0 < \zeta^{(j)} \lhd \dots \lhd \zeta^{(n)}, \textstyle\sum_{i=1}^n \eta^{(i)} = \beta \text{ and } \sum_{i=1}^n |\eta^{(i)}| \zeta^{(i)} = \alpha\Big\},\end{aligned}$$

where $\alpha \lhd \beta$ for $\alpha, \beta \in \mathbb{N}^k$ if $|\alpha| \leqslant |\beta|$ and $\alpha \neq \beta$.

Proof. We have for $\alpha \in \mathfrak{O}_n^k$

$$C_K^h(\alpha) \leqslant \max_{\gamma\sim\alpha} \sum_{1\leqslant|\beta|\leqslant n} \|D^\beta f\|_{g[K]} \sum_{\eta,\zeta\in\mathcal{P}(\gamma,\beta)} \alpha! \prod_{j=1}^n \frac{\prod_{i=1}^m \|(D^{\zeta^{(j)}} g)_i\|_K^{\eta_i^{(j)}}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}$$

$$\leqslant \sum_{1\leqslant|\beta|\leqslant n} C_{g[K]}^f(\mathfrak{o}(\beta)) \max_{\gamma\sim\alpha} \sum_{\eta,\zeta\in\mathcal{P}(\gamma,\beta)} \alpha! \prod_{j=1}^n \frac{C_K^g(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}.$$

Then

$$\left\{\eta, (\mathfrak{o}(\zeta^{(1)}), ..., \mathfrak{o}(\zeta^{(n)}))\middle|(\eta,\zeta)\in\mathcal{P}'(\alpha,\beta)\right\}$$

is invariant in α with respect to $\sim$ and thus

$$C_K^h(\alpha) \leqslant \sum_{1\leqslant|\beta|\leqslant n} C_{g[K]}^f(\mathfrak{o}(\beta)) \sum_{\eta,\zeta\in\mathcal{P}'(\alpha,\beta)} \alpha! \prod_{j=1}^n \frac{C_K^g(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}.$$

Further, notice that

$$\left\{((|\eta^{(1)}|, \eta^{(1)}!), \dots, (|\eta^{(n)}|, \eta^{(n)}!)), \zeta\middle|(\eta,\zeta)\in\mathcal{P}'(\alpha,\beta)\right\}$$

is invariant in β with respect to $\sim$ and the assertion follows. □

Corollary 2. *In the notation of Theorem 5, if f is affine-linear,*

$$C_K^h(\alpha) \leqslant m\alpha! C_{g[K]}^f(e_1) C_K^g(\alpha),$$

where $C_{g[K]}^f(e_1)$ is the maximum weight of the matrix representing f.

Proof. Theorem 5 yields

$$C_K^h(\alpha) \leqslant m\alpha! C_{g[K]}^f(e_1) \sum_{\eta,\zeta\in\mathcal{P}'(\alpha,\beta)} \prod_{j=1}^n \frac{C_K^g(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}},$$

and since $\mathcal{P}'(\alpha, e_1) = \{(0, ..., 0, e_1), (0, ..., 0, \alpha)\}$ the result follows. □

F.2 Step 1 - Concentration of Measure - Bounding the Right-Hand Side of (2)

We are now ready to derive our main concentration of measure results used to derive our risk-bound. This corresponds to bounding term (2) by controlling the integral probability term $d_s(\mu_t, \mu^{(N)})$ in (3), with high probability, where the randomness is due to the randomness of the empirical measure $\mu^{(N)}$.

We state the next bound in the case where the input space if $\mathbb{R}^d$. Note that the results hold for any other input dimension, such as Md, simply by relabeling $d \leftarrow Md$. Thus, it applies to the *finite-dimensional* Markovian lifts $X^M_\cdot$ of data-generating processes $X_\cdot$, where $M \in \mathbb{N}_+$, by relabeling. Therefore, for notational minimality, we chose to label the input dimension d and not dM.

Proposition 5 (Excess Risk-Bound). *Under Assumption 1 and either 2 or 3, let $f^\star : \mathbb{R}^d \to \mathbb{R}^D$, $\ell : \mathbb{R}^{2D} \to \mathbb{R}$, and $R, r > 0$ be a such that the composite map $\mathbb{R}^d \ni x \mapsto \ell(f^\star(x), f(x))$ belongs to $\mathcal{C}_R^s(\mathbb{R}^d)$ for all $f \in C_r^2(\mathbb{R}^d)$. Then, there exists some $\kappa \in (0,1)$ depending only on the Markov chain $X_\cdot$ and some $t_0 \in \mathbb{N}_0$ such that for each $t_0 \leqslant N < t \leqslant \infty$, each "rate-to-constant-tradeoff parameter" $s \in \mathbb{N}_+$, and every "confidence level" $\delta \in (0,1]$ the following*

$$\sup_{g\in\mathcal{C}_R^s(\mathbb{R}^d)} \frac{\left|\mathcal{R}_{\max\{t,N\}}(g) - \mathcal{R}^{(N)}(g)\right|}{R} \lesssim \kappa^t + \frac{\sqrt{2\ln(1/\delta)}}{N^{1/2}} + \begin{cases} \frac{\log\left(c\,N\right)^{d/(2s+1)}}{c\,N^{1/2}} & \text{if } d < 2s \\ \frac{\log\left(c\,N\right)}{c\,N^{1/2}} & \text{if } d = 2s \\ \frac{\log\left(c\,N\right)^{d-2s+(s/d)}}{c_2\,N^{s/d}} & \text{if } d = 2s \end{cases}$$

holds with probability at least $1-\delta$; where $0 < \kappa < 1$, and we use the notation $\kappa^\infty \overset{\text{def.}}{=} 0$.

Proof of Proposition 5. By hypothesis, $\tilde{f} \in C_r^s(\mathbb{R}^d)$ the induced map

$$\begin{aligned} f : \mathbb{R}^d &\to \mathbb{R} \\ x &\mapsto f(x) \overset{\text{def.}}{=} \ell\big(f^\star(x), \tilde{f}(x)\big) \end{aligned} \tag{12}$$

belongs to $C_R^s(\mathbb{R}^d)$.

Conversion to a Concentration of Measure Problem. Denote the empirical (random) measure associated with the samples $\{(X_n,Y_n)\}_{n=1}^N$ by $\mu^{(N)} \stackrel{\text{def.}}{=} \frac{1}{N}\sum_{n=1}^N \delta_{(X_n,Y_n)}$. Note that the generalization bound is 0 for any constant function; therefore, we consider the bound over $C_R^s(\mathbb{R}^d)\setminus \operatorname{Lip}_0$ where Lip_0 denotes the set of constant functions from $\mathbb{R}^d$ to $\mathbb{R}$. Note the bijection between $C_R^s(\mathbb{R}^d)\setminus \operatorname{Lip}_0$ and $C_1^s(\mathbb{R}^d)\setminus \operatorname{Lip}_0$ given by $f\mapsto \frac{1}{\max\{1,\|f\|_{C^s(\mathbb{R}^d)}\}} f$. Therefore, we compute

$$
\begin{aligned}
\left|\mathcal{R}_t(f)-\mathcal{R}^{(N)}(g)\right| \leqslant & \sup_{g\in \mathcal{C}_R^s(\mathbb{R}^d)} \left|\mathcal{R}_t(f)-\mathcal{R}^{(N)}(g)\right| \\
\leqslant & R \sup_{g\in \mathcal{C}_1^s(\mathbb{R}^d)} \left|\mathcal{R}_t(g)-\mathcal{R}^{(N)}(g)\right| \\
\leqslant & R\, d_{C^s}(\mu_{\max\{t,N\}},\mu^{(N)}) \\
\leqslant & R\,\big(\underbrace{d_{C^s}(\mu_t,\bar{\mu})}_{\text{(IV)}}+\underbrace{d_{C^s}(\bar{\mu},\mu^{(N)})}_{\text{(V)}}\big).
\end{aligned} \tag{13}
$$

Next, we bound terms (I) and (II).

Bounding Term (IV). If Assumption 2 holds then: for every $t\in\mathbb{N}_+$ each $x,\tilde{x}\in\mathcal{X}$ we have

$$
\mathcal{W}_1\big(P^t(x,\cdot),P^t(\tilde{x},\cdot)\big) \leqslant \kappa^t\, \mathcal{W}_1(\delta_x,\delta_{\tilde{x}}) = \kappa^t\, \|x-\tilde{x}\|.
$$

If, instead, we operate under the log-Sobolev Assumption 3, then (Bobkov and Götze, 1999, Theorem 1.3) can be applied to $\bar{\mu}$ and $P(x,\cdot)$ for each $x\in\mathcal{X}$, implying that the transport inequalities hold: for each $\nu\in\mathcal{P}(\mathcal{X})$ and each $\tilde{\mu}\in\{\bar{\mu},\mu_0\}\cup\{P(x,\cdot)\}_{x\in\mathcal{X}}$

$$
\mathcal{W}_1(\tilde{\mu},\nu)^2 \leqslant 2C^2\ \mathrm{KL}(\nu|\tilde{\mu}) \tag{14}
$$

where we recall the definition of the Kullback–Leibler divergence $\mathrm{KL}(\nu|\mu)\stackrel{\text{def.}}{=}\mathbb{E}_{X\sim\nu}[\log(\frac{d\nu}{d\mu}(X))]$. Thus, (14) implies that the following exponential contractility property of the Markov kernel: there exists some $\kappa\in(0,1)$ such that for each $x,\tilde{x}\in\mathcal{X}$ and every $t\in\mathbb{N}_+$

$$
\mathcal{W}_1\big(P^t(x,\cdot),P^t(\tilde{x},\cdot)\big) \leqslant \kappa^t\, \|x-\tilde{x}\|. \tag{15}
$$

Furthermore, (15) implies that the conditions for (Riekert, 2022, Theorem 1.5) are met; whence, for every $\varepsilon\geqslant 0$ and each $N\in\mathbb{N}$ the following holds with probability at-least $1-\exp\big(\frac{-N\,\varepsilon^2(1-\kappa)^2}{2C^2}\big)$

$$
\text{(IV)} = d_s(\bar{\mu},\mu^{(N)}) \leqslant \mathbb{E}\big[d_s(\bar{\mu},\mu^{(N)})\big]+\varepsilon, \tag{16}
$$

for some $C>0$. Upon setting $\varepsilon\stackrel{\text{def.}}{=}\frac{C\sqrt{2\ln(1/\delta)}}{\sqrt{N\,(1-\kappa^2)}}$, (16) implies that: for every $N\in\mathbb{N}$ and each $\delta\in(0,1]$ the following holds with probability at-least $1-\delta$

$$
\text{(IV)} = d_s(\bar{\mu},\mu^{(N)}) \leqslant \underbrace{\mathbb{E}\big[d_s(\bar{\mu},\mu^{(N)})\big]}_{\text{(VI)}}+\frac{C\sqrt{2\ln(1/\delta)}}{\sqrt{N\,(1-\kappa^2)}}. \tag{17}
$$

It remains to bound the expectation term (VI) in (17) to bound term (IV).

