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# Setting the Record Straight on Transformer Oversmoothing

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## Abstract

Transformer-based models have recently become wildly successful across a diverse set of domains. At the same time, recent work has shown empirically and theoretically that Transformers are inherently limited. Specifically, they argue that as model depth increases all features become more and more similar. A natural question is: How can Transformers achieve these successes given this shortcoming? In this work we test these observations empirically and theoretically and uncover a number of surprising findings. We find that there are cases where feature similarity increases but, contrary to prior results, this is not inevitable, even for existing pre-trained models. Theoretically, we show that smoothing behavior depends on the eigenspectrum of the value and projection weights and potentially the sign of the layer normalization weights. Our analysis reveals a simple way to parameterize the weights of the Transformer update equations to influence smoothing behavior. We hope that our findings give ML researchers and practitioners additional insight into how to develop future Transformer models.

## 1. Introduction

In recent years, Transformer models (Vaswani et al., 2017) have achieved astounding success across vastly different domains, however their performance can quickly saturate as model depth increases (Kaplan et al., 2020; Wang et al., 2022), as features are observed to become more and more similar to one another (Tang et al., 2021; Zhou et al., 2021a;b; Gong et al., 2021; Yan et al., 2022). Theoretically, these observations were characterized as (a) **Input**

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**Convergence:** Transformer features converge to the exact same vector (Park & Kim, 2022; Wang et al., 2022; Bai et al., 2022); (b) **Angle Convergence:** the angle between Transformer features converges to 0 (Tang et al., 2021; Zhou et al., 2021a; Gong et al., 2021; Yan et al., 2022; Shi et al., 2022; Noci et al., 2022; Guo et al., 2023); or (c) **Rank Collapse:** Transformer features collapse to a rank one matrix (Dong et al., 2021; Shi et al., 2022; Noci et al., 2022; Guo et al., 2023; Ali et al., 2023). We show even for a simplified Transformer setup that: (a) There are cases where all features converge to the same vector, but this is not inevitable, contrary to prior results; (b) Angle convergence is also possible, but not guaranteed; and (c) while rank collapse is likely, it is also not required. Empirically, for existing pre-trained models we find cases where (a) features do not converge to the same vector, (c) feature angles do not converge to 0, and (c) rank does not collapse.

## 2. Background & Related Work

### 2.1. The Transformer Update.

Transformers are a linear combination of a set of ‘heads’; each includes a self-attention function  $\mathbf{X} \in \mathbb{R}^{n \times d}$ ,  $\mathbf{A} := \text{Softmax}\left(\frac{1}{\sqrt{k}} \mathbf{X} \mathbf{W}_Q \mathbf{W}_K^\top \mathbf{X}^\top\right)$ , where the  $\text{Softmax}(\cdot)$  function is applied to each row individually. Further,  $\mathbf{W}_Q, \mathbf{W}_K \in \mathbb{R}^{d \times k}$  are learned query and key weight matrices. This ‘attention map’  $\mathbf{A}$  then transforms the input to produce the output of a single head  $\mathbf{A} \mathbf{X} \mathbf{W}_V \mathbf{W}_{\text{proj}}$ , where  $\mathbf{W}_V, \mathbf{W}_{\text{proj}} \in \mathbb{R}^{d \times d}$  are learned value and projection weights. A residual connection is added to produce the output  $\mathbf{X}_\ell$  of any layer  $\ell$ :

$$\mathbf{X}_\ell := \mathbf{X}_{\ell-1} + \mathbf{A}_\ell \mathbf{X}_{\ell-1} \mathbf{W}_{V,\ell} \mathbf{W}_{\text{proj},\ell}, \quad (1)$$

### 2.2. What Is Oversmoothing?

**Input Convergence.** One way to formalize oversmoothing is through the lens of signal-processing (Wang et al., 2022). : the smoothing of a function can be measured by how much it suppresses higher frequencies in the signal, removing smaller fluctuations to highlight the larger trend. To measure the smoothing of the Transformer update in

eq. (1) we can compute the ratio of high frequency signals to low frequency signals preserved in  $\mathbf{X}_\ell$ . If this goes to 0 as  $\ell \rightarrow \infty$ , all high frequency information is lost: the signal is maximally smoothed. To estimate these signals we can compute the Discrete Fourier Transform (DFT)  $\mathcal{F}$  of  $\mathbf{X}_\ell$ , via  $\mathcal{F}(\mathbf{X}_\ell) := \mathbf{F}\mathbf{X}_\ell$ , where  $\mathbf{F} \in \mathbb{C}^{n \times n}$  is equal to  $\mathbf{F}_{k,l} := e^{2\pi i(k-1)(l-1)}$  for all  $k, l \in \{2, \dots, n\}$  (where  $i := \sqrt{-1}$ ), and is 1 otherwise (i.e., in the first row and column). Define the Low Frequency Component (LFC) of  $\mathbf{X}_\ell$  as  $\text{LFC}[\mathbf{X}_\ell] := \mathbf{F}^{-1} \text{diag}([1, 0, \dots, 0])\mathbf{F}\mathbf{X}_\ell = (1/n)\mathbf{1}\mathbf{1}^\top \mathbf{X}_\ell$ . Further, define the High Frequency Component (HFC) of  $\mathbf{X}_\ell$  as  $\text{HFC}[\mathbf{X}_\ell] := \mathbf{F}^{-1} \text{diag}([0, 1, \dots, 1])\mathbf{F}\mathbf{X}_\ell = (\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^\top)\mathbf{X}_\ell$ . We can now state the first definition of oversmoothing:

