Limits to Depth Efficiencies of Self-Attention

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Abstract

Self-attention architectures, which are rapidly pushing the frontier in natural language processing, demonstrate a surprising depth-inefficient behavior: Empirical signals indicate that increasing the internal representation (network width) is just as useful as increasing the number of self-attention layers (network depth). In this paper, we theoretically study the interplay between depth and width in self-attention, and shed light on the root of the above phenomenon. We invalidate the seemingly plausible hypothesis by which widening is as effective as deepening for self-attention, and show that in fact stacking self-attention layers is so effective that it quickly saturates a capacity of the network width. Specifically, we pinpoint a “depth threshold” that is logarithmic in $d_x$, the network width: $L_{th} = \log_3(d_x)$. For networks of depth that is below the threshold, we establish a double-exponential depth-efficiency of the self-attention operation, while for depths over the threshold we show that depth-inefficiency kicks in. Our predictions strongly accord with extensive empirical ablations in Kaplan et al. [2020], accounting for the different behaviors in the two depth-(in)efficiency regimes. By identifying network width as a limiting factor, our analysis indicates that solutions for dramatically increasing the width can facilitate the next leap in self-attention expressivity.

1 Introduction

The golden age of deep learning has popularized the depth-efficiency notion: From an expressiveness standpoint, increasing a neural network’s size by adding more layers is advantageous relatively to other parameter increase alternatives, such as increasing the dimension of the internal representation (widening). Beyond overwhelming empirical signals for this notion [Simonyan and Zisserman, 2014, He et al., 2016], depth-efficiency was theoretically supported from a variety of angles [Cohen et al., 2016, Eldan and Shamir, 2016, Raghu et al., 2017, Daniely, 2017].

Diminishing returns in the case of very deep networks were mainly attributed to optimization issues, and indeed the alleviation of these issues has allowed network depths to mount from 10s to 100s and beyond [He et al., 2015], enabling deep convolutional networks (ConvNets) to advance the state-of-the-art in computer vision applications. However, as the field matured, a more nuanced perspective emerged. Empirical [Zagoruyko and Komodakis, 2016, Wu et al., 2019] and theoretical [Lu et al., 2017] studies suggest that the interplay between depth and width may be more subtle. Recently, a
heuristic method for increasing width and depth in tandem has lead to the current state-of-the-art on ImageNet to be set by a ConvNet using a fraction of the parameters used by previous leaders [Tan and Le, 2019].

Since the introduction of the Transformer [Vaswani et al., 2017], along with its encoder-only variant, BERT [Devlin et al., 2019], self-attention based deep learning architectures have taken over the field of natural language processing [Liu et al., 2019, Radford et al., 2019, Yang et al., 2019, Raffel et al., 2019, Clark et al., 2020]. However, in contrast to the depth “arms race” that took place in the ConvNet case, the leading self-attention networks are not much deeper than the original depth-12 BERT-base model. In fact, even the strongest self-attention model trained to date, which has increased the parameter count of BERT-base by a factor of 100 [Raffel et al., 2019], has only increased its depth by a factor of 4. The remaining size increase stems from an increase in layer widths, clearly countering the depth-efficiency notion.

A recent extensive empirical ablation study by [Kaplan et al., 2020] provides systematic support for the above signal. Figure [1(a)] taken from this study, shows that the overall (non-embedding) network size, given by \(12 \cdot L \cdot d_x^2\) where \(L\) is the number of self-attention layers (network depth) and \(d_x\) is the hidden representation dimension (network width), is the main predictor of performance regardless of the depth to width ratio (“depth inefficiency”). For \(L \leq 6\), depth-efficiency is clearly demonstrated. Experiments in this figure were performed on the Transformer architecture [Vaswani et al., 2017] while our analysis pertains to its encoder, BERT [Devlin et al., 2019] (we do not expect a qualitative difference in outcome for BERT).

In this paper, we theoretically address the above question of the depth to width trade-off in self-attention networks, and reveal fundamental subtleties in the above picture. We analyze self-attention networks in which all non-linear activations and normalization operations are removed. Otherwise, the analyzed class (presented in section 2) has the regular deep multi-headed Key/Query/Value structure of common self-attention. After presenting this class in detail, we point to recent studies which demonstrate that normalization and position-wise activations are much less pertinent to the ability of self-attention to correlate inputs than its core connectivity, described in full by our analyzed model. More generally, removing non-linearities for analysis of deep network connectivity traits is commonly done: results on expressiveness and optimization of fully-connected [Saxe et al., 2013, Kawaguchi, 2016, Hardt and Ma, 2016], convolutional [Cohen et al., 2016], and recurrent [Khrulkov et al., 2018, Levine et al., 2018a] networks have been attained via this technique.

Theoretical results on Transformers include a proof that they are universal approximators of sequence to sequence functions [Yun et al., 2019], an examination of their robustness [Shi et al., 2020], a comparison between a single self-attention layer and a single convolutional layer [Cordonnier et al., 2020].
We begin by describing the self-attention operation of BERT, and then present the modifications we employ the tool of a function’s separation rank with respect to subsets of its inputs, which quantifies its ability to model input dependencies (presented in section 3). The separation rank was employed for attaining theoretical insights on the dependencies modeled by convolutional and recurrent networks [Cohen and Shashua, 2017] [Levine et al., 2018]

Rather than reinforcing the seemingly plausible hypothesis for the trend in figure 1 by which widening a self-attention network is as effective as deepening it, we confirm the contrary. We show that the operation of stacking self-attention layers is so effective that it quickly saturates the capacity of the network’s width. We establish in section 2.1 the existence of a depth threshold which depends logarithmically on the width \( d_x \), denoted \( L_{th}(d_x) = \log_3(d_x) \). Below the threshold, we prove that depth-efficiency takes place in self-attention networks: a network of depth \( L \leq L_{th}(d_x) \) cannot be replicated by a shallower network, unless the latter’s width grows double-exponentially with \( L \). We prove the above by showing that the separation rank of functions realized by self-attention networks grows double-exponentially with depth, but only polynomially with width, shedding light on the effectiveness of the self-attention mechanism in modeling input interactions when recursively repeated. However, we show that this overwhelming advantage of depth is quickly replaced by a balanced growth. We prove that for self-attention networks with \( L > L_{th}(d_x) \) the ability to model input dependencies, as modeled by the separation rank, increases similarly with depth and width.

A closer observation of the experimental ablation in Kaplan et al. [2020], displayed in figure 1(b), reveals an agreement with our theoretical indications. The figure shows that while for \( L \leq 6 \) there is an advantage for depth, for \( L > 6 \) it completely disappears. When assigning actual width values which range around \( d_x = 1000 \), our theoretical threshold for depth-efficiency agrees with empirical findings, as \( L_{th}(d_x) \approx 6.3 \). Following the presentation of our results, we discuss in section 5 practical outcomes derived from our theoretical insights on the operation of self-attention.

2 The self-attention mechanism

Differentiable attention models in which the output attends over all LSTM-based input representations have been introduced in the context of machine translation [Bahdanau et al., 2014]. Self-attention (also referred to as intra-attention), which relates different inputs to each other, was first employed for machine reading [Cheng et al., 2016], and soon thereafter shown to be useful for a variety of language applications when operating over LSTM-based representations [Parikh et al., 2016] [Paulus et al., 2017] [Lin et al., 2017]. Vaswani et al. [2017] were the first to demonstrate that a model based solely on attention, the Transformer, can be better than LSTM based networks. The Transformer’s encoder, BERT [Devlin et al., 2019], based entirely on self-attention, has demonstrated unprecedented performance across natural language understanding tasks.

2.1 The BERT architecture

We begin by describing the self-attention operation of BERT, and then present the modifications made in our analyzed model. Each layer \( l \in \{L\} := \{1, \ldots, L\} \) of a depth-L BERT is comprised of two sub-layers. The \( H \)-headed self-attention sublayer of layer \( l \) computes the following function at position \( i \in [N] \), over its \( N \) inputs \( \{x^l,j \in \mathbb{R}^{d_x}\}_{j=1}^N \):

\[
f_{\text{SA}}^{l,i}(x^{l,1}, \ldots, x^{l,N}) = \sum_{j=1}^N \sum_{h=1}^H SM_j \left\{ \frac{1}{\sqrt{da}} \langle W_Q^{l,h} x^{l,i}, W_K^{l,h} x^{l,j}\rangle \right\} W^{O,l,h} W^{V,l,h} x^{l,j}
\]  

(1)

where \( SM_j \{ f(j) \} := e^{f(j)} / \sum_{j'} e^{f(j')} \) is the softmax operation and \( \forall h \in [H] \) the learned weights matrices \( W_K^{l,h}, W_Q^{l,h}, W^{V,l,h}, W^{O,l,h} \in \mathbb{R}^{d_a \times d_x} \) convert the representation from its dimension \( d_x \) into the attention dimension \( d_a = d_x / \mu \), creating Key, Query, and Value representations, respectively. The learned weights matrix \( W^{O,l,h} \in \mathbb{R}^{d_a \times d_a} \) converts the attention result back into the representation dimension. The multi-headed self-attention sublayer output in eq. 1 is followed by a residual connection
and layer-norm \cite{Ba et al. 2016}, is inserted into a position-wise feed-forward + ReLU sublayer, such that each layer’s output at position $i \in [N]$ is:

$$
\mathbf{f}_{L,layer}^{l,i} (\mathbf{x}^{1,i}, ..., \mathbf{x}^{N,i}) = \mathbf{W}^{FF,2} \text{ReLU} \left( \mathbf{W}^{FF,1} \text{LayerNorm} \left( \mathbf{f}_{L,layer}^{l,i} + \mathbf{x}^{l,i} \right) \right),
$$

(2)

where the feed-forward matrices are usually taken to be $\mathbf{W}^{FF,1} \in \mathbb{R}^{4d_x \times d_x}$, $\mathbf{W}^{FF,2} \in \mathbb{R}^{d_x \times 4d_x}$, such that the parameter count for an entire layer is $12 \cdot d_x^2$. Finally, the depth-$L$ multi-headed self-attention operation in BERT is obtained by a composition of $L$ such layers, i.e., when setting $\forall l \in \{2, ..., L\}$, $j \in [N] : \mathbf{x}^{l,j} = f_{L,layer}^{l-1,j}$, with $\mathbf{x}^{1,j}$ denoting the input to the deep self-attention network at position $j$.

2.2 The analyzed architecture

We analyze a deep multi-headed self-attention network variant which excludes the layer-norm operation, the softmax normalization, and the ReLU activation \footnote{Focusing on the self-attention operation, we omit a description of the input embedding matrix, as well as of the positional embeddings added at the input, which do not affect our analysis given realistic vocabulary sizes.}, and aggregates the result, depth brings forth an exponential enhancement to the amount of inputs mixed at once as well as to the amount of summed terms. In section 4, we quantify this effect and analyze the limitations posed by the dimension of the internal representation (the width) on the network’s ability to make use of this exponential growth with depth. In the following subsection, we comment on the differences between the BERT architecture described in eqs. 1 and 2 and the self-attention architecture presented in eqs. 3 and 4.

2.3 Relaxations

Empirical evidence indicates that while the ReLU activations and softmax normalization contribute to performance (layer-norm mainly contributes to optimization), the basic mechanism in eqs. 3 and 4 above captures the defining self-attention characteristic of integrating the inputs with each other in a flexible manner:

The ReLU activation relaxation: \cite{Press et al. 2019} demonstrate that a “self-attention first” BERT variant that first performs all of the self-attention operations (eq. 1) consecutively, and only then...
performs all of the position-wise feed-forward+ReLU operations, achieves comparable language modeling performance relatively to the Baseline, which takes the regular approach of interleaving these functionalities (i.e., concatenating the BERT’s layer described in eq. 2). They report that the interleaved Baseline achieves a perplexity score of 18.63±0.26 on the WikiText-103 test [Merity et al., 2016] when averaged over 5 random seeds, while the “self-attention first” model achieves a perplexity score of 18.82 on this test set. The best pre-Transformer perplexity result on the WikiText-103 test, reported by an LSTM-based architecture, was 29.2 [Rae et al., 2018]. Since ReLU and feed-forward do not mix different spatial locations, this outcome directly implies that the self-attention mechanism itself provides all of the elaborate input integration which differentiates BERT from previous models.

The softmax normalization relaxation: Initially, an intuitive interpretation of attention as distributing “fractions” of an overall attention budget among inputs was given to its actual operation of dynamically linking input and output locations. The intuitive interpretation, tightly linked to the need to transform the Key/Query similarity score into a distribution, has been recently challenged, as a growing body of work shows that the attention weights distribution does not directly correlate with predictions [Jain and Wallace 2019; Pruthi et al., 2019; Brunner et al., 2020]. Moreover, Richter and Wattenhofer [2020] recently point out undesirable traits of the softmax operation, demonstrating that its property of confining the outcome to the convex hull of its inputs unnecessarily limits the expressibility of the self-attention mechanism. They experiment on a suite of synthetic tasks with a BERT variant in which the softmax normalization is removed, and find it to perform on par on almost all examined tasks. When replacing the softmax with other normalizations they report improvements. Finally, completely linearized attention (softmax removed) was employed on real tasks as means of reducing costs, since the softmax operation cost scales with the input size [de Brébisson and Vincent, 2016; Wang et al., 2020].

The goal of the above points is not to advocate modifications in BERT’s non-linearity or normalization operations (we leave that to other works), but to note that while these are under examination and are susceptible for alteration, the connectivity of self-attention, manifested by eqs. 3 and 4, is the core mechanism driving its functionality. Our results, to be presented in section 4, demonstrate how conclusions drawn by directly analyzing this mechanism accord with the operation of commonly employed self-attention networks.