Under the exponential moment assumption 4, we have that

$$
\mathbb{E}_{X\sim P(x,\cdot)}[e^{\beta|X|}-1] \leqslant \gamma\,(e^{\beta|x|}-1)+(C-1+\gamma). \tag{18}
$$

Therefore (Riekert, 2022, Proposition 1.3), implies that $\sup_{t\in\mathbb{N}_0}\mathbb{E}[e^{\beta|X_t|}-1]<\infty$. Whence, (Riekert, 2022, Assumption 2) holds with Young function $\Phi(x)=\frac{1}{\max\{1,\sup_{t\in\mathbb{N}_+}\}\,\mathbb{E}[e^{\beta|X_t-1]}}\,(e^{\beta|X_t|}-1)$; namely, $\sup_{t\in\mathbb{N}_0}\mathbb{E}[\Phi(|X_t|)]\leqslant 1$. Consequentially, (Riekert, 2022, Theorem 1.1) applies from which we conclude that there is some $t_0\in\mathbb{N}_+$ such that for all $N\geqslant t_0$

$$
\text{(VI)} = \mathbb{E}\big[d_s(\bar{\mu},\mu^{(N)})\big] \lesssim \log\big((1-\kappa)\,N\big)^s
\begin{cases}
\frac{\log\big((1-\kappa)\,N\big)^{d/(2s)+1}}{(1-\kappa)^{1/2}\,N^{1/2}} & \text{if } 1=d<2s\\
\frac{\log\big((1-\kappa)\,N\big)}{(1-\kappa)^{1/2}\,N^{1/2}} & \text{if } d=2s\\
\frac{\log\big((1-\kappa)\,N\big)^{d-2s+s/d}}{(1-\kappa)^{s/d}\,N^{s/d}} & \text{if } d=2s
\end{cases}. \tag{19}
$$

Combining the order estimate of (VI) in (19) with the estimate in (17) implies that: for every $N \geqslant t_0$ and each $\delta \in (0,1]$ we have

$$\text{(IV)} = d_s(\bar{\mu}, \mu^{(N)}) \lesssim \frac{\sqrt{2\ln(1/\delta)}}{N^{1/2}} + \begin{cases} \frac{\log\left(c\,N\right)^{d/(2s)+1}}{c\,N^{1/2}} & \text{if } 1 = d < 2s \\ \frac{\log\left(c\,N\right)}{c\,N^{1/2}} & \text{if } d = 2s \\ \frac{\log\left(c\,N\right)^{d-2s+s/d}}{c_2\,N^{s/d}} & \text{if } d = 2s \end{cases} \tag{20}$$

where $c \stackrel{\text{def.}}{=} (1-\kappa)$, $c_2 \stackrel{\text{def.}}{=} c^{s/d} \in (0,1)$, and $\lesssim$ suppresses the absolute constant $\max\{1, C\} > 0$.

Bounding Term (V). Next, we bound (V) by computing

$$\begin{aligned}
\text{(V)} = d_{C^s}(\mu_t, \bar{\mu}) \stackrel{\text{def.}}{=} & \sup_{g \in \mathcal{C}_1^s(\mathbb{R}^d)} \mu_t[g] - \bar{\mu}[g] \\
\leqslant & \sup_{g \in \operatorname{Lip}_1(\mathbb{R}^d)} \mu_t[g] - \bar{\mu}[g] && (21)\\
= & \mathcal{W}_1(\mu_t, \bar{\mu}) && (22)\\
= & \mathcal{W}_1(P^t\mu_0, \bar{\mu}) && (23)\\
= & \mathcal{W}_1(P^t\mu_0, P^t\bar{\mu}) && (24)\\
\leqslant & \kappa^t\, \mathcal{W}_1(\mu_0, \bar{\mu}) \stackrel{\text{def.}}{=} \kappa^t\, C && (25)
\end{aligned}$$

where (21) held by definition of the MMD d_{C^s} and by the inclusion of $\mathcal{C}_1^s(\mathbb{R}^d) \subset \operatorname{Lip}_1(\mathbb{R}^d)$, (22) held by Kantorovich duality (see (Villani, 2009, Theorem 5.10)), (24) held since $\bar{\mu}$ is the stationary probability measure for the Markov chain $X_\cdot$, it is invariant to the action of the Markov kernel, and (25) followed from (Olivera and Tudor, 2019, Corollary 21) since we deduced the exponential contractility property (15) of the Markov kernel. Note that $C \stackrel{\text{def.}}{=} \mathcal{W}_1(\mu_0, \bar{\mu})$ is a constant depending only on the initial and stationary distributions of the Markov chain.

Conclusion. Incorporating the estimates for (V) and (IV) into the right-hand side of (13) implies that: for every $t, N \geqslant t_0$, $s \in \mathbb{N}_+$, and each $\delta \in (0,1]$ the following holds

$$\sup_{g \in \mathcal{C}_R^s(\mathbb{R}^d)} \frac{\left|\mathcal{R}_{\max\{t,N\}}(g) - \mathcal{R}^{(N)}(g)\right|}{R} \lesssim I_{t<\infty}\, \kappa^t + \frac{\sqrt{2\ln(1/\delta)}}{N^{1/2}} + \begin{cases} \frac{\log\left(c\,N\right)^{d/(2s+1)}}{c\,N^{1/2}} & \text{if } 1 = d < 2s \\ \frac{\log\left(c\,N\right)}{c\,N^{1/2}} & \text{if } d = 2s \\ \frac{\log\left(c\,N\right)^{d-2s+(s/d)}}{c_2\,N^{s/d}} & \text{if } d = 2s \end{cases}$$

with probability at-least $1-\delta$; where $c \stackrel{\text{def.}}{=} (1-\kappa)$ and $\kappa \in (0,1)$; where $I_{t<\infty} k^{\infty} \stackrel{\text{def.}}{=} 0$ if $t = \infty$. □

F.3 STEP 2 (A) - BOUNDING THE C^s REGULARITY OF TRANSFORMER BUILDING BLOCKS

We begin by the following simple remark, that if the activation function used to defined the transformer is smooth, then so must the entire transformer model.

Proposition 6 (Transformers with Smooth Activation Functions are Smooth). *Fix $\mathcal{TC}$, as in Definition 6, then every transformer $\mathcal{T} \in \mathcal{TC}$ is smooth.*

Theorem 6. The smoothness of Att follows directly from the smoothness of softmax, which immediately implies smoothness of $\mathcal{MH}$ since the operators used for its definition are smooth. Furthermore, the $\mathcal{LN}$ is smooth due to its smooth and lower-bounded denominator and the activation function σ is smooth by definition, therefore we conclude that $\mathcal{TB} \in \mathcal{TBC}$ is smooth for every $\mathcal{TBC}$ as in Definition 5 and we obtain smoothness of $\mathcal{T} \in \mathcal{TC}$ as a consequence. □

F.3.1 THE SOFTMAX FUNCTION

Lemma 4 (Representation of higher-order softmax derivatives). *For $F \in \mathbb{N}$ and*

$$\operatorname{smax} : \mathbb{R}^F \to \mathbb{R}^F, \quad x \mapsto \left(\exp(x_i)/\textstyle\sum_{j=0}^{F-1} \exp(x_j)\right)_{i=1}^F.$$

there exists for any multi-index $\alpha \in \mathbb{N}^F$ *and* $m \in \{1, \ldots, F\}$ *indicators* $(a_{i,j}^k)_{i,j \in I(\alpha)}^{k \in \{1,\ldots,|\alpha|!\}} \subseteq \{0, 1\}$ *such that*

$$\operatorname{smax}^{(\alpha)}(x_m) = \sum_{k=1}^{|\alpha|!} \operatorname{smax}(x_m) \prod_{i,j \in I(\alpha)} (a_{i,j}^k - \operatorname{smax}(x_j)), \tag{26}$$

where $I(\alpha) \overset{\text{def.}}{=} \{(i, j) : i = 1, \ldots, F, j = 1, \ldots, \alpha_i\}$.

Proof. For $|\alpha| = 0$, we have $n \in \{1, \ldots, F\}$ s.t. $\alpha_n = 1$, therfore

$$\operatorname{smax}^{(\alpha)}(x_m) = \frac{\partial \operatorname{smax}}{\partial x_n}(x_m) = \operatorname{smax}(x_m) \left(\delta_{mn} - \operatorname{smax}(x_n)\right),$$

which is of the form (26). Now, let $\alpha \in \mathbb{N}^F$ arbitrary, therefore, by defining $\alpha' \in \mathbb{N}^F$ by $\alpha'_i \overset{\text{def.}}{=} \alpha_i$ for $i \neq n$ and $\alpha'_n \overset{\text{def.}}{=} \alpha_n - 1$ (w.l.o.g. $\alpha_n > 0$). We have

$$\begin{aligned} \operatorname{smax}^{(\alpha)}(x_m) &= \frac{\partial \operatorname{smax}^{(\alpha')}}{\partial x_n}(x_m) \\ &= \frac{\partial}{\partial x_n} \sum_{k=1}^{|\alpha'|!} \operatorname{smax}(x_m) \prod_{i,j \in I(\alpha')} (a'^k_{i,j} - \operatorname{smax}(x_j)). \end{aligned}$$

Since for any k

$$\begin{aligned} &\frac{\partial}{\partial x_n} \operatorname{smax}(x_m) \prod_{i,j \in I(\alpha')} (a'^k_{i,j} - \operatorname{smax}(x_j)) \\ &= \operatorname{smax}(x_m) \left(\delta_{mn} - \operatorname{smax}(x_n)\right) \prod_{i,j \in I(\alpha')} (a'^k_{i,j} - \operatorname{smax}(x_j)) \\ &\quad + \operatorname{smax}(x_m) \sum_{i',j' \in I(\alpha')} - \operatorname{smax}(x_{j'}) \left(\delta_{j',n} - \operatorname{smax}(x_n)\right) \prod_{\substack{i,j \in I(\alpha) \\ (i,j) \neq (i',j')}} (a'^k_{i,j} - \operatorname{smax}(x_j)), \end{aligned}$$

we can define $(a_{i,j}^k)_{i,j \in I(\alpha)}^{k \in \{1,\ldots,|\alpha'|+1\}} \subseteq \{0, 1\}$ such that

$$\frac{\partial}{\partial x_n} \operatorname{smax}(x_m) \prod_{i,j \in I(\alpha')} (a'^k_{i,j} - \operatorname{smax}(x_j)) = \sum_{k=1}^{|\alpha|} \operatorname{smax}(x_m) \prod_{i,j \in I(\alpha)} (a^k_{i,j} - \operatorname{smax}(x_j)).$$

Since $|\alpha|! = |\alpha| \cdot |\alpha'|!$, this concludes the proof. □

Lemma 5 (Bound of higher-order softmax derivatives)**.** *With Notation 3, it holds for any set* $K \in \mathbb{R}^k, k \in \mathbb{N}$ *and any* $\alpha \in \mathfrak{O}^k_{<\infty}$ *that*

$$C^{\text{smax}}(\alpha) \leqslant |\alpha|!.$$

Proof. This is a direct consequence of the representation in Lemma 4 together with $\|\operatorname{smax}\| = 1$. □

F.3.2 The Multi-Head Self-Attention Mechanism

Lemma 6 (Bound of Dot product)**.** *In the notation of Definition 4 and for* $m \in \{1, \ldots, M\}$

$$\operatorname{dp}_m(\,\cdot\,; Q, K) : \mathbb{R}^{M d_{\text{in}}} \longrightarrow \mathbb{R}^M, \quad x \longmapsto \langle Q x_m, K x_j \rangle_{j=0}^M$$

we have using Notation 3

1. $C_K^{\operatorname{dp}_m}(e_1) \leqslant 2 d_{\text{in}} d_K \|K\| C^Q C^K$, *where* $C^Q \overset{\text{def.}}{=} \max_{i,i' \in \{1,\ldots,d_K\} \times \{1,\ldots,d_{\text{in}}\}} |Q_{i,i'}|$, C^K *analogously, and* $\|K\| \overset{\text{def.}}{=} \max_{x \in K} \|x\|$. *Additionally,*
2. $C_K^{\operatorname{dp}_m}(\alpha) \leqslant 2 d_K C^Q C^K$, *for* $|\alpha| = 2$, *and*

3. $C_K^{\mathrm{dp}_m}(\alpha) = 0$ *for* $|\alpha| > 2$.