**Definition 1** (Input Convergence (Wang et al., 2022)). The Transformer update in eq. (1) oversmooths if for all  $\mathbf{X} \in \mathbb{R}^{n \times d}$  we have that  $\lim_{\ell \rightarrow \infty} \frac{\|\text{HFC}[\mathbf{X}_\ell]\|_2}{\|\text{LFC}[\mathbf{X}_\ell]\|_2} = 0$ .

This definition measures the extent to which inputs converge to the same feature vector. To see this, notice that the term in the numerator  $\text{HFC}[\mathbf{X}_\ell] = (\mathbf{I} - (1/n)\mathbf{1}\mathbf{1}^\top)\mathbf{X}_\ell$  goes to 0 iff  $\mathbf{X}_\ell = \mathbf{1}\bar{\mathbf{x}}^\top$  where  $\bar{\mathbf{x}} \in \mathbb{R}^d$  is a vector where entry  $\bar{x}_i$  is the mean of the  $i$ th column of  $\mathbf{X}$ . This is because  $(1/n)\mathbf{1}\mathbf{1}^\top \mathbf{X} = \mathbf{1}\bar{\mathbf{x}}^\top$ . Finally, the required condition  $\mathbf{X}_\ell = \mathbf{1}\bar{\mathbf{x}}^\top$  only holds when all input vectors are equal. In the following we will refer to the ratio in the above definition as HFC/LFC.

**Angle Convergence.** Another way to quantify oversmoothing is via the cosine similarity between inputs:

**Definition 2** (Angle Convergence). The Transformer update in eq. (1) oversmooths if for all  $\mathbf{X} \in \mathbb{R}^{n \times d}$  we have that  $\lim_{\ell \rightarrow \infty} \frac{2}{n(n-1)} \sum_{i=1}^n \sum_{j=i+1}^n \frac{\mathbf{x}_{i,\ell}^\top \mathbf{x}_{j,\ell}}{\|\mathbf{x}_{i,\ell}\|_2 \|\mathbf{x}_{j,\ell}\|_2} = 1$ ,

where  $\mathbf{x}_{i,\ell} \in \mathbb{R}^d$  is the  $i$ th row of  $\mathbf{X}_\ell$ . This measures the cosine of the angle  $\theta$  between every pair of inputs  $\mathbf{x}_{i,\ell}, \mathbf{x}_{j,\ell}$  and is 1 iff  $\theta = 0$ .

**Rank Collapse.** Finally, we can also measure oversmoothing via rank collapse in  $\mathbf{X}_\ell$ . This is usually described as  $\lim_{\ell \rightarrow \infty} \text{rank}(\mathbf{X}_\ell) = 1$ . While rank can be computed via a singular value decomposition (SVD), it is highly-sensitive to the threshold deciding when a singular should be treated as zero. Instead, Guo et al. (2023) use the ‘effective rank’, first introduced by Roy & Vetterli (2007).

**Definition 3** (Rank Collapse). Given  $\mathbf{X}_\ell \in \mathbb{R}^{n \times d}$ , let  $\mathbf{X}_\ell = \mathbf{U}_\ell \boldsymbol{\Sigma}_\ell \mathbf{V}_\ell^\top$  be a singular value decomposition of  $\mathbf{X}$  with singular values  $\text{diag}(\boldsymbol{\Sigma}_\ell) = [\sigma_{1,\ell}, \dots, \sigma_{r,\ell}]$  for  $r \leq \min\{n, d\}$  and  $\sigma_{1,\ell} \geq \dots \geq \sigma_{r,\ell} \geq 0$ . Define the following discrete distribution according to the singular values as  $p_{i,\ell} = \sigma_{i,\ell} / \sum_{j=1}^r \sigma_{j,\ell}$ . The effective rank (Roy

& Vetterli, 2007) is the exponential of the entropy of this distribution:  $\exp(-\sum_{i=1}^r -p_{i,\ell} \log p_{i,\ell})$ . The Transformer update in eq. (1) oversmooths if for all  $\mathbf{X} \in \mathbb{R}^{n \times d}$  we have that  $\lim_{\ell \rightarrow \infty} \exp(-\sum_{i=1}^r p_{i,\ell} \log p_{i,\ell}) = 1$ .