3 A measure of capacity for modeling input dependencies

In this section, we introduce the separation rank of the function realized by a self-attention network as a measure that quantifies its ability to model dependencies between subsets of its variable set \{x^i\}_{j=1}^N. The separation rank, introduced in Beylkin and Mohlenkamp [2002] for high-dimensional numerical analysis, was employed for various applications, e.g., chemistry [Harrison et al., 2003], particle engineering [Hackbusch, 2006], and machine learning [Beylkin et al., 2009]. Importantly, the separation rank has been established as a measure of dependencies modeled by deep convolutional and recurrent networks w.r.t. their inputs [Cohen and Shashua, 2017; Levine et al., 2018a,b].

We provide an intuitive presentation of the concept of the separation rank, see formal definition in the supplementary material. Let \((A, B)\) be a partition of the input locations, i.e., \(A\) and \(B\) are disjoint subsets of \([N]\) whose union gives \([N]\). The separation rank of a scalar function \(y(x^1, \ldots, x^N)\) w.r.t. a partition \((A, B)\), denoted \(sep(y; A, B)\), is the minimal number of summands that together sum up to equal \(y\), where each summand is multiplicatively separable w.r.t. \((A, B)\), i.e., is equal to a product of two functions – one that intakes only inputs from one subset \{x^j\}_{j \in A}\, and another that intakes only inputs from the other subset \{x^j\}_{j \in B}. For the example of \(A = \{1, \ldots, N/2\}\) and \(B = \{N/2+1, \ldots, N\}\), it is equal to the minimal \(k\) such that \(f(x^1, \ldots, x^N) = \sum_{a=1}^k g_a(x^1, \ldots, x^{a/2})h_a(x^{a/2+1}, \ldots, x^N)\) for some \{\alpha, \beta\}_{a \in [k]}.

If the separation rank of a function w.r.t. a partition of its input is equal to 1, the function is separable, meaning it cannot take into account consistency between the values of \{x^j\}_{j \in A}\, and those of \{x^j\}_{j \in B}. In a statistical setting, if \(y\) is a probability density function, this would mean that \{x^j\}_{j \in A}\, and \{x^j\}_{j \in B}\, are statistically independent. The higher \(sep(y; A, B)\), the farther \(y\) is from this situation, i.e. the more it models dependency between \{x^j\}_{j \in A}\, and \{x^j\}_{j \in B}, or equivalently, the stronger the correlation it induces between the inputs indexed by \(A\) and those indexed by \(B\).

The fixed connectivity of ConvNets has been shown to yield high separation ranks w.r.t. partitions which separate neighboring inputs (e.g., where all odd positions are in \(A\) and all even positions are...
in $B$), while suffering from low separation ranks w.r.t. partitions which separate distant inputs (e.g., where $A = 1, ..., N/2$ and $B = N/2 + 1, ..., N$). Our analysis establishes a qualitatively different trait for self-attention networks, which treat all balanced partitions alike:

**Claim 1.** For $p \in [d_z]$, let $y_p^{i, L, d_z, H, \Theta}$ be the scalar function computing the $p$th entry of an output vector at position $i \in [N]$ of the depth-$L$ self-attention network with embedding dimension $d_z$ and $H$ attention heads per layer, defined in eqs. 3 and 4. Then, its separation rank w.r.t. balanced partitions, which obey $A \cup B = [N], |A|, |B| \leq N/2$, is invariant to the identity of the partition, i.e.,

$$\forall A \cup B = [N], \ A \cup \bar{B} = [N], \ s.t. \ |A|, |B|, |\bar{A}|, |\bar{B}| = N/2:$$

$$sep(y_p^{i, L, d_z, H, \Theta}; A, B) = sep(y_p^{i, L, d_z, H, \Theta}; \bar{A}, \bar{B})$$

(5)

Accordingly, we will omit the specification of the partition in future uses, denoting $sep(y_p^{i, L, d_z, H, \Theta})$ as the separation rank of $y_p^{i, L, d_z, H, \Theta}$ w.r.t. any balanced partition of the inputs.

This result accords with the intuition regarding the flexibility of the attention mechanism – it does not integrate the input in a predefined pattern like convolutional networks, but dynamically learns to correlate any inter-dependent subsets of the inputs. Natural text exhibits non-smooth non-local dependency structures, as correlations between input segments can abruptly rise and decay with distance. The fact that self-attention facilitates all correlation patterns equally poses it as a more natural architecture for language modeling related tasks. Convolutional networks, with their local connectivity, may have the right inductive bias for imagery data, but partitions unfavorable to them may reflect more erratic correlations that are nonetheless relevant for natural language inputs.

However, the above property of indifference to the input partition is not enough for succeeding at tasks with elaborate input dependencies, since a function with equally low separation ranks for all input partitions has limited ability to model such dependencies. In the following section, we analyze how different architectural parameters affect the ability of self-attention networks to correlate their inputs. Furthermore, by bounding their separation ranks, we establish different depth-efficiency regimes in self-attention networks.

## 4 The effect of depth in self-attention networks

In this section, we present tight bounds on the separation rank of self-attention networks, which reveal two qualitatively different regimes. In the first regime of $L < \log_3(d_z)$, analyzed in subsection 4.1 we establish that deepening is clearly preferable to widening. In the second regime of $L > \log_3(d_z)$, analyzed in subsection 4.2 we show that deepening and widening play a similar role in enhancing the expressiveness self-attention networks.

### 4.1 Depth efficiency in self-attention

The recursive structure of deep self-attention hints at an exponential increase of input mixing with depth: The output of each layer is introduced 3 times into the Key/Query/Value computation made by the subsequent layer. In this subsection, we formalize this intuition for self-attention networks of sufficient width, $d_z > 3^L$. Theorem 1 below bounds the separation rank of such networks. Subsequent to its statement and brief outline of its proof, we explicitly show in corollary 4.1 the implied exponential requirement from a bounded depth network attempting to replicate a deeper one.

**Theorem 1.** For $p \in [d_z]$, let $y_p^{i, L, d_z, H, \Theta}$ be the scalar function computing the $p$th entry of an output vector at position $i \in [N]$ of the depth-$L$ self-attention network with embedding dimension $d_z$ and $H > 1$ attention heads per layer, defined in eqs. 3 and 4. Let $sep(y_p^{i, L, d_z, H, \Theta})$ be its separation rank (section 2). If $L, d_z$ obey $L < \log_3(d_z)$, then the following holds almost everywhere in the network’s learned parameter space, i.e., for all values of the weight matrices (represented by $\Theta$) but a set of Lebesgue measure zero:

$$a_1 \cdot 3^L (\log_3(d_z - H) + a_2) \leq \log_3(sep(y_p^{i, L, d_z, H, \Theta})) \leq \frac{3^L - 1}{2} \log_3(d_z + H)$$

(6)

with $a_1 = \frac{1}{2}$ and $a_2 = -L + [2 - \log_3 2]$.

(Note that $\log_3(d_z - H) + a_2 > 0$ in this regime of $L < \log_3(d_z)$.)
We provide below a short proof sketch of the lower bound in the above theorem. The derivation of the upper bound is more straightforward, and is left for the supplementary material, along with a formal proof of the lower bound.

**Proof sketch for lower bound on the separation rank in theorem 1**

We make use of grid tensor based function discretization [Hackbusch, 2012] – The function realized by a self-attention network is evaluated for a set of points on an exponentially large grid in the input space, and the outcomes are stored in a matrix $M(y_p^{i, L, d_x, H, \Theta})$, constructed to uphold rank $\left[\mathcal{M} \left( y_p^{i, L, d_x, H, \Theta} \right) \right] \leq \text{sep}(y_p^{i, L, d_x, H, \Theta})$. Observing that the entries of $\mathcal{M} \left( y_p^{i, L, d_x, H, \Theta} \right)$ vary polynomially with the self-attention network’s weights, we note that it suffices to find a single weight assignment for which the rank of the matrix is greater than the desired lower bound, in order to prove the case for almost all of the configurations of the network’s learned weights (but a set of measure zero). Thus, we prove the lower bound in theorem 1 by choosing a simple weight assignment that still represents the self-attention connectivity, and showing that for this value of $\Theta$ rank $\left[\mathcal{M} \left( y_p^{i, L, d_x, H, \Theta} \right) \right]$ achieves the lower bound. □

Theorem 1 bounds the separation rank of a deep self-attention network of sufficient width between two functions that grow double-exponentially with depth and polynomially with width, tightly describing its behavior w.r.t. depth and width. Because equivalence cannot hold between two functions of different separation ranks, the above result implies a double-exponential requirement from the width of a shallow network attempting to replicate the deep one:

**Corollary 1.** With probability 1, the function realized upon randomization of the weights of a deep self-attention network defined in eqs. 3 and 4 with depth $L^{\text{deep}}$ and width $d^{\text{deep}} > 3^{L^{\text{deep}}}$, may only be realized by a shallower network with depth $L^{\text{shallow}} = L^{\text{deep}}/d$ and width $d^{\text{shallow}} = wd^{\text{shallow}}$, where $d > 1, w > 1$ (i.e., the deep network is deeper by a factor of $d$ and the shallow network is wider by a factor of $w$), if the following holds: $w \propto \exp(\exp(d)).$

The above requirement implies clear-cut (double-exponential) depth-efficiency: the shallow network must grow impractically large to match the deeper one. For example, for BERT-large parameters of $d^{\text{deep}} = 1000, H = 16$, by taking the deep network under the depth-efficiency threshold $L^{\text{deep}} = 6$, the width of a depth $L^{\text{shallow}} = 2$ network has to be $d^{\text{shallow}} \approx 2 \cdot 10^{17}$ and the width of a depth $L^{\text{shallow}} = 3$ network has to be $d^{\text{shallow}} \approx 2 \cdot 10^9$ to match the deep network’s operation. These numbers were attained by numerically equating the upper bound in eq. [6] for the shallow network and the lower bound in eq. [6] for the deep network, i.e., by asking when the upper bound on the shallow network is larger than the lower bound on the deep network.

### 4.2 The contribution of depth is limited

Beyond establishing depth-efficiency in early self-attention layers, the above analysis sheds light on the contribution of a self-attention network’s depth to its ability to correlate input subsets. The separation rank (w.r.t. any partition) of a single layer, given by eq. [5], is only linear in $H$ and $d_x$, showcasing a limitation of the class of functions realized by single self-attention layers to model elaborate input dependencies. Theorem 2 quantifies the double exponential growth of this capacity measure with the number of stacked self-attention layers. The following theorem shows that this growth is capped by the dimension of the internal representation:

**Theorem 2.** For $y_p^{i, L, d_x, H, \Theta}$ as defined in theorem 1, if $L > \log_3 (d_x)$, then the following holds almost everywhere in the network’s learned parameter space, i.e., for all values of the weight matrices (represented by $\Theta$) but a set of Lebesgue measure zero:

$$\frac{1}{2}d_x \cdot L + b_1 + b_2 \leq \text{sep}(y_p^{i, L, d_x, H, \Theta}) \leq 2d_x \cdot L + c_1 + c_2$$

with corrections on the order of $L$:

$$b_1 = -L \left( \frac{H}{2} + 1 \right) \quad \text{and} \quad c_1 = L$$

and corrections on the order of $d_x \log_3 (d_x)$:

$$b_2 = -d_x \left( 1 + \frac{1}{2} \log_3 \left( \frac{d_x - H}{2} \right) \right) \quad \text{and} \quad c_2 = -2d_x \cdot \log_3 d_x + \log_3 d_x$$

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We provide below a proof sketch of the upper bound in the above theorem. The formal proof, along with the proof of the lower bound, which is similar to the one illustrated above for the lower bound in theorem\(^1\), are left for the supplementary material.

**Proof sketch for upper bound on the separation rank in theorem\(^2\)**

By observing that \(y_p^{L, d_x, H, \Theta}\) is a polynomial of degree \(2C = 3^L - 1\) (note that \(C\) is as defined in eq. 4), we find a kernel \(\psi(x^1, ..., x^N)\) that maps the input into a space where each of the output monomials is a linear functional. We find a basis for the subspace \(V\) spanned by the output monomials, and bound the separation rank of each element in that basis by a constant. The dimension of \(V\) is exponential in \(Nd_x\) and polynomial in \(3^L - 1\), providing equal groundings for depth and width. A careful analysis that exploits the sums over the indices \(j_1, ..., j_C\) in eq. 4 removes the dependence on \(N\).

Theorem\(^2\) states that when the network’s depth passes a width dependent threshold, the separation rank turns from increasing polynomially with width and double-exponentially with depth to increasing-exponentially with width and depth together. Thus, while an increase in network size increases its capacity to model input dependencies, our result shows that there is no longer a clear cut advantage of depth in this respect:

**Corollary 2.** Let \(y^\text{deep}\) denote the function realized by a deep self-attention network at any output location \(i \in [N]\), defined in eqs. 3 and 4 with depth and width denoted \(L^\text{deep}, d_x^\text{deep}\) such that \(L^\text{deep} > \log_3 d_x^\text{deep}\). Denote \(\beta_1 := \frac{\log d_x^\text{deep}}{\log L^\text{deep}} < 1\). Then, there exists \(\beta_2 = \Theta(\log(H) \cdot \log(d_x^\text{deep}) \cdot \log(L^\text{deep}))\) such that the function realized by a network of depth: \(L^\text{shallow} = \beta_1 \cdot L^\text{deep} + \beta_2\), and width: \(d_x^\text{shallow} = 3^{\beta_2} d_x^\text{deep}\), denoted \(y^\text{shallow}\), has higher separation rank, i.e.:

\[
\text{sep}(y_p^\text{shallow}) > \text{sep}(y_p^\text{deep}) \quad \text{where } p, p' \in [d_x]
\]

The above corollary, which follows from theorems\(^1\) and \(^2\), shows that the separation rank of a function realized by a self-attention network of arbitrary depth \(L > \log_3(d_x)\) can be surpassed by a shallower network of polynomial width, contrarily to the established behavior for networks of depth \(L < \log_3(d_x)\).