Since all bounds are not dependent on m *we write* C^{dp} *short for* C^{dp_m}.

Proof. 1. Let $l = (l_1, l_2) \in \{1, \ldots, M\} \times \{1, \ldots, d_{\text{in}}\}$. Assume $l_1 = m$. If $j \neq m$, then

$$D^{e_l}\,\mathrm{dp}_m(x; Q, K)_j = D^{e_l} \sum_{i=1}^{d_K} (Kx_j)_i \sum_{i'=1}^{d_{\text{in}}} Q_{i,i'}(x_m)_{i'} = \sum_{i=1}^{d_K} \left(\sum_{i'=1}^{d_{\text{in}}} K_{i,i'}(x_j)_{i'} \right) Q_{i,l_2},$$

implying

$$\|D^{e_l}\,\mathrm{dp}_m(x; Q, K)\| \leqslant \|K\| \sum_{i=1}^{d_K} Q_{i,l_2} \sum_{i'=1}^{d_{\text{in}}} K_{i,i'} \leqslant d_{\text{in}} d_K \|K\| C^Q C^K. \tag{27}$$

If $j = m$,

$$\begin{aligned} D^{e_l}\,\mathrm{dp}_m(x; Q, K)_j &= D^{e_l} \sum_{i=1}^{d_K} \left(\sum_{i'=1}^{d_{\text{in}}} K_{i,i'}(x_m)_{i'} \right) \left(\sum_{i'=1}^{d_{\text{in}}} Q_{i,i'}(x_m)_{i'} \right) \\ &= \sum_{i=1}^{d_K} \left(K_{i,l_2} \sum_{i'=1}^{d_{\text{in}}} Q_{i,i'}(x_m)_{i'} + Q_{i,l_2} \sum_{i'=1}^{d_{\text{in}}} K_{i,i'}(x_m)_{i'} \right) \end{aligned}$$

therefore implying

$$\|D^{e_l}\,\mathrm{dp}_m(x; Q, K)\| \leqslant 2 d_{\text{in}} d_K \|K\| C^Q C^K.$$

If $l_1 \neq m$ then for $j \neq l_1$, $D^{e_l}\,\mathrm{dp}_m(x; Q, K)_j = 0$, for $j = l_1$

$$D^{e_l}\,\mathrm{dp}_m(x; Q, K)_j = D^{e_l} \sum_{i=1}^{d_K} (Qx_m)_i \sum_{i'=1}^{d_{\text{in}}} K_{i,i'}(x_j)_{i'} = \sum_{i=1}^{d_K} \left(\sum_{i'=1}^{d_{\text{in}}} Q_{i,i'}(x_m)_{i'} \right) K_{i,l_2},$$

and we obtain (27) analogously.

2. If $l_1 = m$ and $j \neq m$

$$D^{e_l} \left((x_m)_{l_2} \sum_{i=1}^{d_K} \left(\sum_{i'=1}^{d_{\text{in}}} k_{i,i'}(x_j)_{i'} \right) q_{i,l_2} \right) = 0,$$

implying $\|D^{2e_l}\,\mathrm{dp}_m(x; Q, K)\| \leqslant 0$, what analogously holds for $l_1 \neq m$. However, for $l_1 = m$ and $j = m$

$$D^{e_l} \left(\sum_{i=1}^{d_K} K_{i,l_2} \sum_{i'=1}^{d_{\text{in}}} Q_{i,i'}(x_m)_{i'} + Q_{i,l_2} \sum_{i'=1}^{d_{\text{in}}} K_{i,i'}(x_m)_{i'} \right) = \sum_{i=1}^{d_K} K_{i,l_2} Q_{i,l_2} + Q_{i,l_2} K_{i,l_2}$$

we have

$$\|D^{2e_l}\,\mathrm{dp}_m(x; Q, K)\| \leqslant 2 d_K C^Q C^K.$$

3. Let $l' = (l'_1, l'_2) \in \{1, \ldots, M\} \times \{1, \ldots, d_{\text{in}}\}$. Assume $l_1 = m$, $j \neq m$. If $l'_1 \neq j$, $D^{e_l + e_{l'}}\,\mathrm{dp}_m(x; Q, K)_j = 0$. For $l'_1 = j$ follows $D^{e_l + e_{l'}}\,\mathrm{dp}_m(x; Q, K)_j = \sum_{i=1}^{d_K} K_{i,l'_2} Q_{i,l_2}$. If $l_1 = m$, $j \neq m$, we have $D^{e_l + e_{l'}}\,\mathrm{dp}_m(x; Q, K)_j = 0$ in the case that $l'_1 \neq m$, and for $l'_1 \neq m$ we obtain

$$D^{e_l + e_{l'}}\,\mathrm{dp}_m(x; Q, K)_j = \sum_{i=1}^{d_K} K_{i,l_2} Q_{i,l'_2} + Q_{i,l_2} K_{i,l'_2}.$$

This means, we can use the bound

$$\|D^{e_l + e_{l'}}\,\mathrm{dp}_m(x; Q, K)\| \leqslant 2 d_K C^Q C^K.$$

□

Lemma 7 (Bound of Self-Attention for Derivative Type)**.** *Using the notation of Notation 3, Definition 4 and Lemma 6, it holds that*

$$C_K^{\mathrm{Att}}(\alpha) \leqslant d_{\mathrm{in}} M C^V \left(\|K\| C_K^{\mathrm{smax}\circ\mathrm{dp}}(\alpha) + \sum_{l=1}^{M d_{\mathrm{in}}} \alpha_l C_K^{\mathrm{smax}\circ\mathrm{dp}}(\alpha - e_l) \right)$$

where

$$C_K^{\mathrm{smax}\circ\mathrm{dp}}(\alpha) \leqslant \alpha! \sum_{\beta \in \mathfrak{O}^M_{\leqslant n}} N(\beta) C^{\mathrm{smax}}_{\mathrm{dp}[K]}(\beta) \sum_{\eta,\zeta \in \mathcal{P}'(\alpha,\beta)} \prod_{j=1}^{n} \frac{C_K^{\mathrm{dp}}(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}. \tag{28}$$

Proof. Fix $\alpha \in \mathbb{N}^k$, and note that

$$\|D^\alpha \operatorname{Att}(x; Q, K, V)\| \leqslant \max_{m\in\{1,\dots,M\}} \max_{i\in\{0,\dots,d_V\}} \|D^\alpha \operatorname{Att}(x; Q, K, V)_{m,i}\|$$

and

$$\begin{aligned} &\|D^\alpha \operatorname{Att}(x; Q, K, V)_{m,i}\| \\ &\leqslant \sum_{j=1}^{M} \sum_{i'=0}^{d_{\mathrm{in}}} \|D^\alpha \operatorname{smax}\circ\operatorname{dp}(x; Q, K)_j V_{i,i'}(x_j)_{i'}\| \\ &\leqslant d_{\mathrm{in}} M \max_{j\in\{1,\dots,M\}} \max_{i'\in\{0,\dots,d_{\mathrm{in}}\}} \|D^\alpha \operatorname{smax}\circ\operatorname{dp}(x; Q, K)_j V_{i,i'}(x_j)_{i'}\|. \end{aligned}$$

Due to the extended Leibniz rule Hardy (2006), we have

$$\begin{aligned} &\|D^\alpha \operatorname{smax}\circ\operatorname{dp}(x; Q, K)_j V_{i,i'}(x_j)_{i'}\| \\ &\leqslant \|D^\alpha \operatorname{smax}\circ\operatorname{dp}(x; Q, K)_j V_{i,i'}(x_j)_{i'}\| + \sum_{l=1}^{M d_{\mathrm{in}}} V_{i,i'} \alpha_l \|D^{\alpha - e_l} \operatorname{smax}\circ\operatorname{dp}(x; Q, K)_j\|. \end{aligned}$$

Equation (28) follows directly from Theorem 5. □

Corollary 3 (Bound of Self-Attention for Derivative Level)**.** *Using the setting of Lemma 7, for* $n \in \mathbb{N}$*,*

$$C_K^{\mathrm{Att}}(n) \leqslant d_{\mathrm{in}} M C^V C_K^{\mathrm{smax}\circ\mathrm{dp}}(\leqslant n) \left(\|K\| + n d_{\mathrm{in}} M\right) \tag{29}$$

where

$$C_K^{\mathrm{smax}\circ\mathrm{dp}}(\leqslant n) \leqslant C^{\mathrm{smax}}_{\mathrm{dp}[K]}(\leqslant n) C_K^{\mathrm{dp}}(\leqslant n)^n \left[\frac{2nM}{e \ln n}(1 + o(1))\right]^n. \tag{30}$$

Proof. Equation (29) follows directly from Lemma 7; and (30) is a consequence of Corollary 1. □

Corollary 4 (Bound of Multi-head Self-Attention)**.** *In the notation of Definition 4, Theorem 5 and Lemma 6 it holds that*

$$C_K^{\mathcal{MH}}(\alpha) \leqslant \alpha! d_V C^W C_K^{\mathrm{Att}}(\alpha)$$

where

$$C_K^{\mathrm{Att}} \stackrel{\text{def.}}{=} \max_{h\in\{1,\dots,H\}} C_K^{\mathrm{Att}(\,\cdot\,; Q^{(h)}, K^{(h)}, V^{(h)})}, \quad C^W \stackrel{\text{def.}}{=} \max_{h\in\{1,\dots,H\}} W^{(h)}.$$

In particular, we have the following order estimate

$$C_K^{\mathcal{MH}}(\leqslant n) \in \mathcal{O}\left(M^2 \|K\| \|W\| \|V\| (c_{d_{\mathrm{in}},d_K} \|K\| \|Q\| \|K\|)^n \; n^2 \left(\frac{n}{e}\right)^{2n} C_n^n\right).$$

Proof. From Corollary 2 and Lemma 7 we directly obtain

$$\begin{aligned} C_K^{\mathcal{MH}}(\alpha) \leqslant & n! d_V C^W d_{\mathrm{in}} M C^V n! (2 d_{\mathrm{in}} d_K \|K\| C^Q C^K)^n \\ & \times (\|K\| + n d_{\mathrm{in}} M) \left[\frac{2nM}{e \ln n}(1 + o(1))\right]^n. \end{aligned} \tag{31}$$

Applying Stirling's approximation, we have that

$$C_K^{\mathcal{MH}}(\alpha) \in \mathcal{O}\left(M^2 \|K\| \|W\| \|V\| (c_{d_{\mathrm{in}},d_K} \|K\| \|Q\| \|K\|)^n \; n^2 \left(\frac{n}{e}\right)^{2n} C_n^n\right), \tag{32}$$

where $C_n \stackrel{\text{def.}}{=} \frac{2nM}{e \ln n}(1 + o(1))$ and $c_{d_{\mathrm{in}},d_K} \stackrel{\text{def.}}{=} 2 d_{\mathrm{in}} d_K$. □

F.3.3 The Activation Functions

Lemma 8 (Derivatives of splus)**.** *For*

$$\mathrm{splus} : \mathbb{R} \to \mathbb{R}, \quad x \mapsto \ln(1 + \exp(\cdot))$$

it holds

$$\mathrm{splus}^{(1)}(x) = \mathrm{sig}(x) \overset{\text{def.}}{=} 1/(1 + \exp(-x))$$

and for $n \in \mathbb{N}$

$$\mathrm{splus}^{(n+1)}(x) = \mathrm{sig}^{(n)}(x) = \sum_{k=0}^{n} (-1)^{n+k} k! S_{n,k}\, \mathrm{sig}(x)(1 - \mathrm{sig}(x))^k,$$

where $S_{n,k}$ *are the Stirling numbers of the second kind,* $S_{n,k} \overset{\text{def.}}{=} \frac{1}{k!} \sum_{j=0}^{k} (-1)^{k-j} \binom{k}{j} j^n$.