Roy & Vetterli (2007) prove that  $1 \leq \exp(-\sum_{i=1}^r p_{i,\ell} \log p_{i,\ell}) \leq \text{rank}(\mathbf{X}_\ell) \leq r$ .

Notice that Definitions 1-3 are progressively relaxed, i.e., if an update satisfies an oversmoothing definition, it also satisfies any later definitions.

### 3. Do Transformers Always Oversmooth?

#### 3.1. Preliminaries

Our strategy will be to understand the eigenspectrum of the Transformer update in the limit and to use this understanding to derive what the features  $\mathbf{X}_\ell$  converge to as  $\ell \rightarrow \infty$ . All proofs will be left to the appendix. Define the  $\text{vec}(\mathbf{M})$  operator as converting any matrix  $\mathbf{M}$  to a vector  $\mathbf{m}$  by stacking its columns. We can rewrite eq. (1) vectorized as follows

$$\text{vec}(\mathbf{X}_\ell) = (\mathbf{I} + \underbrace{\mathbf{W}_{\text{proj}}^\top \mathbf{W}_V^\top}_{:=\mathbf{H}} \otimes \mathbf{A}) \text{vec}(\mathbf{X}_{\ell-1}). \quad (2)$$

**Assumption 1** ((Ali et al., 2023; Wang et al., 2022)). The attention matrix is positive, i.e.,  $\mathbf{A} > 0$ , and diagonalizable.

**Proposition 1** ((Meyer & Stewart, 2023)). *Given Assumption 1, all eigenvalues of  $\mathbf{A}$  lie within  $(-1, 1]$ . There is one largest eigenvalue that is equal to 1, with corresponding unique eigenvector 1.*

All proofs are left to the Appendix.

#### 3.2. The Eigenvalues

**Lemma 1.** *Let  $\lambda_1^A, \dots, \lambda_n^A$  be the eigenvalues of  $\mathbf{A}$  and let  $\lambda_1^H, \dots, \lambda_r^H$  for  $r \leq d$  be the eigenvalues of  $\mathbf{H}$ . The eigenvalues of  $(\mathbf{I} + \mathbf{H} \otimes \mathbf{A})^\ell$  are equal to  $(1 + \lambda_j^H \lambda_i^A)^\ell$  for  $j \in \{1, \dots, r\}$  and  $i \in \{1, \dots, n\}$ .*

**Definition 4** (Dominating eigenvalue(s)). At least one of the eigenvalues of  $(\mathbf{I} + \mathbf{H} \otimes \mathbf{A})$  has a larger magnitude than all others, i.e., there exists  $j^*, i^*$  (which may be a set of indices if there are ties) such that  $|1 + \lambda_{j^*}^H \lambda_{i^*}^A| > |1 + \lambda_{j'}^H \lambda_{i'}^A|$  for all  $j' \in \{1, \dots, d\} \setminus j^*$  and  $i' \in \{1, \dots, n\} \setminus i^*$ . These eigenvalues are called **dominating**.

**Theorem 1.** *Given the Transformer update in eq. (2), let  $\{\lambda_i^A\}_{i=1}^n$  and  $\{\lambda_j^H\}_{j=1}^r$  for  $r \leq d$  be the eigenvalues of  $\mathbf{A}$  and  $\mathbf{H}$ . Let the eigenvalues be sorted as follows,*

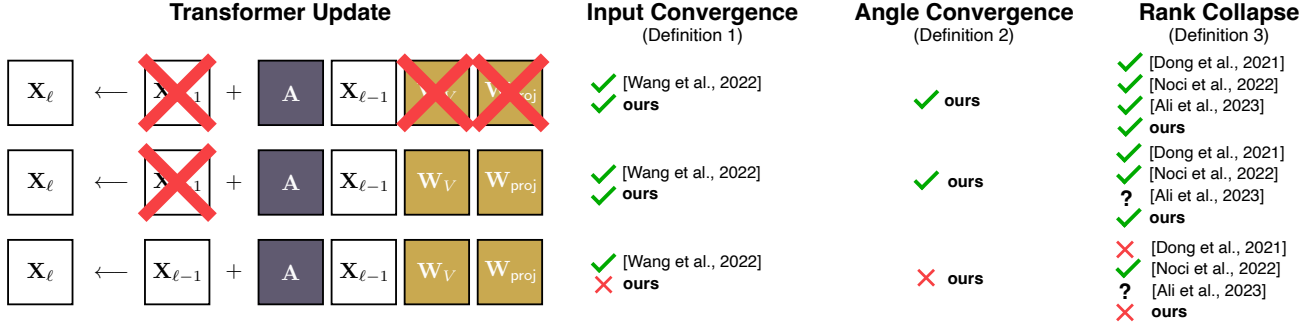


Figure 1. **Theory of Transformer Oversmoothing.** A ✓ indicates prior work says that the corresponding Definition is always satisfied, an ✗ indicates it is not always satisfied. Note that if a work argues a Definition is satisfied, then all later Definitions, which are progressively more relaxed, must also be satisfied.