We leave it as an open conjecture that a polynomially sized shallower network can exactly replicate the operation of a deeper network in this regime. With that, we point out that a variety of results which directly bound different complexity properties of deep networks have been put forward, shedding light on their operation [Montufar et al., 2014; Bianchini and Scarselli, 2014; Raghu et al., 2017; Serra et al., 2017; Inoue, 2019]. Bounds on the separation rank have been used to explain the operation of more veteran architectures, and we find them to be particularly relevant in the case of self-attention: this complexity measure quantifies the amount of input inter-dependency induced by the network, directly reflecting a widespread intuition on the success behind the self-attention mechanism.

5 Discussion

The thorough study of [Kaplan et al., 2020] (figure 1) concludes the existence of a “depth-inefficiency” phenomenon in self-attention networks – in contrast to other successful deep learning architectures, in the case of self-attention there is no clear advantage to deepening vs. widening. This conclusion, which bears formidable impact on design considerations for this popular class of architectures, is clearly reflected within our theoretical framework reported in this paper. However, our analysis suggests an important nuance regarding the origins of this effect.

Rather than an obvious explanation for the above empirical findings, by which the self-attention mechanism does not benefit much from the operation of compounding, our analysis strongly points at the converse: self-attention is so effective at integrating its inputs, that it very quickly reaches saturation in the amount of dependencies that can be supported by the representation dimension. For early self-attention compounding, we prove a rapid growth in expressiveness with depth, and specifically in the ability to flexibly correlate between any input locations, which can not be accounted for by any reasonable widening. We did not find a result which directly upper bounds depth-efficiency in other architecture classes. Works by [Sharir and Shashua, 2018; Levine et al., 2019] shows an exponential growth with depth of a measure related to the separation rank in certain classes of convolutional networks. Comparing this dependence with the double-exponential growth shown in
Theorem 1: For early self-attention layers, it may be conjectured that convolutional networks benefit significantly more from depth than self-attention does, because they do not saturate some width dependent threshold as quickly as self-attention does. We leave investigation of such directions for future works.

Our analysis pinpoints the transition in which the capacity of width to support the above rapid growth exhausts. The experiments in figure 1 show a clear agreement with our theoretical analysis, demonstrating depth-efficiency under the theoretically identified transition point and “depth-in-efficiency” above it. This reinforces consideration of further practical conclusions stemming from our analysis. Firstly, the clear boundaries drawn between the two regimes suggest always to exploit any parameter budget of such that depth does not fall below the threshold of . In this case, we have shown a clear disadvantage in the expressiveness of shallower networks. The adjacent table contains the minimal depths per parameter-budget by these considerations, which accord with empirical evidence in figure 1. Such insights may prove useful given the rapid increase in model sizes [Sharir et al., 2020].

Moreover, the observation that width is the limiting factor for depth-efficiency promotes the development of methods for significantly increasing it. [Lan et al., 2019] present the successful “ALBERT”, a BERT variant which shares parameters between self-attention layers, allowing for wider models to be trained for the same budget. For a more significant increase, that addresses the question of computation efficiency, we point at the concept of ShuffleNet [Ma et al., 2018], which has proven to be very efficient for convolutional networks. They suggest increasing the representation dimension while using only a fraction of it for computation in each layer. This way, the computation costs are contained, but the theoretical limitations posed by our work are relaxed. Similarly, alternative methods for efficiently increasing the representation dimension are also supported by our analysis [Bengio et al., 2013, Shazeer et al., 2017]. Generally, width increases have greater potential for speeding up network inference and training because it can be parallelized, as opposed to depth which yields a sequential computation. A theoretical indication that the contribution of depth and width is indeed on the same order, may motivate further model parallelism methods for Transformers. Indeed, we view our work as part of an effort to provide timely theoretical interpretations as feedback for the tremendous empirical pull of our field, hopefully enabling a more informed and efficient progress.

Acknowledgments

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| size | 10^7 | 10^8 | 10^9 | 10^{10} | 10^{11} |
|------|------|------|------|---------|---------|
| min. depth | 5    | 6    | 7    | 8       | 9       |

Table 1: The minimal depth for efficient parameter distribution. Note the deviation between the and curves in figure 1, which occurs in network sizes predicted by this table.
A Upper bounds on the separation rank

A.1 The function realized by a deep multi-headed self-attention network

In this subsection, we prove facts on the general structure of the function realized by the analyzed self-attention architecture that will be of use to us in the upcoming proofs. For a cleaner presentation, we will rewrite eq. 3 in vectorized notation:

$$Y = \sum_{h=1}^{H} W^{O,h} W^{V,h} X X^T (W^{K,h})^T W^{Q,h} X$$  \hspace{0.5cm} (9)$$

where $X, Y (X) \in \mathbb{R}^{d \times N}$ denote matrices respectively holding $x^j, y^j (x^1, ..., x^N)$ in their $j$'th column. Similarly treating eq. 4, we will denote by $Y_{L,d_x,H,\Theta} (X) \in \mathbb{R}^{d \times N}$ the matrix holding $y^j_{L,d_x,H,\Theta} (X^1, ..., x^N)$ in its $j$'th column.

We begin by proving a lemma that reveals the structure of $g^L$ presented in eq. 4.

**Lemma 1.** Defining $C (L) := \frac{3^L - 1}{2}$, any depth $L$ composition of the self-attention layers defined in eq. 3 can be written as:

$$Y_{L,d_x,H,\Theta} = \sum_{h \in [H]^{[C(L)]}} B^{(0,h)}_T M^{(1,h)}_T \cdots M^{(C(L),h)}_T A^{(0,h)}_T X$$  \hspace{0.5cm} (10)$$

where $\forall h \in [H]^{[C]} 0 \leq c \leq C (L) : M^{(c,h)} = A^{(c,h)} X X^T B^{(c,h)}_T$ and $A^{(c,h)}, B^{(c,h)} \in \mathbb{R}^{d_a \times d_x}$.

**Proof.** By Induction on $L$. Base case:

$$Y^{(1)} (X) = \sum_{h=1}^{H} W^{O,h} W^{V,h} X X^T (W^{K,h})^T W^{Q,h} X$$  \hspace{0.5cm} (9)$$

By Induction on $L$. Base case:
\[ Y^{(L+1)}(X) = \sum_{h=1}^{H} W^{0,h} W^{V,h} Y^{(L)}(X) Y^{(L)}(X)^T (W^{K,h})^T W^{Q,h} Y^{(L)}(X) \]

Now, substituting in the induction hypothesis on the structure of \( Y^{(L)}(X) \) yields:
\[
= \sum_{h=1}^{H} W^{0,h} W^{V,h} \left( \sum_{h_1 \in [H]} B^{(0,h_1)T} M^{(1,h_1)} \cdots M^{(C(L),h_1)} A^{(0,h_1)} X \right)
\[
\left( \sum_{h_2 \in [H]} X^T A^{(0,h_2)T} M^{(C(L),h_2)} \cdots M^{(1,h_2)T} B^{(0,h_2)} \right) (W^{K,h})^T W^{Q,h} \sum_{h_3 \in [H]} B^{(0,h_3)T} M^{(1,h_3)} \cdots M^{(C(L),h_3)} A^{(0,h_3)} X
\]
Finally unifying the summations over \( h, h_1, h_2, h_3 \) to single sum over \([H]^{[C(L)+1=C(L+1)]} \) gives
\[
\sum_{h \in [H]} W^{0,h} W^{V,h} B^{(0,h)T} M^{(1,h)} \cdots M^{(C(L),h)} A^{(0,h)} X X^T A^{(0,h)T} M^{(C(L),h)T} \cdots M^{(1,h)T} B^{(0,h)} X
\]
\[
\text{in the desired form of } M \text{ in the desired form of } M
\]

Note that the number of \( M \) units, each with a sum over a different index \( j \in [N] \), is \( 3C(L)+1 = C(L+1) \), implying \( C(L) = \frac{3^L-1}{2} \) as needed.

**Corollary 3.** Defining \( C(L) := \frac{3^L-1}{2} \), any depth \( L \) composition of \( L \) self-attention layers can be written as:
\[
y^{i,L,d_z,H,\Theta}(x^i, \ldots, x^N) = \sum_{j_1, \ldots, j_C=1}^{N} g^L(x^i, x^{j_1}, \ldots, x^{j_C}) \tag{11}
\]

Where
\[
g^L(x^i, x^{j_1}, \ldots, x^{j_C}) := \sum_{h \in [H]} \sum_{r_1, \ldots, r_{C(L)+1}=1}^{d_h} \left[ B^{(0,h)} \right]_{r_1,p} \left( \prod_{c=1}^{C(L)} \langle A^{(c,h)}_i, x^{(j_c)} \rangle \langle B^{(c,h)}_{r_{c+1}}, x^{(j_c)} \rangle \right) \langle A^{(0,h)}_i, x^{(j)} \rangle
\]

**Proof.** To get the required form, we will use lemma 1 above and write the matrix multiplication in eq. (10) explicitly.
\[
M_{r_1, r_2}^{(c,h)} = \sum_{j=1}^{N} \left[ A^{(c,h)} X \right]_{r_1,j} \left[ X^T B^{(c,h)T} \right]_{j,r_2} = \sum_{j=1}^{N} \langle A^{(c,h)}_i, x^{(j)} \rangle \langle B^{(c,h)}_{r_{c+1}}, x^{(j)} \rangle
\]
Therefore
\[
y^{i,L,d_z,H,\Theta}(x^{(1)}, \ldots, x^{(N)}) = \sum_{h \in [H]} \sum_{r_1, p} B^{(0,h)T} M^{(1,h)} \cdots M^{(C(L),h)} A^{(0,h)} x^{(i)}
\]
\[
= \sum_{j_1, \ldots, j_C=1}^{N} \sum_{h \in [H]} \sum_{r_1, \ldots, r_{C(L)+1}=1}^{d_h} \left[ B^{(0,h)} \right]_{r_1,p} \left( \prod_{c=1}^{C(L)} \langle A^{(c,h)}_i, x^{(j_c)} \rangle \langle B^{(c,h)}_{r_{c+1}}, x^{(j_c)} \rangle \right) \langle A^{(0,h)}_i, x^{(j)} \rangle
\]
\[
= \sum_{j_1, \ldots, j_C=1}^{N} \sum_{h \in [H]} \sum_{r_1, \ldots, r_{C(L)+1}=1}^{d_h} \left[ B^{(0,h)} \right]_{r_1,p} \left( \prod_{c=1}^{C(L)} \langle A^{(c,h)}_i, x^{(j_c)} \rangle \langle B^{(c,h)}_{r_{c+1}}, x^{(j_c)} \rangle \right) \langle A^{(0,h)}_i, x^{(j)} \rangle
\]

In the next two subsections, we will use the above lemma 1 to prove the two competing upper bounds on the separation rank of self-attention networks.
A.2 Proof of the upper bound in theorem 1

In the following theorem, we show how an upper bound on the separation rank is implied by the form of eq. 10 in the statement of lemma 1.

**Theorem 3.** Defining $C(L) := \frac{2L+1}{2}$, for any depth $L \geq 1$ input size $N > 1$ partition $P \cup Q = [N]$ and output locations $i \in [N]$, $p \in [d_z]$, the following holds:

$$\text{sep} \left( y_p^{i,L,d_z,H}, P, Q \right) \leq (H (d_a + 1))^{C(L)}$$

**Proof.** We begin by writing the matrix multiplication in eq. 10 explicitly.

$$M^{(c,h)}_{r_s,r_t} = \sum_{j=1}^{N} A^{(c,h)} X \quad \sum_{j=1}^{P} \left( A^{(c,h)} \right) \quad \sum_{j=1}^{Q} \left( A^{(c,h)} \right)$$

Therefore, rewriting the summation to be over $\{ P_c \in \{ P, Q \} \}_{C(L)}$ that correspond to the two partition segments $P/Q$.

$$y_p^{i,L,d_z,H} \left( x^{(1)}, ..., x^{(N)} \right) = \sum_{h \in [H][C(L)]} B^{(0,h)} M^{(1,h)} \cdot \sum_{h \in [H][C(L)]} B^{(0,h)} M^{(C(L),h)} A^{(0,h)} x^{(i)}$$

Now we reorder the above sum by summing over indices of swaps between $P$ and $Q$, i.e. $\beta \in [C]$ such that $P_{\beta} \neq P_{\beta+1}$, and split the multiplication $\prod_{C(L)}^{C(L)}$ according to the crossing indices:
Where we assume w.l.o.g that $i \in P$ and therefore $P_{\beta_1}, P_{\beta_1+1}, \ldots, P_{\beta_h-1}, P_{\beta_h} = P$. The above reordering allows pushing the summation of non swapping $r_c$ indices into the $P, Q$ parentheses:

$$
\sum_{h \in [H]} \sum_{b=0}^{C(L)} \sum_{r=0}^{d_a} \sum_{r_1=1}^{d_a} \sum_{r_2m+1=1}^{d_a} \sum_{m=0}^{d_a} \beta_{2m} \sum_{r_2m+1=1}^{d_a} \sum_{e=\beta_{2m+1}+1}^{d_a} \left( \sum_{j \in P} \left( A_{x_a}^{(c,h)}, x(j) \right) \right) \left( B_{r_{c+1}}^{(c,h)}, x(j) \right)
$$

(12)

Since the separation rank of each term in the above summation is 1, we proved the following upper bound on the separation rank:

$$
sep \left( y_p^{L,d_x,H,\Theta}, P, Q \right) \leq \sum_{h \in [H]} \sum_{b=0}^{C(L)} \sum_{r=0}^{d_a} \sum_{r_1=1}^{d_a} \sum_{r_2m+1=1}^{d_a} \sum_{m=0}^{d_a} \beta_{2m} \sum_{r_2m+1=1}^{d_a} \sum_{e=\beta_{2m+1}+1}^{d_a} \left( \sum_{j \in P} \left( A_{x_a}^{(c,h)}, x(j) \right) \right) \left( B_{r_{c+1}}^{(c,h)}, x(j) \right)
$$

$$
= H^{C(L)} \sum_{b=0}^{C(L)} \left( C \left( L \right) \right) (d_a)^b = H^{C(L)} (d_a + 1)^{C(L)} = (H (d_a + 1))^{C(L)}
$$

We note that unlike the $d_a$ case, the same $H$ index can affect nonconsecutive $M^{(c_1, h)}, M^{(c_2, h)}$, therefore we can’t simply push the $h$ indices as done for the $r$ indices in eq. 12.