Proof. We start with Faà di Bruno's formula,

$$\frac{d^n}{dt^n} \mathrm{sig}(x) = \frac{d^n}{dx^n} \frac{1}{f(x)} = \sum_{k=0}^{n} (-1)^k k! f^{-(k+1)}(x) B_{n,k}(f(x)),$$

where $f(x) \overset{\text{def.}}{=} 1 + \exp(-x)$ and $B_{n,k}(f(x))$ denotes the Bell polynomials evaluated on $f(x)$. Next, we know the k-th derivative of $f(x)$ is given by

$$\frac{d^k}{dt^k} f(x) = (1 - k)_k + k e^{-x}.$$

Now, using the definition of the Bell polynomials $B_{n,k}(f(t))$, we have

$$B_{n,k}(f(x)) = (-1)^n S_{n,k} e^{-kx},$$

where $S_{n,k}$ represents the Stirling numbers of the second kind. Substituting the expression for $B_{n,k}(f(x))$ into the derivative of $\mathrm{sig}(x)$, we obtain

$$\frac{d^n}{dx^n} \mathrm{sig}(x) = \sum_{k=0}^{n} (-1)^{n+k} k! S_{n,k}\, \mathrm{sig}(x)(1 - \mathrm{sig}(x))^k.$$

□

Corollary 5. *In the setting of Lemma 8, for* $n \in \mathbb{N}$*,*

$$C^{\mathrm{splus}}(n) \leqslant \sum_{k=0}^{n} \frac{k^k k! S_{n,k}}{(k+1)^{k+1}}.$$

Proof. For $k \in \mathbb{N}$ and $x \in [0, 1]$, we have

$$f^k(x) \overset{\text{def.}}{=} x(1 - x)^k, \quad (f^k)'(x) = (1 - (k+1)x)(1 - x)^{k-1};$$

which amounts to $(f^k)'(x) = 0$ at $1/(k + 1)$, i.e.

$$\max_{x \in [0,1]} f(x) = \frac{1}{k+1} \left(\frac{k}{k+1} \right)^k = \frac{k^k}{(k+1)^{k+1}}.$$

□

Lemma 9 (Derivatives of GELU)**.** *For*

$$\mathrm{GELU} : \mathbb{R} \to \mathbb{R}, \quad x \mapsto x\Phi(x),$$

it holds

$$\begin{aligned} \mathrm{GELU}'(x) &= \Phi(x) + x\varphi(x), \\ \mathrm{GELU}^{(n)}(x) &= n\varphi^{(n-2)}(x) + x\varphi^{(n-1)}(x), \quad n \geqslant 2, \end{aligned} \tag{33}$$

with $\varphi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2}$, $\Phi(x) = \int_{-\infty}^{x} \varphi(u) du$. *The* n*-th derivative of* $\varphi(x)$ *is given by*

$$\frac{d^n}{dx^n} \varphi(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \Big[\sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} 2^k \frac{\Gamma(\frac{2k+1}{2})}{\Gamma(\frac{1}{2})} x^{n-2k} \Big].$$

Proof. By induction we can show that (33) holds. And the representation of the n-th derivative of $\varphi(x)$ follows from de Oliveira and Ikeda (2012). □

Corollary 6. *For $n \geqslant 2$, it holds in the setting of Lemma 9*

$$C^{\text{GELU}}(n) \leqslant \frac{1}{\sqrt{2\pi}\Gamma(\frac{1}{2})}\left(na_{n-2}b_{n-2} + a_{n-1}c_{n-1}\right),$$

where

$$a_n \stackrel{\text{def.}}{=} \sum_{k=0}^{\lfloor n/2 \rfloor} \binom{n}{2k} 2^k \Gamma\left(\frac{2k+1}{2}\right), \quad b_n \stackrel{\text{def.}}{=} \max_{x\in\mathbb{R}} e^{-\frac{x^2}{2}} \sum_{k=0}^{\lfloor n/2 \rfloor} x^{n-k}, \quad c_n \stackrel{\text{def.}}{=} \max_{x\in\mathbb{R}} e^{-\frac{x^2}{2}} x \sum_{k=0}^{\lfloor n/2 \rfloor} x^{n-k}.$$

Lemma 10 (Derivatives of tanh)**.** *For $\tanh : \mathbb{R} \mapsto \mathbb{R}$, the n-th derivatives have the representation*

$$\frac{d^n}{dx^n}\tanh x = C_n(\tanh x),$$

$$C_n(z) = (-2)^n(z+1)\sum_{k=0}^{n}\frac{k!}{2^k}\binom{n}{k}(z-1)^k, \quad n \geqslant 1.$$

Proof. See Boyadzhiev (2007). □

Corollary 7. *In the setting of Lemma 10, for $n \in \mathbb{N}$, $C^{\tanh}(n) = \max_{z\in[-1,1]} C_n(z)$.*

Lemma 11 (Derivatives of SWISH)**.** *For*

$$\text{SWISH} : \mathbb{R} \to \mathbb{R}, \quad x \mapsto \frac{x}{1+e^{-x}}$$

it holds for $n \geqslant 1$

$$\frac{d^n}{dx^n}\text{SWISH}(x) = n\sum_{k=1}^{n}(-1)^{k-1}(k-1)!S_{n,k}\,\text{sig}^k(x) + x\sum_{k=1}^{n+1}(-1)^{k-1}(k-1)!S_{n+1,k}\,\text{sig}^k(x),$$

where $S_{n,k}$ are Stirling numbers of the second kind, i.e.,

$$S_{n,k} = \frac{1}{k!}\sum_{j=0}^{k}(-1)^j\binom{k}{j}(k-j)^n.$$

Proof. By induction, we can show that

$$\frac{d^n}{dx^n}\text{SWISH}(x) = n\,\text{sig}^{(n-1)}(x) + x\,\text{sig}^{(n)}(x), \quad n \geqslant 1.$$

By (Minai and Williams, 1993, Theorem 2), the derivatives of the sigmod function can be represented as

$$\text{sig}^{(n)}(x) = \sum_{k=1}^{n+1}(-1)^{k-1}(k-1)!S_{n+1,k}\,\text{sig}^k(x),\; n \geqslant 1.$$

Combining the above two equations, we obtain the general form of the n-th derivative of the SWISH function. □

F.3.4 The Layer Norm

Lemma 12 (Bound of the Layer Norm for Derivative Type)**.** *Fix $k \in \mathbb{N}$, $\beta \in \mathbb{R}^k$, $\gamma \in \mathbb{R}$, and $w \in [0,1]$. For the layer norm, given by*

$$\mathcal{LN} : \mathbb{R}^k \to \mathbb{R}^k, \quad x \mapsto \gamma\, f(x) g \circ \Sigma(x) + \beta;$$

$$f : \mathbb{R}^k \to \mathbb{R}^k, \quad x \mapsto x - M(x); \qquad g : \mathbb{R} \to \mathbb{R}, \quad u \mapsto \frac{1}{\sqrt{1+u}};$$

$$M : \mathbb{R}^k \to \mathbb{R}, \quad x \mapsto \frac{w}{k}\sum_{i=1}^{k} x_i; \qquad \Sigma : \mathbb{R}^k \to \mathbb{R}, \quad x \mapsto \frac{w}{k}\sum_{i=1}^{k}(x_i - M(x))^2;$$

holds for a compact symmetric set K (using Notation 3)

$$C_K^{\mathcal{LN}}(\alpha) \leqslant \alpha!\gamma \sum_{m=1}^{n=1} \frac{(2m+1)!!}{2^{2m}} \Bigg(\sum_{\substack{\alpha' \leqslant \alpha \\ |\alpha'|=n-1}} \sum_{\eta,\zeta \in \mathcal{P}'(\alpha',m)} \prod_{j=1}^{n} \frac{C_K^{\Sigma}(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} + \sum_{\eta,\zeta \in \mathcal{P}'(\alpha,m)} \prod_{j=1}^{n} \frac{C_K^{\Sigma}(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} \Bigg),$$

where $C_K^{\Sigma}(\alpha) = 2w\|K\|$ for $|\alpha| = 1$, $C_K^{\Sigma}(\alpha) = 2w$ for $|\alpha| = 2$, and $C_K^{\Sigma}(\alpha) = 0$ otherwise.

Proof. Note that

$$g^{(n)}(x) = (-1)^n \frac{(2n+1)!}{n!2^{2n}} (1+x)^{-\frac{1}{2}-n},$$

implying $C_K^g(n) \leqslant (2n+1)!!2^{-2n}$, !! denoting the double factorial. We have further $C_K^f(\alpha) \leqslant \mathbb{1}_{|\alpha|=1}$ and a direct computation yields

$$C_K^{\Sigma}(\alpha) \leqslant \begin{cases} 2w\|K\| & \text{for } |\alpha| = 1 \\ 2w & \text{for } |\alpha| = 2 \\ 0 & \text{else.} \end{cases}$$

By Theorem 5,

$$C_K^{g\circ\Sigma}(\alpha) \leqslant \alpha! \sum_{m=1}^{n} C_{\Sigma[K]}^g(m) \sum_{\eta,\zeta \in \mathcal{P}'(\alpha,m)} \prod_{j=1}^{n} \frac{C_K^{\Sigma}(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}.$$

According to the general multivariate Leibnitz rule, it holds that

$$D^\alpha(f \cdot (g \circ \Sigma)) = \sum_{\beta \leqslant \alpha} \frac{\alpha!}{\beta!(\alpha-\beta)!} D^\beta f \cdot D^{\alpha-\beta}(g \circ \Sigma)$$

which implies

$$C_K^{\mathcal{LN}}(\alpha) \leqslant C_K^{g\circ\Sigma}(\alpha)\|K\| + \sum_{\beta \leqslant \alpha, |\beta|=1} \frac{\alpha!}{(\alpha-\beta)!} C_K^{g\circ\Sigma}(\alpha-\beta).$$

□

Corollary 8 (Bound of the Layer Norm for Derivative Level)**.** *In the setting of Lemma 12, it holds that*

$$C_K^{\mathcal{LN}}(\leqslant n) \leqslant 2w\|K\|(2n+1)!!2^{-2n}(\|K\| + kn)\left[\frac{2n}{e \ln n}(1+o(1))\right]^n.$$