From here, the upper bound in theorem follows by

$$
\log_3 \left( sep \left( y_p^{L,d_x,H,\Theta}, P, Q \right) \right) \leq \log_3 \left( (H (d_a + 1))^{C(L)} \right) = \frac{3L-1}{2} \log_3 (d_x + H)
$$

(13)

A.3 Proof of the upper bound in theorem

In the following theorem, we show how an upper bound on the separation rank is implied by the polynomial degree of $y_p^{L,d_x,H,\Theta}$ in eq. 12. We will use the notation of $\binom{n}{k}$ – the multiset coefficient, given in the binomial form by $\binom{n+k-1}{k}$. We will use the identity $|\{a_1 \ldots a_n \in \mathbb{Z} \geq 0 : \sum_{r=1}^{n} a_r = k\}| = \binom{n+k-1}{k}$.

**Theorem 4.** Defining $C(L) := \frac{3L-1}{2}$, for any depth $L \geq 1$ input size $N > 1$ partition $P : Q = [N]$ and output locations $i \in [N]$, $p \in [d_x]$, the following holds:

$$
sep \left( y_p^{i,L,d_x,H,\Theta}, P, Q \right) \leq d_x (C (L) + 1) \left( \left( \frac{d_x}{2C (L)} + 1 \right)^{d_x}
$$

\}^{1/2} \binom{n-1}{k-1}
$$

(14)

We will use the notation of $\binom{n}{k}$ – the multiset coefficient, given in the binomial form by $\binom{n+k-1}{k}$. We will use the identity $|\{a_1 \ldots a_n \in \mathbb{Z} \geq 0 : \sum_{r=1}^{n} a_r = k\}| = \binom{n+k-1}{k}$.

**Theorem 4.** Defining $C(L) := \frac{3L-1}{2}$, for any depth $L \geq 1$ input size $N > 1$ partition $P : Q = [N]$ and output locations $i \in [N]$, $p \in [d_x]$, the following holds:

$$
sep \left( y_p^{i,L,d_x,H,\Theta}, P, Q \right) \leq d_x (C (L) + 1) \left( \left( \frac{d_x}{2C (L)} + 1 \right)^{d_x}
$$

\}^{1/2} \binom{n}{k}
$$

(14)
Proof. We begin by opening the inner products in eq. 11, explicitly writing the indices:

\[ y_p^{j, L, d_x, H, \Theta} = \sum_{j_1, \ldots, j_{C(L)}}^{N} \sum_{h \in [H]}^{C(L)} \sum_{r_1, \ldots, r_{C(L)+1} = 1}^{d_a} B_{r_1, h}^{0, (0, h)} \left( \prod_{c=1}^{C(L)} A_{r_c}^{(c, h), x(j_c)} \right) \langle B_{r_{C(L)+1}}^{(c, h), x(j_{C(L)+1})} \rangle \langle A_{r_{C(L)+1}}^{(0, h), x(i)} \rangle \]

Now we can group monomials by the powers \( n_1, \ldots, n_{d_x} \) of each coordinate:

\[ = \sum_{\alpha_1, \ldots, \alpha_{C(L)+1}, \beta_1, \ldots, \beta_{C(L)} = 1}^{d_a} \left( \sum_{h \in [H]}^{C(L)} \sum_{r_{C(L)+1} = 1}^{d_a} B_{r_{C(L)+1}, h}^{0, (0, h)} \left( \prod_{c=1}^{C(L)} A_{r_c}^{(c, h), x(j_c)} \right) \langle B_{r_{C(L)+1}}^{(c, h), x(j_{C(L)+1})} \rangle \langle A_{r_{C(L)+1}}^{(0, h), x(i)} \rangle \right) \]

And separating between coefficients and \( x \)'s:

\[ = \sum_{\alpha_1, \ldots, \alpha_{C(L)+1}, \beta_1, \ldots, \beta_{C(L)} = 1}^{d_a} \left( \sum_{h \in [H]}^{C(L)} \sum_{r_{C(L)+1} = 1}^{d_a} B_{r_{C(L)+1}, h}^{0, (0, h)} \left( \prod_{c=1}^{C(L)} A_{r_c}^{(c, h), x(j_c)} \right) \langle B_{r_{C(L)+1}}^{(c, h), x(j_{C(L)+1})} \rangle \langle A_{r_{C(L)+1}}^{(0, h), x(i)} \rangle \right) \]

Now we can group monomials by the powers \( n_1, \ldots, n_{d_x} \) of each coordinate:

\[ \sum_{\alpha_1, \ldots, \alpha_{C(L)+1}, \beta_1, \ldots, \beta_{C(L)} = 1}^{d_a} \left( \sum_{h \in [H]}^{C(L)} \sum_{r_{C(L)+1} = 1}^{d_a} B_{r_{C(L)+1}, h}^{0, (0, h)} \left( \prod_{c=1}^{C(L)} A_{r_c}^{(c, h), x(j_c)} \right) \langle B_{r_{C(L)+1}}^{(c, h), x(j_{C(L)+1})} \rangle \langle A_{r_{C(L)+1}}^{(0, h), x(i)} \rangle \right) \]

Where:

\[ \chi_{n_1, \ldots, n_{d_x}, \alpha_{C(L)+1}} \left( x^{(1)}, \ldots, x^{(N)} \right) := \sum_{\alpha_1, \ldots, \alpha_{C(L)} = 1}^{C(L)} x^{(i)}_{\alpha_{C(L)+1}} \prod_{j=1}^{N} \prod_{m=1}^{d_x} x^{(j)}_m \left( n_{m,j} \right) \]

Finally, we need to bound the separation rank of \( \chi_{n_1, \ldots, n_{d_x}, \alpha_{C(L)+1}} \). W.l.o.g we choose the partition \( P = \{1, \ldots, \frac{N}{2} \} \), \( Q = \{ \frac{N}{2} + 1, \ldots, N \} \) and \( i \in P \) then we can divide the powers between \( P, Q \) in the following way:
\[
\chi_{n_1 \ldots n_d, \alpha C(L)+1} \left( x^{(1)}, \ldots, x^{(N)} \right) = \sum_{0 \leq r_1, \ldots, r_d, p \leq 2C(L)} \sum_{\forall m \in [d_x]} \sum_{\forall j \in [N]} \sum_{n_{m,j} = 2a_j}^{n_{m,j} \leq 2C(L)} x^{(i)}_{\alpha_{C(L)+1}} \prod_{j \in P, m=1}^{d_x} \left( x^{(j)}_{m} \right)^{n_{m,j}}.
\]

Thus, since each summand is of separation rank 1, the separation rank of \( \chi_{n_1 \ldots n_d, \alpha C(L)+1} \) is bounded by the number of summands:

\[
(C(L) + 1) \prod_{\beta=1}^{d_x} \left( \binom{2}{r_{\beta}} \right) \leq (C(L) + 1) \left( \frac{2C(L)}{d_x} + 1 \right)^{d_x},
\]

where the inequality followed from lemma 2. Since we have at most \( d_x \left( \binom{d_x}{2C(L)} \right) \) different \( \chi \) we conclude that:

\[
\text{sep} \left( y_p^{i:L,d_x,H,\Theta}, P, Q \right) \leq d_x \left( \binom{d_x}{2C(L)} \right) (C(L) + 1) \left( \frac{2C(L)}{d_x} + 1 \right)^{d_x}.
\]

From here, theorem 2 follows by the multiset identity in lemma 3.

\[
\log_3 \left[ \text{sep} \left( y_p^{i:L,d_x,H,\Theta}, P, Q \right) \right] \leq \log_3 \left[ d_x (C(L) + 1) \left( \binom{d_x}{2C(L)} \right) \left( \frac{2C(L)}{d_x} + 1 \right)^{d_x} \right] \tag{14}
\]

\[
\leq \log_3 \left[ d_x (C(L) + 1) \left( \frac{2C(L)}{d_x} + 1 \right)^{d_x} \right]
\]

\[
\leq \log_3 \left[ 3^4 (2e)^{2d_x} \left( \frac{3L}{d_x} - 1 \right)^{2d_x} \right]
\]

\[
\leq L + \log_3 d_x + d_x 2 \log_3 2e + 2d_x \log_3 \left( \frac{3^L}{d_x} \right)
\]

\[
\leq (2d_x + 1) L + \log_3 d_x + 2d_x (\log_3 2e - \log_3 d_x)
\]
A.4 Technical lemmas

Lemma 2. (inequality of arithmetic and geometric multiset coefficient means)

Let \( n, k \in \mathbb{N} \) and \( \phi : \mathbb{N}^k \rightarrow \mathbb{N} := r_1, \ldots, r_k \vdash \prod_{j=1}^{k} \binom{n}{r_j} \) then:

\[
\forall r_1, \ldots, r_k \in \mathbb{N} \quad \phi(r_1, \ldots, r_k) \leq \left( \prod_{t=1}^{n-1} \frac{M + t}{(n-1)!} \right)^{k}
\]

where \( M := \sum_{j=1}^{k} r_j \)

Proof. Define \( f_t := \prod_{j=1}^{k} (r_j + t) \) and \( \psi := \prod_{t=1}^{n-1} f_t \) than by the inequality of arithmetic and geometric means

\[
\forall t \in [k] \quad f_t = \left( \frac{1}{k} \sum_{j=1}^{k} (r_j + t) \right)^{k} = \left( \frac{M + t}{k} \right)^{k}
\]

Therefore

\[
\phi(r_1, \ldots, r_k) = \prod_{j=1}^{k} \binom{n}{r_j} = \prod_{j=1}^{k} \binom{n + r_j - 1}{r_j} = \prod_{j=1}^{k} \frac{(n + r_j - 1)!}{r_j!(n-1)!} = \frac{1}{((n-1)!)^{k}} \prod_{j=1}^{n} (r_j + t) \leq \frac{1}{((n-1)!)^{k}} \prod_{t=1}^{n-1} \left( \frac{M + t}{(n-1)!} \right)^{k}
\]

One can see that when \( M \) divided by \( k \) it hold that

\[
\phi \left( \frac{M}{k}, \ldots, \frac{M}{k} \right)^{k} = \frac{1}{((n-1)!)^{k}} \prod_{t=1}^{n-1} f_t = \frac{1}{((n-1)!)^{k}} \prod_{t=1}^{n-1} \left( \frac{M}{k} + t \right)^{k} = \left( \prod_{t=1}^{n-1} \left( \frac{M}{k} + t \right) \right)^{k}
\]

hence the name of this lemma.

\[\Box\]

Lemma 3. \( \binom{n}{k} \leq \left( \frac{2e(n+k)}{n} \right)^{n} \)

Proof. : by using the inequality \( \binom{n}{k} \leq \left( \frac{en}{k} \right)^{k} \) we have

\[
\binom{n}{k} = \binom{n+k-1}{n-1} \leq \left( \frac{2e(n+k)}{n} \right)^{n}
\]

\[\Box\]

B Lower bounds on the separation rank

B.1 preliminaries

B.1.1 Tensors and their matricization

We begin by laying out basic concepts in tensor theory required for the upcoming analysis. The core concept of a tensor may be thought of as a multi-dimensional array. The order of a tensor is defined to be the number of indexing entries in the array, referred to as modes. The dimension of a tensor in a particular mode is defined as the number of values taken by the index in that mode. If \( A \) is a tensor of order \( N \) and dimension \( M_i \) in each mode \( i \in [N] \), its entries are denoted \( A_{d_1, \ldots, d_N} \), where the index in each mode takes values \( d_i \in [M_i] \).

We will make use of the concept of the matricization of \( A \) w.r.t. the balanced partition \((I, J)\), denoted \( [A]_{I,J} \in \mathbb{R}^{M_i/N/2 \times M_j/N/2} \), which is essentially the arrangement of the tensor elements as a matrix.
whose rows correspond to \( I \) and columns to \( J \). Suppose \( A \in \mathbb{R}^{M \times \cdots \times M} \) is a tensor of order \( N \), and let \((I, J)\) be a balanced partition of \([N]\), \(i.e.\) \( I \) and \( J \) are disjoint subsets of \([N]\) whose union gives \([N]\). The matricization of \( A \) w.r.t. the partition \((I, J)\), denoted \( [A]_{I,J} \), is the \( M^{N/2} \)-by-\( M^{N/2} \) matrix holding the entries of \( A \) such that \( A_{d_1,\ldots,d_N} \) is placed in row index \( 1 + \sum_{\ell=1}^{N/2} (d_{i\ell} - 1)M^{N/2-\ell} \) and column index \( 1 + \sum_{\ell=1}^{N/2} (d_{j\ell} - 1)M^{N/2-\ell} \).

### B.1.2 Grid tensors provide lower bounds for the separation rank

We now present the concept of grid tensors, which are a form of function discretization \cite{Hackbusch12}. Essentially, the function is evaluated for a set of points on an exponentially large grid in the input space and the outcomes are stored in a tensor. Formally, fixing a set of \textit{template vectors} \( x^{(1)}, \ldots, x^{(M)} \in \mathbb{R}^{d_x} \), the points on the grid are the set \( \{(x^{(d_1)}, \ldots, x^{(d_N)})\}^{M}_{d_1,\ldots,d_N=1} \). Given a function \( y(x^{1}, \ldots, x^{N}) \), the set of its values on the grid arranged in the form of a tensor are called the grid tensor induced by \( y \), denoted \( A(y)_{d_1,\ldots,d_N} \equiv y(x^{(d_1)}, \ldots, x^{(d_N)}) \).

The following claim establishes a fundamental relation between a function’s separation rank (intuitively defined in section \ref{sec:sep-rank}), see formal definition in section \ref{sec:appendix} of this supplementary) and the rank of the matrix obtained by the corresponding grid tensor matricization. This relation, which holds for all functions, is formulated below for functions realized by self-attention networks:

**Claim 2.** For \( p \in [d_x] \), let \( y_p^{i, L, d_x, H, \Theta} \) be the scalar function computing the \( p \)th entry of an output vector at position \( i \in [N] \) of the depth-\( L \) self-attention network with embedding dimension \( d_x \) and \( H \) attention heads per layer, defined in eqs. \ref{eq:head} and \ref{eq:ffn}. Then, for any integer \( M \) and any set of template vectors \( x^{(1)}, \ldots, x^{(M)} \in \mathbb{R}^{d_x} \), it holds that:

\[
\text{sep}_{(I,J)}(y_p^{i, L, d_x, H, \Theta}) \geq \text{rank} \left( [A(y_p^{i, L, d_x, H, \Theta})]_{I,J} \right),
\]

where \( A(y_p^{i, L, d_x, H, \Theta}) \) is the grid tensor of \( y_p^{i, L, d_x, H, \Theta} \) with respect to the above template vectors.

**Proof.** If \( \text{sep}_{(I,J)}(y_p^{i, L, d_x, H, \Theta}) = \infty \) then the inequality is trivially satisfied. Otherwise, assume that \( \text{sep}_{(I,J)}(y_p^{i, L, d_x, H, \Theta}) = K \in \mathbb{N} \), and let \( \{g^I_\nu, g^J_\nu\}_{\nu=1}^K \) be the functions of the respective decomposition to a sum of separable functions, \(i.e.\) the following holds:

\[
y_p^{i, L, d_x, H, \Theta}(x^{1}, \ldots, x^{N}) = \sum_{\nu=1}^K g^I_\nu(x^j : j \in I) \cdot g^J_\nu(x^j : j \in J).
\]

Then, by definition of the grid tensor, for any template vectors \( x^{(1)}, \ldots, x^{(M)} \in \mathbb{R}^{d_x} \) the following equality holds:

\[
A(y_p^{i, L, d_x, H, \Theta})_{d_1,\ldots,d_N} = \sum_{\nu=1}^K g^I_\nu(x^{(d_j)} : j \in I) \cdot g^J_\nu(x^{(d_j)} : j \in J)
\]

\[
\equiv \sum_{\nu=1}^K V^\nu_{d_j : j \in I} U^\nu_{d_j : j \in J},
\]

where \( V^\nu \) and \( U^\nu \) are the tensors holding the values of \( g^I_\nu \) and \( g^J_\nu \), respectively, at the points defined by the template vectors. Under the matricization according to the \((I, J)\) partition, it holds that \( [V^\nu]_{I,J} \) and \( [U^\nu]_{I,J} \) are column and row vectors, respectively, which we denote by \( v_\nu \) and \( u_\nu \). It follows that the matricization of the grid tensor is given by:

\[
[A(y_p^{i, L, d_x, H, \Theta})]_{I,J} = \sum_{\nu=1}^K v_\nu u_\nu^T,
\]

which means that \( \text{rank} \left( [A(y_p^{i, L, d_x, H, \Theta})]_{I,J} \right) \leq K = \text{sep}_{(I,J)}(y_p^{i, L, d_x, H, \Theta}) \).
B.1.3 Method for bounding the grid tensor’s rank

Claim 2 assures us that the separation rank of the function realized by a self-attention network is lower bounded by the rank of the matrix obtained by the corresponding grid tensor matricization, for any choice of template vectors. Specifically:

$$\text{sep}_{(I,J)} (y_p^{i,L,d_x,H,\Theta}) \geq \text{rank} (\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J}).$$

Thus, proving that $$\text{rank} (\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J})$$ is higher than the lower bounds stated in theorems 1 and 2 for all of the values of the parameters $$\Theta$$ but a set of Lebesgue measure zero, would satisfy the theorems.

We note that since the network’s operation is polynomial in $$\Theta$$, then the entries of the grid tensor are also polynomial. Sharir et al. [2016] prove a claim regarding the prevalence of the maximal matrix rank for matrices whose entries are polynomial functions. Essentially, they show that it suffices to find a single configuration of the parameters, denoted $$\theta \in \mathbb{R}^K$$ (where $$K$$ is the number of scalar parameters), for which the resultant matrix is of rank $$r$$, in order to show the rank is at least $$r$$ for all configurations in $$\mathbb{R}^K$$ but a set of measure zero in $$\mathbb{R}^K$$. For simplicity of the proof we will find a single configuration $$\theta \in \mathbb{C}^K$$ for which the resultant matrix is of the required rank. We therefore modify the original claim to fit this setting, still proving the rank is lower bounded for all configurations in $$\mathbb{R}^K$$ but a set of measure zero in $$\mathbb{R}^K$$:

**Claim 3.** Let $$M, N, K \in \mathbb{N}, 1 \leq r \leq \min\{M, N\}$$ and an $$M \times N$$ matrix $$A$$ where each entry is a polynomial mapping $$A_{ij}$$ over $$K$$ variables for every $$i \in [M]$$ and $$j \in [N]$$, if there exists a point $$\theta \in \mathbb{R}^K$$, where $$F$$ is either $$\mathbb{R}$$ or $$\mathbb{C}$$, s.t. $$\text{rank}(A(\theta)) \geq r$$, then the set $$\{\theta \in \mathbb{R}^K : \text{rank}(A(\theta)) < r\}$$ has zero measure (w.r.t. the Lebesgue measure over $$\mathbb{R}^K$$).

**Proof.** (based on a proof in Sharir et al. [2016]) Recall that $$\text{rank}(A(\theta)) \geq r$$ iff there exists a non-zero $$r \times r$$ minor of $$A(\theta)$$. Note that a minor of $$A(\theta)$$ is polynomial in the entries of $$A(\theta)$$, and so it is polynomial in $$\theta$$ as well. Let $$c = \binom{M}{r} \cdot \binom{N}{r}$$ be the number of minors in $$A$$, denote the minors by $$\{f_i(\theta)\}_{i=1}^c$$, and define a new polynomial function $$f(\theta) = \sum_{i=1}^c f_i(\theta)^2$$. It thus holds that $$f(\theta) = 0$$ iff for all $$i \in [c]$$ it holds that $$f_i(\theta) = 0$$, i.e. $$f(\theta) = 0$$ iff rank $$(A(\theta)) < r$$.

Now, $$f(\theta)$$ is a polynomial in the entries of $$\theta$$, and so it either vanishes on a set of zero measure in $$\mathbb{R}^K$$, or it is the zero polynomial (see Caron and Traynor [2005] for proof). Since we assumed that there exists $$\theta \in \mathbb{R}^K$$ s.t. $$\text{rank}(A(\theta)) \geq r$$, the latter option is not possible. 

B.2 Proof of the lower bounds in theorems 1 and 2

In this section, we show there exists an assignment for the weight matrices of a self-attention network, along with a specific choice of template vectors, for which $$\text{rank} (\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J})$$ surpasses the lower bounds stated in theorems 1 and 2 for the appropriate depth to width ratios. In accordance with Claim 3 the lower bounds in the theorems will follow since such an assignment implies this rank is achieved for all configurations of the self-attention network weights but a set of Lebesgue measure zero.

**Proof.** (of lower bounds in theorems 1 and 2).

Relying on Claim 2 we will bound the separation rank from below via the rank of the matricization w.r.t. a partition $$(I,J)$$ of a grid tensor induced by $$y_p^{i,L,d_x,H,\Theta}$$, computed by any set of template vectors: $$\text{sep}_{(I,J)} (y_p^{i,L,d_x,H,\Theta}) \geq \text{rank} (\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J})$$. Relying on Claim 3 we ensure that the rank of $$\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J}$$ is above a certain value almost everywhere by finding an assignment of the network parameters for which it achieves this value.

Lemma 4 assures us that for any matrix $$V \in \mathbb{R}^{M/2 \times (d_x - H)/2}$$ with $$l^2$$ normalized rows, there exists a choice of $$M + 1$$ template vectors $$x^{(1)}, \ldots, x^{(M+1)} \in \mathbb{R}^{d_x}$$, as well as an assignment to the self-attention network weights for which:

$$\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J} = \text{Const.} \cdot (VV^T)^{\otimes (L-2)},$$

where $$\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J}$$ is a sub-matrix of the grid tensor matricization $$\mathcal{A}(y_p^{i,L,d_x,H,\Theta})_{I,J}$$ of size $$M/2 \times M/2$$ and $$\otimes$$ represents the Hadamard power operation, i.e., $$(A^{\otimes k})_{ij} = A_{ij}^k$$. Since proving
the existence of a sub-matrix of a certain rank lower-bounds the rank of the full matrix by this rank, it suffices to find a matrix $V$ such that rank $\left((VV^T)^{\otimes(3^{L-2})}\right)$ upholds the stated dependence.

Noting that the operation of raising a rank $r$ matrix to the Hadamard power of $p$ results in a matrix upper bounded by $\binom{d}{r}^p$ (see proof in [Amini et al., 2012] for example) with the notation of the multiset coefficient $\binom{q}{k} := \binom{n+k-1}{k}$, and that the rank of $VV^T$ is upper bounded by $(d_1-H)/2$, we choose the dimension $M/2 = (\binom{d_1-H}{3L-2})/2$ to facilitate the rank increase.

For this choice, observe that it suffices to prove that the sub-matrix $\binom{q}{k}$ is fully ranked in order to satisfy the theorems. This follows by using the identity $\binom{n+k-1}{k} \geq \binom{\binom{n+k-1}{k}}{k}$. We have:

$\binom{(n+k-1)}{k} = \binom{(n+k-1)}{n-1} \geq \max \left\{ \left( \frac{n-1}{k} + 1 \right)^k, \left( \frac{k}{n+1} + 1 \right)^{n-1} \right\}

$and accordingly:

$\left(\frac{(d_1-H)/2}{3L-2}\right) \geq \max \left\{ \left( \frac{(d_1-H)/2 - 1}{3L-2} + 1 \right)^{3L-2}, \left( \frac{3L-2}{(d_1-H)/2 - 1} + 1 \right)^{(d_1-H)/2-1} \right\}$

and the log of this bounds the expressions in the theorems’ lower bounds, where for each regime the tighter lower bound is used.

Defining for brevity $d := (d_1-H)/2$ and $\lambda := 3L-2$, it remains only to find a specific matrix $V \in \mathbb{R}^{(\lambda)} \times d$ with $\ell^2$ normalized rows such that the operation of taking the rank $d$ matrix $VV^T$ to the Hadamard power of $\lambda$ would result in a fully ranked matrix. We will provide such a matrix, and prove for it that:

$$(VV^T)^{\otimes\lambda} = \sum_{k=1}^{\binom{d}{\lambda}} a^{(k)} \otimes b^{(k)}$$

(17)

for $\{a^{(k)}\}_{k=1}^{\binom{d}{\lambda}}$ and $\{b^{(k)}\}_{k=1}^{\binom{d}{\lambda}}$ which are two sets of linearly independent vectors.