Furthermore, we have the asymptotic estimate

$$C_K^{g\circ\Sigma}(\leqslant n) \in \mathcal{O}\Big(w\|K\|\, n^{1/2} \big(\frac{n^{5/2}}{e^{3/4}\ln(n)}\,(1+o(1))\big)^n\Big).$$

Proof. Analogue to the proof of Lemma 12,

$$C_K^{\mathcal{LN}}(\leqslant n) \leqslant \|K\| C_K^{g\circ\Sigma}(\leqslant n) + kn C_K^{g\circ\Sigma}(\leqslant n-1) \leqslant (\|K\| + kn) C_K^{g\circ\Sigma}(\leqslant n),$$

where we can use Corollary 1 to bound

$$\begin{aligned} C_K^{g\circ\Sigma}(\leqslant n) &\leqslant C_{\Sigma[K]}^g(\leqslant n) C_K^{\Sigma}(\leqslant n)^n \left[\frac{2n}{e \ln n}(1+o(1))\right]^n \\ &\leqslant 2w\|K\|(2n+1)!!2^{-2n}\left[\frac{2n}{e \ln n}(1+o(1))\right]^n. \end{aligned} \tag{34}$$

Since $2n+1$ is odd, for each $n \in \mathbb{N}_+$, then sterling approximation *for double factorial* yields the asymptotic

$$(2n+1)!! \in \mathcal{O}\Big(\sqrt{2n}\left(\frac{n}{e}\right)^{n/2}\Big). \tag{35}$$

Merging (35) with the right-hand side of (34) yields

$$C_K^{g\circ\Sigma}(\leqslant n) \in \mathcal{O}\Big(w\|K\|\, n^{1/2} \big(\frac{n^{5/2}}{e^{3/4}\ln(n)}\,(1+o(1))\big)^n\Big).$$

□

F.3.5 THE MULTILAYER PERCEPTRON (FEEDFORWARD NEURAL NETWORK) WITH SKIP CONNECTION

Definition 7 (Single-Layer Feedforward Neural Network with Skip Connection)**.** *Fix a non-affine activation function* $\sigma \in C^\infty(\mathbb{R})$ *and dimensions* $d_{\text{in}}, d_{\text{ff}}, d_{\text{out}} \in \mathbb{N}$. *A feedforward neural network is a map* $\mathcal{PL} : \mathbb{R}^{d_{\text{in}}} \to \mathbb{R}^{d_{\text{out}}}$ *represented for each* $x \in \mathbb{R}^{d_{\text{in}}}$ *by*

$$\mathcal{PL}(x) \stackrel{\text{def.}}{=} B^{(1)}x + B^{(2)}\big(\sigma \bullet (A\,x + a)\big) \tag{36}$$

for $A \in \mathbb{R}^{d_{\text{ff}} \times d_{\text{in}}}$, $a \in \mathbb{R}^{d_{\text{ff}}}$, $B^{(1)} \in \mathbb{R}^{d_{\text{out}} \times d_{\text{in}}}$, *and* $B^{(2)} \in \mathbb{R}^{d_{\text{out}} \times d_{\text{ff}}}$.

Lemma 13 (Bound of Neural Networks for Derivative Type)**.** *In the notation of Notation 3, Lemma 6, and Definition 7, it holds that*

$$C_K^{\mathcal{PL}}(\alpha) \leqslant C^{B^{(1)}} \mathbb{1}_{|\alpha|=1} + d_{\text{ff}} (\alpha!)^2 C^{B^{(2)}} \sum_{m=1}^{n} C^{\sigma}_{h[K]}(m) \cdot (C^A)^m \sum_{\eta,\zeta \in \mathcal{P}'(\alpha,m)} \prod_{j=1}^{n} \frac{\mathbb{1}_{|\zeta^{(j)}| \leqslant 1}}{\eta^{(j)}!},$$

where $h[K]$ *is defined as the image of* $h(x) \stackrel{\text{def.}}{=} Ax + a$ *on* K.

Proof. Write $\mathcal{PL}(x) = B^{(1)}x + B^{(2)}((g_i(x))_{i=1}^{d_{\text{ff}}})$, where for $i \in \{1, \ldots, d_{\text{ff}}\}$

$$g_i(x) \stackrel{\text{def.}}{=} \sigma((Ax + a)_i).$$

If we define $h_i(x) \stackrel{\text{def.}}{=} h(x)_i$, we follow with Theorem 5

$$C_K^{g_i}(\alpha) \leqslant \alpha! \sum_{m=1}^{n} C^{\sigma}_{h[K]}(m) \cdot (C^A)^m \sum_{\eta,\zeta \in \mathcal{P}'(\alpha,m)} \prod_{j=1}^{n} \frac{\mathbb{1}_{|\zeta^{(j)}| \leqslant 1}}{\eta^{(j)}!} \stackrel{\text{def.}}{=} C_K^{g}(\alpha),$$

and due to the component wise application of the activation function it holds that

$$\|D^\alpha \max_{i \in \{1,\ldots,d_{\text{ff}}\}} g_i(x)\|_K = \max_{i \in \{1,\ldots,d_{\text{ff}}\}} C_K^{g_i}(\alpha) \leqslant C_K^{g}(\alpha).$$

Using Corollary 2, we obtain

$$C_K^{\mathcal{PL}}(\alpha) \leqslant C^{B^{(1)}} \mathbb{1}_{|\alpha|=1} + d_{\text{ff}} \alpha! C^{B^{(2)}} C_K^{g}(\alpha).$$

□

Corollary 9 (Bound of Neural Networks for Derivative Level)**.** *In the setting of Lemma 13,*

$$C_K^{\mathcal{PL}}(\leqslant n) \leqslant C^{B^{(1)}} + d_{\text{ff}} n! C^{B^{(2)}} C^{\sigma}_{h[K]}(\leqslant n)(C^A)^n \left[\frac{2n}{e \ln n}(1 + o(1))\right]^n.$$

If, moreover, $K = [-M_1, M_2]^{d_{\text{in}}}$ *then*

$$C_K^{\mathcal{PL}}(\leqslant n) \in \mathcal{O}\Big(\|B^{(1)}\|_\infty + \|B^{(2)}\|_\infty \|A\|_\infty^n \|\sigma\|_{n:\text{Ball}(a,\sqrt{d_{\text{in}}|M_1+M_2|})} \operatorname{Width}(\mathcal{PL})\, n^{1/2} \big(\frac{n}{e}\big)^n C_n^n\Big)$$

Proof. Arguing analogously to the proof of Lemma 13, barring the usage of Corollary 1, we obtain the estimate

$$C_K^{\mathcal{PL}}(\leqslant n) \leqslant C^{B^{(1)}} + d_{\text{ff}} n! C^{B^{(2)}} C^{\sigma}_{h[K]}(\leqslant n)(C^A)^n \left[\frac{2n}{e \ln n}(1 + o(1))\right]^n. \tag{37}$$

Let $C_n \stackrel{\text{def.}}{=} \frac{2n}{e \ln n}(1 + o(1))$ Using Stirling's approximation and the definition of the component-wise $\|\cdot\|_\infty$ norm of a matrix, (37) becomes

$$C_K^{\mathcal{PL}}(\leqslant n) \in \mathcal{O}\Big(\|B^{(1)}\|_\infty + \|B^{(2)}\|_\infty \|A\|_\infty^n C^{\sigma}_{h[K]}(\leqslant n) d_{\text{ff}}\, n^{1/2} \big(\frac{n}{e}\big)^n C_n^n\Big). \tag{38}$$

If, there is some $M_1, M_2 \leqslant 0$, such that $K = [0, \beta]^d$ then using the estimate between the $\|\cdot\|_2$ and $\|\cdot\|_\infty$ norms on $\mathbb{R}^{d_{\text{in}}}$ and the linearity of A we estimate

$$C^{\sigma}_{h[K]}(\leqslant n) \leqslant C^{\sigma}_{\text{Ball}(a,\sqrt{d_{\text{in}}|M_1+M_2|})}(\leqslant n) \leqslant \|\sigma\|_{n:\text{Ball}(a,\sqrt{d_{\text{in}}|M_1+M_2|})}.$$

Upon $\operatorname{Width}(\mathcal{PL}) \stackrel{\text{def.}}{=} \max\{d_{\text{in}}, d_{\text{out}}, d_{\text{ff}}\}$, the estimate (37) implies that $C_K^{\mathcal{PL}}(\leqslant n)$ is of the order of

$$\mathcal{O}\Big(\|B^{(1)}\|_\infty + \|B^{(2)}\|_\infty \|A\|_\infty^n \|\sigma\|_{n:[-\|a\|_\infty - \sqrt{d_{\text{in}}|M_1+M_2|}, \|a\|_\infty + \sqrt{d_{\text{in}}|M_1+M_2|}]} \times \operatorname{Width}(\mathcal{PL})\, n^{1/2} \big(\frac{n}{e}\big)^n C_n^n\Big). \tag{39}$$

□

F.4 STEP 2 (B) - TRANSFORMERS

We may now merge the computations in Subsection F.3, with the Fa‘a di Bruno-type from Section F.1 to uniformly bound the C^s-norms of the relevant class transformer networks. Our results are derived in two verions: the first is of “derivative type” (which is much smaller and more precise but consequentially more complicated) and the second is in “derivative level” form (cruder but simpler but also looser).

Theorem 6 (By Derivative Type)**.** *Let K be a compact set, $\mathcal{TB}$ a transformer block as in Definition 5, and $\alpha \in \mathfrak{D}_n^{M d_{\text{in}}}, n \in \mathbb{N}$. Then,*

$$C_K^{\mathcal{TB}}(\alpha) \leqslant \alpha! \sum_{\beta \in \mathfrak{D}_{\leqslant n}^{d_{\text{out}}}} N(\beta) C_{K^{(3)}}^{\mathcal{LN}}(\beta) \sum_{\eta,\zeta \in \mathcal{P}'(\alpha,\beta)} \prod_{j=1}^{n} \frac{C_K^{(3)}(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}},$$

where for all $\gamma \in \mathfrak{D}_{\leqslant n}^{M d_{\text{in}}}$:

$$C_K^{(3)}(\gamma) \stackrel{\text{def.}}{=} \gamma! \sum_{\beta \in \mathfrak{D}_{\leqslant n}^{d_{\text{in}}}} N(\beta) C_{K^{(2)}}^{\mathcal{PL}}(\beta) \sum_{\eta,\zeta \in \mathcal{P}'(\gamma,\beta)} \prod_{j=1}^{n} \frac{C_K^{(2)}(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}},$$

$$C_K^{(2)}(\gamma) \stackrel{\text{def.}}{=} \gamma! \sum_{\beta \in \mathfrak{D}_{\leqslant n}^{d_{\text{in}}}} N(\beta) C_{K^{(1)}}^{\mathcal{LN}}(\beta) \sum_{\eta,\zeta \in \mathcal{P}'(\gamma,\beta)} \prod_{j=1}^{n} \frac{C_K^{(1)}(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}},$$

$$C_K^{(1)}(\gamma) \stackrel{\text{def.}}{=} \mathbb{1}_{|\gamma|=1} + C_K^{\mathcal{MH}}(\gamma).$$

In the above, $K^{(1)} = \bigcup_{m=0}^{M} \mathcal{MH}_m[K]$, $K^{(2)} = \mathcal{LN}[K^{(1)}]$, and $K^{(3)} = \mathcal{PL}[K^{(2)}]$.

For respective multi-indices, a bound for $C_{K^{(3)}}^{\mathcal{LN}}, C_{K^{(1)}}^{\mathcal{LN}}$ is given by Lemma 12, $C_{K^{(2)}}^{\mathcal{PL}}$ is bounded in Lemma 13, and a bound for $C_K^{\mathcal{MH}}$ is given in Corollary 4.

Proof. This is a direct consequence of Theorem 5. □

Theorem 7 (By Derivative Level)**.** *Let K be a compact set, $\mathcal{TB}$ a transformer block as in Definition 5, and $n \in \mathbb{N}$. Then,*

$$C_K^{\mathcal{TB}}(\leqslant n) \leqslant C_{K^{(3)}}^{\mathcal{LN}}(\leqslant n) \left(d_{\text{out}} C_{K^{(2)}}^{\mathcal{PL}}(\leqslant n)\right)^n \left(d_{\text{in}}^2 C_{K^{(1)}}^{\mathcal{LN}}(\leqslant n)\right)^{n^2} \cdot \left(1 + C_K^{\mathcal{MH}}(\leqslant n)\right)^{n^3} \left[\frac{2n}{e \ln n}(1+o(1))\right]^{n+n^2+n^3}$$

where, $K^{(1)} = \bigcup_{m=0}^{M} \mathcal{MH}_m[K]$, $K^{(2)} = \mathcal{LN}[K^{(1)}]$, and $K^{(3)} = \mathcal{PL}[K^{(2)}]$.

A bound for $C_{K^{(3)}}^{\mathcal{LN}}, C_{K^{(1)}}^{\mathcal{LN}}$ is given by Corollary 8, $C_{K^{(2)}}^{\mathcal{PL}}$ is bounded in Corollary 9, and a bound for $C_K^{\mathcal{MH}}$ is given in Corollary 4.

Proof. Corollary 1 yields

$$C_K^{\mathcal{TB}}(\leqslant n) \leqslant C_{K^{(3)}}^{\mathcal{LN}}(\leqslant n) C_K^{(3)}(\leqslant n)^n \left[\frac{2 d_{\text{out}} n}{e \ln n}(1+o(1))\right]^n.$$

where

$$C_K^{(3)}(\leqslant n) \stackrel{\text{def.}}{=} C_{K^{(2)}}^{\mathcal{PL}}(\leqslant n) C_K^{(2)}(\leqslant n)^n \left[\frac{2 d_{\text{in}} n}{e \ln n}(1+o(1))\right]^n,$$

$$C_K^{(2)}(\leqslant n) \stackrel{\text{def.}}{=} C_{K^{(1)}}^{\mathcal{LN}}(\leqslant n) C_K^{(1)}(\leqslant n)^n \left[\frac{2 d_{\text{in}} n}{e \ln n}(1+o(1))\right]^n,$$

$$C_K^{(1)}(\leqslant n) \stackrel{\text{def.}}{=} 1 + C_K^{\mathcal{MH}}(\leqslant n),$$

which concludes the proof. □

Theorem 8 (C^s-Norm Bound of Transformers)**.** *Fix $n, L, H, C, D, d, M \in \mathbb{N}_+$ for a transformer class $\mathcal{TC}$. For any $\mathcal{T} \in \mathcal{TC}$, any compact $K_0 \subset \mathbb{R}^{M \times D}$, and any $\alpha \in \mathbb{N}^{M \times D}$, $|\alpha| \stackrel{\text{def.}}{=} n$ we have*

$$C_{K_0}^{\mathcal{T}}(\alpha) \leqslant d_{\text{out}}^L M \alpha! \cdot C^A \cdot C^L(\alpha), \tag{40}$$

where $C^1(\alpha) \overset{\text{def.}}{\equiv} C^{\mathcal{TB}_1}_{K_0}(\alpha)$ *and for* $l \in \{2, \ldots, L\}$,

$$C^l(\alpha) \overset{\text{def.}}{\equiv} \leqslant \alpha! \sum_{\beta \in \mathfrak{O}^{\tilde{d}_l}_{\leqslant n}} N(\beta) C^{\mathcal{TB}_l}_{K_{l-1}}(\beta) \sum_{\eta,\zeta \in \mathcal{P}'(\mathfrak{o}(\alpha),\beta)} \prod_{j=1}^{n} \frac{C^l(\mathfrak{o}(\zeta^{(j)}))^{|\eta^{(j)}|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}} \tag{41}$$

where $K_l \overset{\text{def.}}{\equiv} \mathcal{TB}_l[K_{l-1}]$, $\tilde{d}_l \overset{\text{def.}}{\equiv} M_l d^l_{\text{in}}$, *and a bound for* $C^{\mathcal{TB}_l}_{K_{l-1}}(\beta)$ *is given by Theorem 6, only depending on the transformer block class* $\mathcal{TBC}_l$.

Proof of Theorem 8. The bounds (40) are a direct consequence of Theorem 5 and (41) follows directly from Corollary 2. □

F.5 STEP 2 (C) - MERGING THE C^s-NORM BOUNDS FOR TRANSFORMERS WITH THE LOSS FUNCTION

In this section, we consider the following generalization of the class in Definition 2. As before, each result holds for input dimensions d just as much as any other input dimension, e.g. Md, with the only change being relabeling $d \leftarrow Md$. Therefore, for notational minimality, we chose to label the input dimension d and not dM.

Definition 8 (Smoothness Growth Rate)**.** *Let* $d, D \in \mathbb{R}$*. A smooth function* $g : \mathbb{R}^d \to \mathbb{R}^D$ *is said to belong to the class* $C^\infty_{poly:C,r}(\mathbb{R}^d, \mathbb{R}^D)$ *(resp.* $C^\infty_{exp:C,r}(\mathbb{R}^d, \mathbb{R}^D)$*) if there exist* $C, r \geqslant 0$ *such that: for each* $s \in \mathbb{N}_+$

(i) ***Polynomial Growth -*** $C^\infty_{poly:C,r}(\mathbb{R}^d, \mathbb{R}^D)$*:* $\|g\|_{C^s} \leqslant C\, s^r$,

(ii) ***Exponential Growth -*** $C^\infty_{exp:C,r}(\mathbb{R}^d, \mathbb{R}^D)$*:* $\|g\|_{C^s} \leqslant C\, e^{s\,r}$,

The next lemma will help us relate the C^s-regularity of a model, a target function, and a loss function to their composition and product. We use it to relate the C^s-regularity of a transformed model $\mathcal{T} : \mathbb{R}^d \to \mathbb{R}^D$, the target function $f^\star : \mathbb{R}^d \to \mathbb{R}^D$, and the loss function $\ell : \mathbb{R}^{2D} \to \mathbb{R}$ to their composition

$$\begin{aligned} \ell_{\mathcal{T}} : \mathbb{R}^d &\to \mathbb{R} \\ x &\mapsto \ell\big(\mathcal{T}(x), f^\star(x)\big). \end{aligned} \tag{42}$$

One we computed have the C^s-regularity of $\ell_{\mathcal{T}}$, we can apply a concentration of measure-type argument based on an optimal transport-type duality, as in Amit et al. (2022); Hou et al. (2023b); Benitez et al. (2023); Kratsios et al. (2024), to obtain our generalization bounds. A key technical point where our analysis largely deviates from the mentioned derivations, is that we are not relying on any i.i.d. assumptions.

More generally, the next lemma allows us to bound the size of $\|\ell(\hat{f}, f^\star)\|_{C^s}$ using bounds on C^s norms of $\mathcal{TC}$ computed in Theorem 8, the target function $f^\star$, and on the loss function ℓ. Naturally, to use this result, we must assume a given level of regularity of the target function, as in Definition 2.

Lemma 14 (C^s-Norm of loss of between two functions)**.** *Let* $d, D, s \in \mathbb{N}_+$, $f_1, f_2 : \mathbb{R}^d \to \mathbb{R}^D$ *be of class* C^s *and* $\ell : \mathbb{R}^{2D} \to \mathbb{R}$ *be smooth. If there are constants* $C_1, C_2, \widetilde{C}_1, \ldots, \widetilde{C}_s \geqslant 0$ *such that:* $\|f_i\|_{C^s} \leqslant C_i$ *for* $i = 1, 2$ *and for* $j = 1, \ldots, s$ *we have* $\|\ell\|_{C^j} \leqslant \widetilde{C}_j$ *then for all* $s > 0$ *large it satisfies*

$$\big\|\ell(f_1, f_2)\big\|_{C^s} = \begin{cases} \mathcal{O}\Big[\Big(\frac{2Ds}{e \ln s}(1 + o(1))\Big)^s\Big], & \text{if } \max_{1 \leqslant k} \widetilde{C}_k (C_1 C_2)^k \text{ is bounded}, \\ \mathcal{O}\Big[\widetilde{C}_s \Big(C_1 C_2 \frac{2Ds}{e \ln s}(1 + o(1))\Big)^s\Big], & \text{if } \max_{1 \leqslant k} \widetilde{C}_k (C_1 C_2)^k \text{ is unbounded}. \end{cases} \tag{43}$$

Particularly, if $\ell \in C^\infty_{poly:C,r}(\mathbb{R}^{2D}, \mathbb{R})$*, i.e.,* $\|\ell\|_{C^j} \leqslant C\, j^r$ *, then*

$$\big\|\ell(f_1, f_2)\big\|_{C^s} = \mathcal{O}\Big[C s^r \Big(C_1 C_2 \frac{2Ds}{e \ln s}(1 + o(1))\Big)^s\Big]; \tag{44}$$

if $\ell \in C^\infty_{exp:C,r}(\mathbb{R}^{2D}, \mathbb{R})$*, i.e.,* $\|\ell\|_{C^j} \leqslant C\, e^{j\,r}$*, then*

$$\big\|\ell(f_1, f_2)\big\|_{C^s} = \mathcal{O}\Big[C e^{sr} \Big(C_1 C_2 \frac{2Ds}{e \ln s}(1 + o(1))\Big)^s\Big]. \tag{45}$$

Lemma 14 allows us to obtain a bound on the term $\sup_{\hat{f}\in C^s_R(\mathbb{R}^d)} \|\ell(\hat{f},f^\star)\|_{C^s}$ in (3), using Theorem 8 and our assumptions on ℓ and on $f^\star$.