For $\alpha, \beta \in \left(\binom{d}{\lambda}\right)$, observing an entry of $(VV^T)^{\otimes\lambda}$:

$$\left((VV^T)^{\otimes\lambda}\right)_{\alpha\beta} = (VV^T)^{\lambda}_{\alpha\beta} = \left(\sum_{r=1}^{d} \psi_r^{(\alpha)} \psi_r^{(\beta)}\right)^{\lambda} = \sum_{k_1,\ldots,k_d = \lambda}^{d} \left(\prod_{r=1}^{d} \psi_r^{(\alpha)} \psi_r^{(\beta)}\right)^k$$

(18)

$$\left(\prod_{r=1}^{d} \psi_r^{(\alpha)} \psi_r^{(\beta)}\right)^k$$

(19)

where the first equality follows from the definition of the Hadamard power, in the section we denoted $\psi_r^{(\alpha)}$, $\psi_r^{(\beta)}$ as the $r$th entries in rows $\alpha$ and $\beta$ of $V$, and in the second line we expanded the power with the multinomial identity. Identifying the form of eq. [19] with the schematic form of eq. [17] it remains to find a specific matrix $V \in \mathbb{R}^{(\lambda)} \times d$ with $\ell^2$ normalized rows for which the size $\left(\binom{d}{\lambda}\right)$ set $\{a^{(k_1,\ldots,k_d)}\}_{k_1,\ldots,k_d = \lambda}$ is linearly independent, where $a^{(k_1,\ldots,k_d)} = \prod_{r=1}^{d} \psi_r^{(\alpha)} \psi_r^{(\beta)}$.

We show this is the case for $V$ in which the rows are each associated with one of $\left(\binom{d}{\lambda}\right)$ configurations of distributing $d$ integer numbers that sum up to $\lambda$, i.e., in which each row is associated with specific $\{q_r^{(\alpha)}, q_r^{(\beta)} \geq 0, \sum_{r=1}^{d} q_r^{(\alpha)} = \lambda\}$. Explicitly, we take the rows $\psi_r^{(\alpha)}$ to be:

$$\forall r \in [d] : \psi_r^{(\alpha)} = \Omega r / \sqrt{\sum_{r'=1}^{d} \Omega r'^{2}}.$$
Given this \( V \), each vector in the above defined set \( \{ a^{(k_1, \ldots, k_d)} \}_{k_1 + \cdots + k_d = \lambda} \) is equal to:

\[
a^{k_1, \ldots, k_d} = \prod_{r=1}^{d} a^{(k_r)} = \prod_{r=1}^{d} \left( \frac{\Omega q_r}{\sqrt{\sum_{r'=1}^{d} \Omega q_{r'}}} \right) = \frac{\prod_{r=1}^{d} \Omega q_r}{\prod_{r=1}^{d} \left( \sum_{r'=1}^{d} \Omega q_{r'} \right)^{\frac{1}{2}}} = \left( \sum_{r'=1}^{d} \Omega q_{r'} \right)^{-\frac{1}{2}} \cdot \left[ \Omega \prod_{r=1}^{d} q_r \right]
\]

Observing that the factor attained from the normalization depends only on the rows and doesn’t vary with the different vectors labeled by \((k_1, \ldots, k_d)\), we note it does not affect their linear dependence (amounts to a multiplication by a diagonal matrix with non-zero entries on the diagonal - does not affect the rank).

We prove that the set \( \{ a^{(k_1, \ldots, k_d)} \}_{k_1 + \cdots + k_d = \lambda} \) for \( a^{(k_1, \ldots, k_d)} = \Omega \prod_{r=1}^{d} q_r \) is linearly independent by arranging it as the columns of the matrix \( A \in \mathbb{R}^{\binom{d}{\lambda} \times \binom{d}{\lambda}} \), and showing that \( A \) is fully ranked.

Since the elements of \( A \) are polynomial in \( \Omega \), then as lemma [5] shows, it is sufficient to show that there exists a single contributor to the determinant of \( A \) that has the highest degree of \( \Omega \) in order to ensure that the matrix is fully ranked for all values of \( \Omega \) but a finite set, so \( \Omega \) should simply be chosen to be any number that is outside of this set. Observing the summands of the determinant, i.e. \( \Omega \prod_{r=1}^{d} q_r \), where \( \sigma \) is a permutation on the columns of \( A \), lemma [6] assures us the existence of a strictly maximal contributor, satisfying the conditions of lemma [5], thus the set \( \{ a^{(k_1, \ldots, k_d)} \}_{k_1 + \cdots + k_d = \lambda} \) is linearly independent, and the lower bounds in the theorems follow.  

### B.3 Technical lemmas

The following lemma details the assignment of the self-attention network weights and the choice of template vectors which help us establish theorem [1].

**Lemma 4.** For any balanced partition of \([N]\), denoted \((I, J)\), for any even \( M \), and for any matrix \( V \in \mathbb{R}^{M/2 \times (d_x - M/2)} \) with rows that are \( \ell^2 \) normalized, there exists a choice of \( M + 1 \) template vectors \( x^{(1)} \), \ldots, \( x^{(M+1)} \) in \( \mathbb{R}^{d_x} \), as well as an assignment to the self-attention network weights, for which:

\[
[ A(y_p^{1, L, d_x, H, \Theta}) ]_{I, J} = \text{Const} \cdot (VV^T)^{\otimes 3L-2}, \tag{20}
\]

where \([ A(y_p^{1, L, d_x, H, \Theta}) ]_{I, J} \) is a sub-matrix of the grid tensor matricization \([ A(y_p^{1, L, d_x, H, \Theta}) ]_{I, J} \) of size \( M/2 \times M/2 \) and \( \otimes \) represents the Hadamard power operation, i.e., \((A^{\otimes k})_{ij} = A_{ij}^k\).

**Proof.** We present below a choice of weights and template vectors that yields the stated form for a sub-matrix of \([ A(y_p^{1, L, d_x, H, \Theta}) ]_{I, J} \). Subsequently we will plug these values into the self attention operation stated in eq.\([3]\) and prove that this form follows.

Though the proof has many technical details, it has 3 essential parts. We first choose the weights of the first layer so that the outputs in all locations are the same and equal to a summation of the input vectors. Because the weight matrices are not \( d_x \times d_x \) but are decomposed through the attention dimension \( d_x \times d_x \) or \( d_x \times d_y \), then we divide the coordinates of the \( d_x \)-dimensional vectors into contiguous segments of length \( d_x \), and set the weights to either project these segments to the \( d_x \)-dimensional space or invert this mapping with added zero-padding. For the second part, we set the key and query matrices to use the same “projections” we used in the first layer to compute inner-products between each segment, while setting the value and output matrices to preserve each head’s segment (with zero-padded coordinates). For the remainder of the network’s layers, we use the previous step to compute increasingly larger powers of the norm of the vector computed in the first layer, by reconstructing the squared-norm from the inner products of each segment. The template vectors (and parameters) are chosen such that the square of this norm will be equal to \( VV^T \).
The assignment to the network weights:

\[
W_{i,j}^{V,1,h} = \frac{1}{N} \cdot \begin{cases} 
1_{i=j-d_a(h-1)} & d_a(h-1) < j \leq d_a(h-1) + \frac{d_a-1}{2} \\
1 \cdot 1_{i=j-d_a(h-1)-\frac{d_a-1}{2}} & 0 < i \leq \frac{d_a-1}{2} \\
-1_{i=j-d_a(h-1)} & d_a(h-1) + \frac{d_a-1}{2} < j \leq d_a h - 1 \\
-i \cdot 1_{i=j-d_a(h-1)-\frac{d_a-1}{2}} & 0 < i \leq \frac{d_a-1}{2} \\
0 & d_a(h-1) < j \leq d_a(h-1) + \frac{d_a-1}{2} \\
1 & d_a(h-1) + \frac{d_a-1}{2} < j \leq d_a h - 1 \\
N & \frac{d_a-1}{2} < i \leq d_a - 1 \\
1 & j = d_a h, \frac{d_a-1}{2} < i \leq d_a \\
0 & \text{Otherwise}
\end{cases}
\]

\[
W_{i,j}^{O,l,h} = \begin{cases} 
1_{j-i-d_a(h-1)} & d_a(h-1) < i \leq d_a h \\
0 & \text{Otherwise}
\end{cases}
\]

\[
W_{i,j}^{L,h} = i \cdot 1_{j=d_a}
\]

\[
W_{i,j}^{V,1,h} = W_{i,j}^{Q,1,h} = 1_{i=1 \land j=d_a}
\]

\[
W_{i,j}^{V,2,h} = W_{i,j}^{Q,2,h} = \begin{cases} 
1_{i=j-d_a(h-1)} & d_a(h-1) < j \leq d_a(h-1) + \frac{d_a-1}{2} \\
0 & \text{Otherwise}
\end{cases}
\]

\[
W_{i,j}^{K,l,h} = W_{i,j}^{Q,l,h} = \begin{cases} 
1 & i = 1 \land j \mod d_a \neq 0 \\
0 & \text{Otherwise}
\end{cases}
\]

In the above, we denoted the complex root of \(-1\) as \(i\), to differentiate it from the index \(i\). The choice of template vectors:

\[
x^{(i)}_j = \begin{cases} 
V_{i,\phi(j)} & i \leq M/2 \land (j - 1) \mod d_a < \frac{d_a-1}{2} \\
V_{i-M/2+1,\phi(j-\frac{d_a-1}{2})} & \frac{M}{2} < i \leq M \land \frac{d_a-1}{2} \leq (j - 1) \mod d_a < d_a - 1 \\
1 & (j - 1) \mod d_a = d_a - 1 \\
0 & \text{Otherwise}
\end{cases}
\]

where \(\phi(j) \equiv \lfloor j-1/d_a \rfloor \cdot (d_a - 1) + (j - 1 \mod d_a) + 1\).

W.l.o.g. we can assume that \(I = \{1, \ldots, N/2\}, J = \{N/2 + 1, \ldots, N\}\). We examine the sub-matrix defined by the following indices:

\[
\tilde{I} = \{(i_1, \ldots, i_{N/2}) : 1 \leq i_1 \leq M/2 \land \forall k > 1, i_k = M + 1\}
\]

\[
\tilde{J} = \{(j_1, \ldots, j_{N/2}) : M/2 < j_1 \leq M \land \forall k > 1, j_k = M + 1\}
\]
With all of the above in place, we are ready to prove that the resulting sub-matrix has the form of eq. [20]. We begin with the output of the first self-attention layer:

\[
y^{(1,i)}(x^{(d_1)}, \ldots, x^{(d_N)})_k = \sum_{j=1}^{N} \sum_{h=1}^{H} \left(W^{Q,1,h}x^{(d_1)}, W^{K,1,h}x^{(d_j)}\right) (W^{O,1,h}W^{V,1,h}x^{(d_j)})_k
\]

\[
= \sum_{j=1}^{N} \sum_{h=1}^{H} x^{(d_j)}_{d_a} \cdot x^{(d_j)}_{d_a} (W^{Q,1,h}W^{V,1,h}x^{(d_j)})_k
\]

\[
= 2 \left(\sum_{h=1}^{H} W^{Q,1,h}W^{V,1,h} \right) (x^{(i_1)} + x^{(j_1)} + (N-2)x^{(M+1)})
\]

where (1) is because \(W^{Q,1,h} = W^{K,1,h}\) are matrices that are zero everywhere except for entry \((1, d_a)\), (2) because when summing over the locations, only \(i_1\) and \(j_1\) are different from \(M+1\), and (3) because applying the value and output matrices on any template vector \(u\) results in:

\[
(W^{O,1,h}W^{V,1,h}u)_k = \sum_{\alpha=1}^{d_a} W^{Q,1,h}_{k,\alpha} \sum_{\beta=1}^{d_a} W^{V,1,h}_{\alpha,\beta} u_{\beta}
\]

\[
= d_a \sum_{\alpha=1}^{d_a} W^{Q,1,h}_{k,\alpha} \left\{\left[u_{d_a,h+\alpha-1} + i \cdot u_{d_a,h+\alpha-1} + \frac{d_a-1}{2}\right] \alpha \leq \frac{d_a-1}{2} \right. \\
\left. \frac{1}{N} \cdot u_{d_a,h+\alpha-1} - i \cdot u_{d_a,h+\alpha-1} + \frac{d_a-1}{2}\right\] \quad \frac{d_a-1}{2} \leq \alpha < d_a
\]

\[
= \hat{u}_{l((k-1) \mod d_a) + 1} \quad d_a(h-1) \leq k < d_a h
\]

At this point, notice that for any \(i \in [N]\), \(y^{(1,i)}\) is the same, and we denote it with \(v\). Note that it is a vector composed of \(H d_a\)-dimensional sub-vectors, each composed of a \(\frac{d_a-1}{2}\)-dimensional sub-vector and its complement in the next \(\frac{d_a-1}{2}\) indices, followed by a fixed value of 1.