Proof of Lemma 14. We first derive the general bound; which we then specialize to the case where the growth rate of ℓ is known. We first observe that

$$\big\|\ell(f_1,f_2)\big\|_{C^s} = \underbrace{\max_{k=1,\cdots,s-1}\max_{\alpha\in\{1,\cdots,d\}^k}\|D^\alpha\ell(f_1(x),f_2(x))\|_\infty}_{\text{(VII)}} + \underbrace{\max_{\alpha\in\{1,\cdots,d\}^{s-1}}\operatorname{Lip}\big(D^\alpha\ell(f_1(x),f_2(x))\big)}_{\text{(VIII)}}.$$

General Case - Term Term (VII): By Corollary 1, we have

$$\Big\|(D^\alpha\ell)(f_1(x),f_2(x))\Big\|_\infty \leqslant \big[\max_{1\leqslant k\leqslant s-1}\widetilde{C}_k(C_1C_2)^k\big]\cdot\mathcal{O}\Big[\Big(\frac{2Dk}{e\ln k}(1+o(1))\Big)^k\Big], \tag{46}$$

From (46) we have for all large $s>0$ that

$$\max_{k=1,\cdots,s-1}\max_{\alpha\in\{1,\cdots,d\}^k}\|D^\alpha\ell(f_1(x),f_2(x))\|_\infty = \begin{cases}\mathcal{O}\big[\big(\frac{2Ds}{e\ln s}(1+o(1))\big)^s\big], & \text{if } \max_{1\leqslant k}\widetilde{C}_k(C_1C_2)^k \text{ is bounded,}\\ \mathcal{O}\Big[\widetilde{C}_s\Big(C_1C_2\frac{2Ds}{e\ln s}(1+o(1))\Big)^s\Big], & \text{if } \max_{1\leqslant k}\widetilde{C}_k(C_1C_2)^k \text{ is unbounded.}\end{cases}$$

General Case - Term Term (VIII): For each $\alpha\in\{1,\cdots,d\}^{s-1}$, by the multivariate Faà di Bruno formula, we have

$$D^\alpha\ell(f_1(x),f_2(x)) = \sum_{1\leqslant|\beta|\leqslant s-1}(D^\beta\ell)(f_1(x),f_2(x))\sum_{\eta,\zeta\in\mathcal{P}(\alpha,\beta)}\alpha!\prod_{j=1}^{s-1}\frac{[D^{\zeta^{(j)}}(f_1(x),f_2(x))]^{\eta^{(j)}}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}.$$

The Lipschitz constants of the derivatives satisfy

$$\begin{aligned}
&\operatorname{Lip}\big(D^\alpha\ell(f_1(x),f_2(x))\big)\\
=&\sum_{1\leqslant|\beta|\leqslant s-1}\operatorname{Lip}\big((D^\beta\ell)(f_1(x),f_2(x))\big)\sum_{\eta,\zeta\in\mathcal{P}(\alpha,\beta)}\alpha!\prod_{j=1}^{s-1}\frac{\operatorname{Lip}\big([D^{\zeta^{(j)}}(f_1(x),f_2(x))]^{\eta^{(j)}}\big)}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}\\
\leqslant&\sum_{1\leqslant|\beta|\leqslant s-1}\widetilde{C}_{|\beta|+1}\sum_{\eta,\zeta\in\mathcal{P}(\alpha,\beta)}\alpha!\prod_{j=1}^{s-1}\frac{(C_1C_2)^{|\eta(j)|}}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}\\
=&\sum_{1\leqslant|\beta|\leqslant s-1}\widetilde{C}_{|\beta|+1}(C_1C_2)^{|\beta|}\sum_{\eta,\zeta\in\mathcal{P}(\alpha,\beta)}\alpha!\prod_{j=1}^{s-1}\frac{1}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}\\
\leqslant&\big[\max_{1\leqslant k\leqslant s-1}\widetilde{C}_{k+1}(C_1C_2)^k\big]\sum_{1\leqslant|\beta|\leqslant s-1}\sum_{\eta,\zeta\in\mathcal{P}(\alpha,\beta)}\alpha!\prod_{j=1}^{s-1}\frac{1}{\eta^{(j)}!(\zeta^{(j)}!)^{|\eta^{(j)}|}}\\
=&\big[\max_{1\leqslant k\leqslant s-1}\widetilde{C}_{k+1}(C_1C_2)^k\big]\cdot\mathcal{O}\Big[\Big(\frac{2Ds}{e\ln s}(1+o(1))\Big)^s\Big],
\end{aligned}\tag{47}$$

where the last equality is due to Lemma 3.

From (47) we have for all $s>0$ large that

$$\max_{\alpha\in\{1,\cdots,d\}^{s-1}}\operatorname{Lip}\big(D^\alpha\ell(f_1(x),f_2(x))\big) = \begin{cases}\mathcal{O}\big[\big(\frac{2Ds}{e\ln s}(1+o(1))\big)^s\big], & \text{if } \max_{1\leqslant k}\widetilde{C}_k(C_1C_2)^k \text{ is bounded,}\\ \mathcal{O}\big[\widetilde{C}_s\big(C_1C_2\frac{2Ds}{e\ln s}(1+o(1))\big)^s\big], & \text{if } \max_{1\leqslant k}\widetilde{C}_k(C_1C_2)^k \text{ is unbounded.}\end{cases}$$

Completing the General Case: Combining our estimates for terms Term (VII) and Term (VIII) respectively obtained in (46) and (47), we obtain an upper-bound for $\|\ell(f_1, f_2)\|_{C^s}$ via

$$\|\ell(f_1, f_2)\|_{C^s} = \begin{cases} \mathcal{O}\big[\big(\frac{2Ds}{e\ln s}(1+o(1))\big)^s\big], & \text{if } \max_{1\leqslant k} \widetilde{C}_k(C_1C_2)^k \text{ is bounded,} \\ \mathcal{O}\big[\widetilde{C}_s\big(C_1C_2\frac{2Ds}{e\ln s}(1+o(1))\big)^s\big], & \text{if } \max_{1\leqslant k} \widetilde{C}_k(C_1C_2)^k \text{ is unbounded.} \end{cases}$$

Special Cases of Interest: In particular, if ℓ belongs either to $C^\infty_{poly:C,r}(\mathbb{R}^d, \mathbb{R}^D)$ or to $C^\infty_{exp:C,r}(\mathbb{R}^d, \mathbb{R}^D)$, , as in Definition (2), then: there exists constants $C_\ell, r_\ell > 0$ s.t. for each $j = 1, \ldots, s$ we have

(i) **Polynomial Growth - $C^\infty_{poly:C,r}(\mathbb{R}^{2D}, \mathbb{R})$ Case:**

$$\|\ell\|_{C^j} \leqslant C\, j^r \overset{\text{def.}}{=} \tilde{C}_j,$$

(ii) **Exponential Growth - $C^\infty_{exp:C,r}(\mathbb{R}^{2D}, \mathbb{R})$ Case:**

$$\|\ell\|_{C^j} \leqslant C\, e^{j\,r} \overset{\text{def.}}{=} \tilde{C}_j.$$

Consequentially, in cases (i) and (ii), the bound in (43) respectively becomes

(i) **Polynomial Growth - $C^\infty_{poly:C,r}(\mathbb{R}^{2D}, \mathbb{R})$ Case:**

$$\|\ell(f_1, f_2)\|_{C^s} \leqslant \mathcal{O}\Big[Cs^r\Big(C_1C_2\frac{2Ds}{e\ln s}(1+o(1))\Big)^s\Big],$$

(ii) **Exponential Growth - $C^\infty_{exp:C,r}(\mathbb{R}^{2D}, \mathbb{R})$ Case:**

$$\|\ell(f_1, f_2)\|_{C^s} \leqslant \mathcal{O}\Big[Ce^{sr}\Big(C_1C_2\frac{2Ds}{e\ln s}(1+o(1))\Big)^s\Big].$$

□

F.6 Step 3 - Combining Steps 1 and 2 and Completing The Proof of Theorem 1

We are now ready to complete the proof of our main result, namely Theorem 1. Before doing so, we state a more technical and general version, which we instead prove and which directly implies the simpler version found in the main body of our manuscript.

We operate under the following more general, but more technical set of assumptions than those considered in the main body of our text (in Setting 2.1).

Setting F.1 (Generalized Setting)**.** *Let $D, d, L, H, *C', C^A, C^b \in \mathbb{N}_+$, set $M \overset{\text{def.}}{=} 0$, and $C \overset{\text{def.}}{=} (*C', C^A, C^b)$, $r_f, r_\ell, C_f, C_\ell \geqslant 0$. Suppose that Assumptions 3 and 4 hold.*

Fix a target function $f^\star : \mathbb{R}^d \to \mathbb{R}^D$ and a loss function $\ell : \mathbb{R}^D \times \mathbb{R}^D \to \mathbb{R}$. Assume either that:

*(i) **Polynomial Growth:** $f^\star \in C^\infty_{poly:C_f,r_f}(\mathbb{R}^d, \mathbb{R}^D)$ and $\ell \in C^\infty_{poly:C_\ell,r_\ell}(\mathbb{R}^{2D}, \mathbb{R})$,*

*(ii) **Exponential Growth:** $f^\star \in C^\infty_{exp:C_f,r_f}(\mathbb{R}^d, \mathbb{R}^D)$ and $\ell \in C^\infty_{exp:C_\ell,r_\ell}(\mathbb{R}^{2D}, \mathbb{R})$,*

*(iii) **No Growth:** There is a constant $\bar{C} \geqslant 0$ such that for all $s > 0$ we have $\|f^\star\|_{C^s}, \|\ell\|_{C^s} \leqslant \bar{C}$.*

Example 3 (Example of Generalized Setting (iii))*.* For every $d \in \mathbb{R}^d$, the function $f : \mathbb{R}^d \ni x \mapsto \cos \bullet x = \big(\cos(x_i)\big)_{i=1}^d$ satisfies $\|\frac{\partial^s}{\partial x_i^s} f\|_\infty \leqslant 1$ for each $s \in \mathbb{N}$ and each $i = 1, \ldots, d$. Thus, it is an example of a function satisfying Assumption F.1. ◁

We are now ready to prove our main theorem, which is a combination of Theorems 1 and 2.

Table 6: Bounds on the terms in defining the constant $C_{\ell,\mathcal{TC},K,s}$, in Theorem 9, for a single attention block.

Term	Bound ($\mathcal{O}$)
$c_{\ell,f^\star}$	$C_f^s\, s^{r_\ell+2s^2} C_s^s$
$\mathcal{LN}$	$s^{(1+s)/2} C_s^s$
$\mathcal{PL}$	$\Vert B^{(1)}\Vert + \Vert B^{(2)}\Vert \Vert A\Vert^s \Vert\sigma\Vert_{s:\left[\pm\Vert a\Vert_\infty \pm\sqrt{d_{\text{in}}}\right]}$ Width$(\mathcal{PL})\, \tilde{C}_s^s$
$\mathcal{MH}$	$\Vert W\Vert \Vert V\Vert (\tilde{d}\Vert Q\Vert \Vert K\Vert)^s \left(s^2\left(\frac{s}{e}\right)^{2s} C_s^s\right)$

Here $C_s \overset{\text{def.}}{=} \frac{2s}{e\ln s}(1+o(1))$, $\tilde{C}_s \overset{\text{def.}}{=} s^{1/2}\left(\frac{n}{e}\right)^s C_s^s$, $c_d \overset{\text{def.}}{=} 2\max\{d_{\text{in}}, d_K, d_V, d_{\text{ff}}, d_{\text{out}}\}$, Width$(\mathcal{PL})$ is the width of the neural network $\mathcal{PL}$, where $\Vert\cdot\Vert$ denotes the componentwise max matrix/vector norm.