Next, we will compute the result of the second layer, where we use the fact that every position is equal to \(v\) to drop the reference to a specific location \(i\), i.e., \(y^{(1,i)} = y^{(1)}\):

\[
y^{(2)} = N \sum_{h=1}^{H} \left(W^{Q,2,h}v, W^{K,2,h}v\right) (W^{O,2,h}W^{V,2,h}v)_k
\]

\[
= N \sum_{h=1}^{H} \left(\hat{v}^{(h)}, \hat{v}^{(h)}\right) v^{(h)},
\]

where we used the notation \(v^{(h)}_k = v_k \cdot 1_{d_a(h-1) \leq k < d_a h}\), i.e., a vector that is equal to \(v_k\) on the \(h\)th \(d_a\)-dimensional segment and otherwise filled with zeros, as well as the notation \(\hat{v}^{(h)}_k = v_k \cdot 1_{d_a(h-1) \leq k < d_a(h-1) + \frac{d_a-1}{2}}\). The last equality is because all matrices in this layer essentially just project the \(d_a\)-dimensional sub-vector of \(v\) for its respective head \(h\).
For the third layer we get:

\[
y^{(3)} = N \sum_{h=1}^{H} \left< W^{Q,2,h} y^{(2)}, W^{K,2,h} y^{(2)} \right> (W^{O,2,h} W^{V,2,h} y^{(2)})
\]  

(32)

\[
\frac{1}{N} \sum_{h=1}^{H} \sum_{r \mod d_a \neq 0} y^{(2)}_{y_{rmod_h}}^2 y^{(2),h}
\]  

(33)

\[
2 \sum_{h=1}^{H} \left< N \sum_{h'=1}^{H} \langle \tilde{v}^{(h')}, \tilde{v}^{(h')} \rangle \rangle \right> 2 N \langle \tilde{v}^{(h)} , \tilde{v}^{(h)} \rangle v^{(h)}
\]  

(34)

\[
3 N^4 \| \tilde{v} \|_2^2 \sum_{h=1}^{H} \langle \tilde{v}^{(h')}, \tilde{v}^{(h')} \rangle v^{(h)}
\]  

(35)

where we define \( \tilde{v} = \sum_{h=1}^{H} \tilde{v}^{(h)} \). Equality (1) is because in both \( W^{K,3,h} \) and \( W^{Q,3,h} \) on the first row is non-zero, and it has ones everywhere except in coordinates that are multiples of \( d_a \), resulting in summing over all of these non-zero elements of the vector \( y^{(2)} \). Equality (2) is because in the vector \( v^{(h)} \) every entry has a corresponding entry equal to its complement, which upon summation is equal to one, leaving only the \( \langle \tilde{v}^{(h')}, \tilde{v}^{(h')} \rangle \) coefficients of the vector \( y^{(2)} \). Equality (3) is because

\[
\| \tilde{v} \|^2 = \langle \tilde{v}, \tilde{v} \rangle = \sum_{h_1, h_2} \langle \tilde{v}^{(h_1)}, \tilde{v}^{(h_2)} \rangle = \sum_{h=1}^{H} \langle \tilde{v}^{(h)}, \tilde{v}^{(h)} \rangle
\]  

(36)

where the last equality stems from the fact that every \( \tilde{v}^{(h)} \) is non-zero on a different segment of its \( d_a \) coordinates.

For any subsequent layer \( l < L \) we use the same set of parameters, and since the input of each preceding layer has the same form of \( y^{(l)} = N^{\alpha_l} \| \tilde{v} \|^2^{2\beta_l} \sum_{h=1}^{H} \langle \tilde{v}^{(h)}, \tilde{v}^{(h)} \rangle v^{(h)} \), then we can just compute its recurrence relation:

\[
y^{(l+1)} = N^{\alpha_l} \| \tilde{v} \|^2^{2\beta_l} \sum_{h=1}^{H} \langle \tilde{v}^{(h)}, \tilde{v}^{(h)} \rangle \right> \sum_{h'=1}^{H} \langle \tilde{v}^{(h')}, \tilde{v}^{(h')} \rangle \rangle \right> 2 N^{\alpha_l} \| \tilde{v} \|^2^{2\beta_l} \langle \tilde{v}^{(h)} , \tilde{v}^{(h)} \rangle v^{(h)}
\]  

(37)

\[
N^{1+3\alpha_l} \| \tilde{v} \|^6^{2\beta_l} \sum_{h=1}^{H} \left( \sum_{h'=1}^{H} \langle \tilde{v}^{(h')}, \tilde{v}^{(h')} \rangle \right) \right> \langle \tilde{v}^{(h)}, \tilde{v}^{(h)} \rangle v^{(h)}
\]  

(38)

\[
N^{3\alpha_l+1} \| \tilde{v} \|^2 \langle \tilde{v}^{(h)}, \tilde{v}^{(h)} \rangle v^{(h)}
\]  

(39)

\[
\Rightarrow \alpha_{l+1} = 3\alpha_l + 1, \beta_{l+1} = 3\beta_l + 2
\]  

(40)

Using the initial conditions of \( \alpha_3 = 4 \) and \( \beta_3 = 2 \), we get that \( \alpha_l = \frac{3^{l-1}-1}{2}, \beta_l = 3^{l-2} - 1 \). For the \( L \)th layer, the only difference is that \( W^{V,L,h} \) is defined such that it returns a 1-hot vector that picks the \( d_a \)’th element of the previous step. Putting it all together we get:

\[
y^{(L)} = N^{\frac{3^{L-1}-1}{2}} \| \tilde{v} \|^{2-2^{L-2}} \sum_{h=1}^{H} \langle \tilde{v}^{(h)}, \tilde{v}^{(h)} \rangle i \cdot v^{(h)}_{d_a} 
\]  

(41)

\[
y^{(L)} = N^{\frac{3^{L-1}-1}{2}} \| \tilde{v} \|^{2-2^{L-2}} 
\]  

(42)
Finally, we can evaluate $\|\bar{v}\|^2$:

$$\|\bar{v}\|^2 = \sum_{k=1}^{d_x} \hat{v}_k^2 = \sum_{h=1}^{d_x - 1/2} \sum_{i=1}^{H} \left( \sum_{k=1}^{\text{normalized}} (V_{i1,(d_a-1)\cdot(h-1)+k} + i \cdot V_{j1,(d_a-1)\cdot(h-1)+k})^2 \right)$$

which concludes the proof.

Next, we show two lemmas that aid in the proof of the lower bound. We first quote an identity by which for a matrix with entries that are polynomials in $x$, if a single contributor to the determinant has the highest degree of $x$, then the matrix is fully ranked for all values of $x$ but a finite set.

**Lemma 5.** (from Levine et al. [2018a].) Let $A \in \mathbb{R}^{N \times N}$ be a matrix whose entries are polynomials in $x \in \mathbb{R}$. In this case, its determinant may be written as $\det(A) = \sum_{\sigma \in S_N} sgn(\sigma)p_\sigma(x)$, where $S_N$ is the symmetric group on $N$ elements and $p_\sigma(x)$ are polynomials defined by $p_\sigma(x) = \prod_{i=1}^{N} A_{i\sigma(i)}(x)$, $\forall \sigma \in S_N$. Additionally, there exist $\bar{x}$ such that $\deg(p_\bar{x}(x)) > \deg(p_\sigma(x)) \forall \sigma \neq \bar{x}$. Then, for all values of $x$ but a finite set, $A$ is fully ranked.

**Proof.** We show that in this case $\det(A)$, which is a polynomial in $x$ by its definition, is not the zero polynomial. Accordingly, $\det(A) \neq 0$ for all values of $x$ but a finite set. Denoting $t = \deg(p_\sigma(x))$, since $t > \deg(p_\sigma(x)) \forall \sigma \neq \bar{x}$, a monomial of the form $c \cdot x^t$, $c \in \mathbb{R} \setminus \{0\}$ exists in $p_\sigma(x)$ and doesn't exist in any $p_\bar{x}(x)$, $\sigma \neq \bar{x}$. This implies that $\det(A)$ is not the zero polynomial, since its leading term has a non-vanishing coefficient $sgn(\bar{x}) \cdot c \neq 0$, and the lemma follows from the basic identity: $\det(A) \neq 0 \iff A$ is fully ranked.

The following quoted lemma, establishes a relation referred to as the vector rearrangement inequality, which helped us ensure that our matrix of interest upholds the conditions of lemma 5 and is thus fully ranked.

**Lemma 6.** (from Levine et al. [2018a]). Let $\{v^{(i)}\}_{i=1}^{N}$ be a set of $N$ different vectors in $\mathbb{R}^R$ such that $\forall i \in [N]$, $j \in [R] : v_{ij}^{(i)} \geq 0$. Then, for all $\sigma \in S_N$ such that $\sigma \neq \mathbb{I}_N$, where $S_N$ is the symmetric group on $N$, it holds that:

$$\sum_{i=1}^{N} \langle v^{(i)}, v^{(\sigma(i))} \rangle \leq \sum_{i=1}^{N} \|v^{(i)}\|^2$$

**Proof.** We rely on theorem 368 in Hardy et al. [1952], which implies that for a set of non-negative numbers $\{a^{(1)}, \ldots, a^{(N)}\}$ the following holds for all $\sigma \in S_N$:

$$\sum_{i=1}^{N} a^{(i)} a^{(\sigma(i))} \leq \sum_{i=1}^{N} (a^{(i)})^2,$$

with equality obtained only for $\sigma$ which upholds $\sigma(i) = j \iff a^{(i)} = a^{(j)}$. The above relation, referred to as the rearrangement inequality, holds separately for each component $j \in [R]$ of the given vectors:

$$\sum_{i=1}^{N} v_{ij}^{(i)} v_{ij}^{(\sigma(i))} \leq \sum_{i=1}^{N} (v_{ij}^{(i)})^2.$$
We now prove that for all $\sigma \in S_N$ such that $\sigma \neq 1_N$, $\exists j \in [R]$ for which the above inequality is hard, i.e.: 
\[
\sum_{i=1}^{N} v_{j}^{(i)} v_{j}^{(\sigma(i))} < \sum_{i=1}^{N} (v_{j}^{(i)})^2.
\] (48)

By contradiction, assume that $\exists \tilde{\sigma} \neq 1_N$ for which $\forall j \in [R]$:
\[
\sum_{i=1}^{N} v_{j}^{(i)} v_{j}^{(\tilde{\sigma}(i))} \geq \sum_{i=1}^{N} (v_{j}^{(i)})^2.
\]

From the conditions of achieving equality in the rearrangement inequality defined in Equation (47), it holds that $\forall j \in [R]: v_{j}^{(\tilde{\sigma}(i))} = v_{j}^{(i)}$, trivially entailing: $v_{j}^{(\tilde{\sigma}(i))} = v_{j}^{(i)}$. Thus, $\tilde{\sigma} \neq 1_N$ would yield a contradiction to $\{v_{j}^{(i)}\}_{i=1}^{N}$ being a set of $N$ different vectors in $\mathbb{R}^R$. Finally, the hard inequality of the lemma for $\sigma \neq 1_N$ is implied from Equation (48):
\[
\sum_{i=1}^{N} \langle v_{i}^{(i)}, v_{i}^{(\sigma(i))} \rangle = \sum_{i=1}^{N} \left( \sum_{j=1}^{R} v_{j}^{(i)} v_{j}^{(\sigma(i))} \right) = \sum_{j=1}^{R} \left( \sum_{i=1}^{N} v_{j}^{(i)} v_{j}^{(\sigma(i))} \right) < \sum_{j=1}^{R} \left( \sum_{i=1}^{N} (v_{j}^{(i)})^2 \right) = \sum_{i=1}^{N} \left\| v_{i}^{(i)} \right\|^2.
\]

\[\square\]

### C Separation rank: Definition and identities

#### C.1 Formal definition of the separation rank

In this section we define the concept of separation rank for functions realized by real functions that take as input $X = (x_1, \ldots, x_N) \in (\mathbb{R}^{d_x})^N$. The separation rank serves as a measure of the correlations such functions induce between different sets of input patches, i.e. different subsets of the variable set $\{x_1, \ldots, x_N\}$.

Let $(I, J)$ be a partition of input indexes, i.e. $I$ and $J$ are disjoint subsets of $[N]$ whose union gives $[N]$. We may write $I = \{i_1, \ldots, i_{|I|}\}$ where $i_1 < \cdots < i_{|I|}$, and similarly $J = \{j_1, \ldots, j_{|J|}\}$ where $j_1 < \cdots < j_{|J|}$. For a function $h : (\mathbb{R}^{d_x})^N \rightarrow \mathbb{R}$, the separation rank w.r.t. the partition $(I, J)$ is defined as follows:

\[
\text{sep}(h; I, J) := \min \left\{ R \in \mathbb{N} \cup \{0\} : \exists g_1 \ldots g_R : (\mathbb{R}^{d_x})^{|I|} \rightarrow \mathbb{R}, g'_1 \ldots g'_R : (\mathbb{R}^{d_x})^{|J|} \rightarrow \mathbb{R} \text{ s.t.} \right.
\]

\[
h(x_1, \ldots, x_N) = \sum_{\nu=1}^{R} g_{\nu}(x_{i_{\nu}}, \ldots, x_{i_{\nu}(|I|)})g'_{\nu}(x_{j_{\nu}}, \ldots, x_{j_{\nu}(|J|)}) \}
\]

(49)

In words, it is the minimal number of summands that together give $h$, where each summand is separable w.r.t. $(I, J)$, i.e. is equal to a product of two functions – one that intakes only segments indexed by $I$, and another that intakes only segments indexed by $J$.

#### C.2 Proof of claim 1 on the separation rank symmetry

**Claim 4.** For any depth $L \geq 1$ input size $N > 1$ and output locations $i \in [N]$, $p \in [d_x]$ The separation rank w.r.t. balanced partitions, which obey $A \cup B = [N], |A|, |B| = N/2$, is invariant to the identity of the partition, i.e., $\forall A \cup B = [N], \bar{A} \cup \bar{B} = [N], \text{ s.t. } |A|, |B|, |\bar{A}|, |\bar{B}| = N/2$:

\[
\text{sep}(y_{p,L,d_x,H,\Theta}, A, B) = \text{sep}(y_{p,L,d_x,H,\Theta}, \bar{A}, \bar{B})
\]

(50)

**Proof.** We will denote $A = (a_1, \ldots, a_{\frac{N}{2}}), B = (b_1, \ldots, b_{\frac{N}{2}}), \bar{A} = (\bar{a}_1, \ldots, \bar{a}_{\frac{N}{2}}), \bar{B} = (\bar{b}_1, \ldots, \bar{b}_{\frac{N}{2}})$ and by $\pi \in S_N$ the unique permutation that satisfy

\[
\forall m \in \left[ \frac{N}{2} \right] \pi(a_m) = \bar{a}_m \land \pi(b_m) = \bar{b}_m
\]

\[\text{If } I = \emptyset \text{ or } J = \emptyset \text{ then by definition } \text{sep}(h; I, J) = 1 \text{ (unless } h \equiv 0, \text{ in which case } \text{sep}(h; I, J) = 0).\]
w.l.o.g we will assume that $a_1 = \tilde{a}_1 = i$.

Assuming that $\text{sep}(y; A, B) = R$, then there exist $g_1, \ldots, g_R, g'_1, \ldots, g'_R$ s.t.

$$\forall x^{(1)}, \ldots, x^{(N)} \in \mathbb{R}^{d_x} \exists y_p^{i, L, d_x, H, \Theta}(x^{(1)}, \ldots, x^{(N)}) = \sum_{v=1}^{R} g_v \left( x^{(a_1)}, \ldots, x^{\left(\frac{a}{2}\right)} \right) g'_v \left( x^{(b_1)}, \ldots, x^{\left(\frac{b+N}{2}\right)} \right)$$

$i = \pi(a_1) = a_1$ therefore the summations over $j_1, \ldots, j_N$ in Eq [11] implies that for any $x^{(1)}, \ldots, x^{(N)} \in \mathbb{R}^{d_x}$ we have

$$y_p^{i, L, d_x, H, \Theta}(x^{(1)}, \ldots, x^{(N)}) = y_p^{i, L, d_x, H, \Theta}(x^{(\pi(1))}, \ldots, x^{(\pi(N))})$$

And therefore

$$= \sum_{v=1}^{R} g_v \left( x^{(\pi(a_1))}, \ldots, x^{\left(\pi\left(\frac{a}{2}\right)\right)} \right) g'_v \left( x^{(\pi(b_1))}, \ldots, x^{\left(\pi\left(\frac{b+N}{2}\right)\right)} \right)$$

$$= \sum_{v=1}^{R} g_v \left( x^{(\tilde{a}_1)}, \ldots, x^{\left(\frac{\tilde{a}}{2}\right)} \right) g'_v \left( x^{(b_1)}, \ldots, x^{\left(\frac{b+N}{2}\right)} \right)$$

So we proved that

$$\text{sep}(y_p^{i, L, d_x, H, \Theta}; \tilde{A}, \tilde{B}) \leq \text{sep}(y_p^{i, L, d_x, H, \Theta}; A, B)$$

Finally by switching the roles of $\tilde{A}, \tilde{B}$ and $A, B$ we can get the inverse inequality so we conclude that

$$\text{sep}(y_p^{i, L, d_x, H, \Theta}; \tilde{A}, \tilde{B}) = \text{sep}(y_p^{i, L, d_x, H, \Theta}; A, B)$$

\[\square\]
Nadav Cohen and Amnon Shashua. Inductive bias of deep convolutional networks through pooling geometry. In 5th International Conference on Learning Representations (ICLR), 2017.

Nadav Cohen, Or Sharir, and Amnon Shashua. On the expressive power of deep learning: A tensor analysis. Conference On Learning Theory (COLT), 2016.

Jean-Baptiste Cordonnier, Andreas Loukas, and Martin Jaggi. On the relationship between self-attention and convolutional layers. arXiv preprint arXiv:1911.03584, 2019.

Amit Daniely. Depth separation for neural networks. arXiv preprint arXiv:1702.08489, 2017.

Alexandre de Brébisson and Pascal Vincent. A cheap linear attention mechanism with fast lookups and fixed-size representations. arXiv preprint arXiv:1609.05866, 2016.

Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. BERT: pre-training of deep bidirectional transformers for language understanding. In Jill Burstein, Christy Doran, and Thamar Solorio, editors, Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2019, Minneapolis, MN, USA, June 2-7, 2019, Volume 1 (Long and Short Papers), pages 4171–4186. Association for Computational Linguistics, 2019. doi: 10.18653/v1/n19-1423. URL https://doi.org/10.18653/v1/n19-1423

Ronen Eldan and Ohad Shamir. The power of depth for feedforward neural networks. In Conference on learning theory, pages 907–940, 2016.

Wolfgang Hackbusch. On the efficient evaluation of coalescence integrals in population balance models. Computing, 78(2):145–159, 2006.

Wolfgang Hackbusch. Tensor spaces and numerical tensor calculus, volume 42. Springer Science & Business Media, 2012.

Moritz Hardt and Tengyu Ma. Identity matters in deep learning. arXiv preprint arXiv:1611.04231, 2016.

G. H. Hardy, J. E. Littlewood, and G. Pólya. Inequalities. Cambridge university press, 1952.

Robert J Harrison, George I Fann, Takeshi Yanai, and Gregory Beylkin. Multiresolution quantum chemistry in multiresolution bases. In Computational Science-ICCS 2003, pages 103–110. Springer, 2003.

Kaiming He, Xiangyu Zhang, Shaoqing Ren, and Jian Sun. Deep residual learning for image recognition. In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition, pages 770–778, 2016.

K. Inoue. Expressive numbers of two or more hidden layer relu neural networks. In 2019 Seventh International Symposium on Computing and Networking Workshops (CANDARW), pages 129–135, 2019.

Sarthak Jain and Byron C. Wallace. Attention is not explanation. In Jill Burstein, Christy Doran, and Thamar Solorio, editors, Proceedings of the 2019 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, NAACL-HLT 2019, Minneapolis, MN, USA, June 2-7, 2019, Volume 1 (Long and Short Papers), pages 3543–3556. Association for Computational Linguistics, 2019. doi: 10.18653/v1/n19-1357. URL https://doi.org/10.18653/v1/n19-1357

Jared Kaplan, Sam McCandlish, Tom Henighan, Tom B Brown, Benjamin Chess, Rewon Child, Scott Gray, Alec Radford, Jeffrey Wu, and Dario Amodei. Scaling laws for neural language models. arXiv preprint arXiv:2001.08361, 2020.

Kenji Kawaguchi. Deep learning without poor local minima. In Advances in neural information processing systems, pages 586–594, 2016.

Valentin Khrulkov, Alexander Novikov, and Ivan Oseledets. Expressive power of recurrent neural networks. In 6th International Conference on Learning Representations (ICLR), 2018.

Zhenzhong Lan, Mingda Chen, Sebastian Goodman, Kevin Gimpel, Piyush Sharma, and Radu Soricut. Albert: A lite bert for self-supervised learning of language representations. arXiv preprint arXiv:1909.11942, 2019.

Yoav Levine, Or Sharir, Alon Ziv, and Amnon Shashua. Benefits of depth for long-term memory of recurrent networks. (ICLR 2018) International Conference on Learning Representations workshop, 2018a.

Yoav Levine, David Yakira, Nadav Cohen, and Amnon Shashua. Deep learning and quantum entanglement: Fundamental connections with implications to network design. In 6th International Conference on Learning Representations (ICLR), 2018b.
Yoav Levine, Or Sharir, Nadav Cohen, and Amnon Shashua. Quantum entanglement in deep learning architectures. *Phys. Rev. Lett.*, 122:065301, Feb 2019. doi: 10.1103/PhysRevLett.122.065301. URL https://link.aps.org/doi/10.1103/PhysRevLett.122.065301

Zhouhan Lin, Minwei Feng, Cicero Nogueira dos Santos, Mo Yu, Bing Xiang, Bowen Zhou, and Yoshua Bengio. A structured self-attentive sentence embedding. *arXiv preprint arXiv:1703.03130*, 2017.

Yinhan Liu, Myle Ott, Naman Goyal, Jingfei Du, Mandar Joshi, Danqi Chen, Omer Levy, Mike Lewis, Luke Zettlemoyer, and Veselin Stoyanov. Roberta: A robustly optimized BERT pretraining approach. *CoRR*, abs/1907.11692, 2019. URL http://arxiv.org/abs/1907.11692

Zhou Lu, Hongming Pu, Feicheng Wang, Zhiqiang Hu, and Liwei Wang. The expressive power of neural networks: A view from the width. In *Advances in neural information processing systems*, pages 6231–6239, 2017.

Ningning Ma, Xiangyu Zhang, Hai-Tao Zheng, and Jian Sun. Shufflenet v2: Practical guidelines for efficient cnn architecture design. In *Proceedings of the European conference on computer vision (ECCV)*, pages 116–131, 2018.

Stephen Merity, Caiming Xiong, James Bradbury, and Richard Socher. Pointer sentinel mixture models. *arXiv preprint arXiv:1609.07843*, 2016.

Guido F Montufar, Razvan Pascanu, Kyunghyun Cho, and Yoshua Bengio. On the number of linear regions of deep neural networks. In *Advances in neural information processing systems*, pages 2924–2932, 2014.

Ankur P Parikh, Oscar Täckström, Dipanjan Das, and Jakob Uszkoreit. A decomposable attention model for natural language inference. *arXiv preprint arXiv:1606.01933*, 2016.

Romain Paulus, Caiming Xiong, and Richard Socher. A deep reinforced model for abstractive summarization. *arXiv preprint arXiv:1705.04304*, 2017.

Ofir Press, Noah A Smith, and Omer Levy. Improving transformer models by reordering their sublayers. *arXiv preprint arXiv:1911.03864*, 2019.

Danish Pruthi, Mansi Gupta, Bhuvan Dhingra, Graham Neubig, and Zachary C Lipton. Learning to deceive with attention-based explanations. *arXiv preprint arXiv:1909.07913*, 2019.

Alec Radford, Jeff Wu, Rewon Child, David Luan, Dario Amodei, and Ilya Sutskever. Language models are unsupervised multitask learners. 2019.

Jack W Rae, Chris Dyer, Peter Dayan, and Timothy P Lillicrap. Fast parametric learning with activation memorization. *arXiv preprint arXiv:1803.10049*, 2018.

Colin Raffel, Noam Shazeer, Adam Roberts, Katherine Lee, Sharan Narang, Michael Matena, Yanqi Zhou, Wei Li, and Peter J Liu. Exploring the limits of transfer learning with a unified text-to-text transformer. *arXiv preprint arXiv:1910.10683*, 2019.

Maithra Raghu, Ben Poole, Jon Kleinberg, Surya Ganguli, and Jascha Sohl-Dickstein. On the expressive power of deep neural networks. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pages 2847–2854. JMLR. org, 2017.

Oliver Richter and Roger Wattenhofer. Normalized attention without probability cage. *arXiv preprint arXiv:2005.09561*, 2020.

Andrew M Saxe, James L McClelland, and Surya Ganguli. Exact solutions to the nonlinear dynamics of learning in deep linear neural networks. *arXiv preprint arXiv:1312.6120*, 2013.

Thiago Serra, Christian Tjandraatmadja, and Srikumar Ramalingam. Bounding and counting linear regions of deep neural networks. *arXiv preprint arXiv:1711.02114*, 2017.

Or Sharir and Amnon Shashua. On the expressive power of overlapping architectures of deep learning. In *6th International Conference on Learning Representations (ICLR)*, 2018.

Or Sharir, Ronen Tamari, Nadav Cohen, and Amnon Shashua. Tractable generative convolutional arithmetic circuits. 2016.

Or Sharir, Barak Peleg, and Yoav Shoham. The cost of training nlp models: A concise overview. *arXiv preprint arXiv:2004.08900*, 2020.
Utkarsh Sharma and Jared Kaplan. A neural scaling law from the dimension of the data manifold, 04 2020.

Noam Shazeer, Azalia Mirhoseini, Krzysztof Maziarz, Andy Davis, Quoc Le, Geoffrey Hinton, and Jeff Dean. Outrageously large neural networks: The sparsely-gated mixture-of-experts layer. arXiv preprint arXiv:1701.06538, 2017.

Zhouxing Shi, Huan Zhang, Kai-Wei Chang, Minlie Huang, and Cho-Jui Hsieh. Robustness verification for transformers. In ICLR, 2020.

Karen Simonyan and Andrew Zisserman. Very deep convolutional networks for large-scale image recognition. arXiv preprint arXiv:1409.1556, 2014.

Mingxing Tan and Quoc V Le. Efficientnet: Rethinking model scaling for convolutional neural networks. arXiv preprint arXiv:1905.11946, 2019.

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, 4-9 December 2017, Long Beach, CA, USA, pages 5998–6008, 2017. URL http://papers.nips.cc/paper/7181-attention-is-all-you-need.

Chengwei Wang, Tengfei Zhou, Chen Chen, Tianlei Hu, and Gang Chen. Off-policy recommendation system without exploration. In Pacific-Asia Conference on Knowledge Discovery and Data Mining, pages 16–27. Springer, 2020.

Zifeng Wu, Chunhua Shen, and Anton Van Den Hengel. Wider or deeper: Revisiting the resnet model for visual recognition. Pattern Recognition, 90:119–133, 2019.

Zhilin Yang, Zihang Dai, Yiming Yang, Jaime G. Carbonell, Ruslan Salakhutdinov, and Quoc V. Le. Xlnet: Generalized autoregressive pretraining for language understanding. In Hanna M. Wallach, Hugo Larochelle, Alina Beygelzimer, Florence d’Alché-Buc, Emily B. Fox, and Roman Garnett, editors, Advances in Neural Information Processing Systems 32: Annual Conference on Neural Information Processing Systems 2019, NeurIPS 2019, 8-14 December 2019, Vancouver, BC, Canada, pages 5754–5764, 2019. URL http://papers.nips.cc/paper/8812-xlnet-generalized-autoregressive-pretraining-for-language-understanding.

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.

Sergey Zagoruyko and Nikos Komodakis. Wide residual networks. arXiv preprint arXiv:1605.07146, 2016.