Theorem 9 (Pathwise Generalization Bounds for Transformers)**.** *In Setting F.1, there is a $\kappa \in (0,1)$, depending only on $X_\cdot$, and a $t_0 \in \mathbb{N}_0$ such that: for each $t_0 \leqslant N \leqslant t \leqslant \infty$ and $\delta \in (0,1]$ the following holds with probability at-least $1-\delta$*

$$\sup_{\mathcal{T}\in\mathcal{TC}} \left|\mathcal{R}_{\max\{t,N\}}(\mathcal{T}) - \mathcal{R}^{(N)}(\mathcal{T})\right| \lesssim \sum_{s=1}^\infty I_{N\in[\tau_s,\tau_{s+1})}\, C_{\ell,\mathcal{TC},K,s-1}\left(I_{t<\infty}\,\kappa^t + \frac{\sqrt{2\ln(1/\delta)}}{N^{1/2}} + \text{rate}_s(N)\right)$$

where $\text{rate}_s(N)$ *is defined in (rate), the constant $C_{\ell,\mathcal{TC},K,s} \overset{\text{def.}}{=} \sup_{\mathcal{T}\in\mathcal{TC}} \Vert\ell(\mathcal{T},f^*)\Vert_{C^s}$, is of order*

$$\mathcal{O}\Big(\underbrace{C^{\ell,f^\star}}_{\textit{Loss \& Target}} \quad \underbrace{C^{\mathcal{LN}}_{K^{(3)}}(\leqslant s)^s C^{\mathcal{LN}}_{K^{(1)}}(\leqslant s)^{s^3}}_{\textit{Layernorms}} \underbrace{C^{\mathcal{PL}}_{K^{(2)}}(\leqslant s)^{s^2}}_{\textit{Perceptron}} \underbrace{\left(1 + C_K^{\mathcal{MH}}(\leqslant s)\right)^{s^4}}_{\textit{Multihead Attention}} \underbrace{D^{s^2}\, d^{2s^3}}_{\textit{dimensions}} \underbrace{c_s^{s^s+s^3+s^4}}_{\textit{Generic: s-th order Derivative}} \Big)$$

with terms according to Table 6 and the transition phases $(\tau_s)_{s=0}^\infty$ are given iteratively by $\tau_0 \overset{\text{def.}}{=} 0$ and for each $s \in \mathbb{N}_+$

$$\tau_s \overset{\text{def.}}{=} \inf\left\{t \geqslant \tau_{s-1} :\, C_{\ell,\mathcal{TC},K,s}(\kappa^t + \text{rate}_s(N) + \frac{\sqrt{\log(1/\delta)}}{\sqrt{N}}) \leqslant C_{\ell,\mathcal{TC},K,s-1}(\kappa^t + \text{rate}_{s-1}(N) + \frac{\sqrt{\log(1/\delta)}}{\sqrt{N}})\right\}.$$

Furthermore, $c \overset{\text{def.}}{=} 1-\kappa$, $c_2 \overset{\text{def.}}{=} c^{s/d}$, $\kappa^\infty \overset{\text{def.}}{=} \lim_{t\to\infty} \kappa^t = 0$, and $\lesssim$ hides an absolute constant.

Proof of Theorem 1. Since N is given, we may pick $s \in \mathbb{N}_+$ to ensure that $N \in [\tau_s, \tau_{s+1})$; where these are defined as in the statement of Theorem 9.

Since we are in Setting 2.1, then $\ell \in C^\infty_{poly:C_\ell,r_\ell}(\mathbb{R}^{2D},\mathbb{R})$ (resp. $\ell \in C^\infty_{exp:C_\ell,r_\ell}(\mathbb{R}^{2D},\mathbb{R})$) and $f^\star : \mathbb{R}^d \to \mathbb{R}^D$ is smooth. Therefore, Lemma 14 implies that there is an absolute constant $c_{\text{abs}} > 0$ such that for any transformer network $\mathcal{T} \in \mathcal{TC}$, the following bound holds

(i) **No Growth Case:** Using (43) we find that

$$\left\Vert\ell(\mathcal{T},f^\star)\right\Vert_{C^s} \leqslant c_{\text{abs}} \left(\frac{2Ds}{e\ln s}(1+o(1))\right)^s \Vert\mathcal{T}\Vert^s_{C^s} \tag{48}$$

(ii) **Polynomial Growth Case -** $\ell \in C^\infty_{poly:C_\ell,r_\ell}(\mathbb{R}^{2D},\mathbb{R})$ **Case:**

$$\left\Vert\ell(\mathcal{T},f^\star)\right\Vert_{C^s} \leqslant c_{\text{abs}}\, s^{r_\ell} \left(\frac{2Ds}{e\ln s}(1+o(1))\right)^s \Vert f^\star\Vert^s_{C^s} \Vert\mathcal{T}\Vert^s_{C^s} \tag{49}$$

(iii) **Exponential Growth -** $C^\infty_{exp:C_\ell,r_\ell}(\mathbb{R}^{2D},\mathbb{R})$ **Case:**

$$\left\Vert\ell(\mathcal{T},f^\star)\right\Vert_{C^s} \leqslant c_{\text{abs}}\, e^{s\,r_\ell} \left(\frac{2Ds}{e\ln s}(1+o(1))\right)^s \Vert f^\star\Vert^s_{C^s} \Vert\mathcal{T}\Vert^s_{C^s}. \tag{50}$$

Since we have assumed that $f^\star \in C^\infty_{poly:C_f,r_f}(\mathbb{R}^d,\mathbb{R}^D)$ (resp. $C^\infty_{exp:C_f,r_f}(\mathbb{R}^d,\mathbb{R}^D)$ or the "no growth condition" in Setting F.1 (iii)) then the bounds in (48), (49), and (50), respectively, imply that

(i) **No Growth Case:**

$$\left\|\ell(\mathcal{T},f^{\star})\right\|_{C^s} \leqslant c_{\text{abs}}\,\Big(\frac{2Ds}{e\ln s}(1+o(1))\Big)^s\, C_K^{\mathcal{TC}}(s)^s \tag{51}$$

(ii) **Polynomial Growth Case -** $\ell\in C^{\infty}_{poly:C_\ell,r_\ell}(\mathbb{R}^{2D},\mathbb{R})$ **Case:**

$$\left\|\ell(\mathcal{T},f^{\star})\right\|_{C^s} \leqslant c_{\text{abs}}\, s^{r_\ell+2s^2}\left(\frac{C_f\,2D}{e\ln s}(1+o(1))\right)^s\, C_K^{\mathcal{TC}}(s)^s \tag{52}$$

(iii) **Exponential Growth -** $C^{\infty}_{exp:C_\ell,r_\ell}(\mathbb{R}^{2D},\mathbb{R})$ **Case:**

$$\left\|\ell(\mathcal{T},f^{\star})\right\|_{C^s} \leqslant c_{\text{abs}}\, e^{s\,r_\ell+s^2 r_f}\left(\frac{2D\,s}{e\ln s}(1+o(1))\right)^s\, C_f^s\, C_{K_0}^{\mathcal{TC}}(s)^s, \tag{53}$$

where we have used the definition of the constant $C_K^{\mathcal{TC}}(s)$ as a uniform upper bound of $\sup_{\mathcal{T}\in\mathcal{TC}}$. Using Theorem 6 for the "derivative type estimate" (resp.7 for the "derivative level estimate") concludes the implies yields a uniform upper bound (of "derivative type" or "derivative level" respectively) on $C_{K_0}^{\mathcal{TC}}(s)$, i.e. independent of the particular transformer instance $\mathcal{T}\in\mathcal{TC}$. In either case, we respectively define $R>0$ to be the right-hand side of (52) or (53) depending on the respective assumptions made on ℓ and on $f^\star$.

The conclusion now follows upon applying Proposition 5 due to the inequality in (2). □

G Example of Additive Noise Using Stochastic Calculus

In this appendix, we briefly discuss why the seemingly *realizable* learning setting which we have placed ourselves in, i.e. $Y_n = f^\star(X_n)$, does not preclude additive noise. Our illustration considers the class of following Markov processes.

Assumption 5 (Structure on $X_\cdot$)**.** *Let $g:\mathbb{R}^d\to[0,1]^d$ be a twice continuously differentiable function. Let $W_\cdot \overset{\text{def.}}{=} (W_t)_{t\geqslant 0}$ be d-dimensional Brownian motion and, for each $n\in\mathbb{N}$, define*

$$X_n \overset{\text{def.}}{=} g(W_n).$$

By construction, the boundedness of the change of variables-type function g in Assumption 5, implies that the process $X_\cdot = (X_n)_{n\in\mathbb{N}}$ is bounded (and can easily be seen to be Markovian since Brownian motion has the strong Markov property). However, we can say more, indeed under Assumption 5, the Itô Lemma (see e.g. (Cohen and Elliott, 2015, Theorem 14.2.4)) implies that X_n is given as the following stochastic differential equation (SDE) evaluated at integer times $n\in\mathbb{N}$

$$X_n = g(0) + \int_0^n \mu_s\,ds + \int_0^n \sigma_t^\top\,dW_s \tag{54}$$

where $\mu_\cdot = (\mu_t)_{t\geqslant 0}$ and $\sigma_\cdot = (\sigma_t)_{t\geqslant 0}$ are given by

$$\mu_t \overset{\text{def.}}{=} \frac{1}{2}\,\mathrm{tr}\,\big(H(g)(W_s)\big) \text{ and } \sigma_t \overset{\text{def.}}{=} \nabla g(W_t)$$

and $H(g)$ is the Hessian of g and tr is the trace of a matrix.

Example 4. Set $d=1$ and $g(x) = (\sin(x)+1)/2$. Then, for each $n\in\mathbb{N}$ we have

$$X_n = \int_0^n -\sin(W_s)/4ds + \int_0^t \cos(W_s)/2\,dW_s.$$

◁

In particular, the expression (54) shows that the input process $X_\cdot$ is also defined for all intermediate times between non-negative integer times; i.e. for each $t\geqslant 0$ the process

$$X_t = g(0) + \int_0^t \mu_s\,ds + \int_0^t \sigma_t^\top\,dW_s \tag{55}$$

is well-defined and coincides with X_n whenever $t = n \in \mathbb{N}$. We may, therefore, also consider the "continuous-time extension" $Y_\cdot \stackrel{\text{def.}}{=} (Y_t)_{t \geqslant 0}$ of the target process defined for all intermediate times using (55) by

$$Y_t \stackrel{\text{def.}}{=} f^\star(X_t).$$

Note that Y_t coincides with the target process on non-negative integer times, as defined in our main text, by definition.

The convenience of these continuous-time extensions, of the discrete versions considered in our main text, is that now $Y_\cdot$ is the transformation of a continuous-time (Itô) process of satisfying the SDE (55) by a smooth function[4], namely $f^\star$. Therefore, we may again apply the Itô Lemma (again see e.g. (Cohen and Elliott, 2015, Theorem 14.2.4)) this time to the process $X_\cdot$ to obtain the desired signal and noise decomposition of the target process $Y_\cdot$ (both in discrete and continuous time). Doing so yields the following decomposition

$$\begin{aligned} Y_t = & \underbrace{f^\star(X_0) + \int_0^t \Big(\left(\nabla f^\star(X_s)\right)^\top \mu_t + \frac{1}{2} \operatorname{tr}\left(\sigma_s^\top H(f^\star)(X_s)\sigma_s\right)\Big)\, ds}_{\text{Signal (Target)}} \\ & + \underbrace{\int_0^t \left(\nabla f^\star\right)^\top \sigma_s \, dW_s}_{\text{Additive Noise}} . \end{aligned} \tag{56}$$

This shows that even if it a priori seemed that we are in the *realizable PAC setting* due to the structural assumption that $Y_n = f^\star(X_n)$ made when defining the target process, we are actually in the standard setting where the target data $(Y_n)_{n=0}^\infty$ can be written as a signal plus an additive noise term. Indeed, when $X_\cdot$ is simply a transformation of a Brownian motion by a bounded C^2-function, as in Assumption 5, then Assumption 1 held and Y_n admitted the signal-noise decomposition in (56).

[4] Note that $f^\star$ was assumed to be smooth in our main result (Theorem 1).