$\lambda_1^A \leq \dots \leq \lambda_n^A$  and  $|1 + \lambda_1^H| \leq \dots \leq |1 + \lambda_r^H|$ . As the number of layers  $\ell \rightarrow \infty$ , there are two types of dominating eigenvalues: (1)  $(1 + \lambda_{j^*}^H \lambda_n^A)$ . and (2)  $(1 + \lambda_{j^*}^H \lambda_1^A)$

### 3.3. The Features

**Theorem 2.** Given the Transformer update in eq. (2), if a single eigenvalue dominates, as the number of total layers  $\ell \rightarrow \infty$ , the feature representation  $\mathbf{X}_\ell$  converges to one of two representations: (1) If  $(1 + \lambda_j^H \lambda_n^A)$  dominates then,  $\mathbf{X}_\ell \rightarrow (1 + \lambda_j^H \lambda_n^A)^\ell s_{j,n} \mathbf{1} \mathbf{v}_j^{H^\top}$ , (2) If  $(1 + \lambda_j^H \lambda_1^A)$  dominates then,  $\mathbf{X}_\ell \rightarrow (1 + \lambda_j^H \lambda_1^A)^\ell s_{j,1} \mathbf{v}_1^A \mathbf{v}_j^{H^\top}$  where  $\mathbf{v}^H, \mathbf{v}^A$  are eigenvectors of  $\mathbf{H}, \mathbf{A}$  and  $s_{j,i} := \langle \mathbf{v}_{j,i}^{Q^{-1}}, \text{vec}(\mathbf{X}) \rangle$  and  $\mathbf{v}_{j,i}^{Q^{-1}}$  is row  $ji$  in the matrix  $\mathbf{Q}^{-1}$  (here  $\mathbf{Q}$  is the matrix of eigenvectors of  $(\mathbf{I} + \mathbf{H} \otimes \mathbf{A})$ ). (3) If multiple eigenvalues have the same dominating magnitude,  $\mathbf{X}_\ell$  converges to the sum of the dominating terms.

**Corollary 1.** If the residual connection is removed in the Transformer update, then the eigenvalues are of the form  $(\lambda_j^H \lambda_i^A)$ . Further,  $(\lambda_{j^*}^H \lambda_n^A)$  is always a dominating eigenvalue, and  $\mathbf{X}_\ell \rightarrow (\lambda_{j^*}^H \lambda_n^A)^\ell s_{j,n} \mathbf{1} \bar{\mathbf{v}}_{j^*}^{H^\top}$  as  $\ell \rightarrow \infty$ , where  $\bar{\mathbf{v}}_{j^*}^H$  is the sum of all eigenvectors with eigenvalue equal to the dominating eigenvalue  $\lambda_{j^*}^H$ .

### 3.4. When Oversmoothing Happens

**Theorem 3.** Given the Transformer update eq. (2), as the number of total layers  $\ell \rightarrow \infty$ , if (1) one eigenvalue  $(1 + \lambda_j^H \lambda_n^A)$  dominates, we have input convergence, angle convergence, and rank collapse. If (2) one eigenvalue  $(1 + \lambda_j^H \lambda_1^A)$  dominates, we do not have input convergence or angle convergence, but we do have rank collapse. If (3) multiple eigenvalues have the same dominating magnitude and: (a) there is at least one dominating eigenvalue  $(1 + \lambda_{j^*}^H \lambda_i^A)$

where  $\lambda_{i^*}^A \neq \lambda_n^A$ , then we do not have input convergence or angle convergence, or (b) the geometric multiplicity of  $\lambda_1^A$  and  $\lambda_{j^*}^H$  are both greater than 1, then we also do not have rank collapse.

**Corollary 2.** If the residual connection is removed in the Transformer update, input convergence, angle convergence, and rank collapse are guaranteed.

The above statements follow directly from Theorem 2 and Corollary 1. They tell us that whenever a single eigenvalue  $(1 + \lambda_j^H \lambda_n^A)$  dominates, every input in  $\mathbf{X}_\ell$  converges to the same feature vector. This happens because  $\mathbf{v}_n^A = \mathbf{1}$  and so  $\mathbf{x}_{\ell,i} \sim \mathbf{v}_j^H$ , for all  $i$  as  $\ell \rightarrow \infty$ . But there is a second case: whenever the single eigenvalue  $(1 + \lambda_j^H \lambda_1^A)$  dominates, each feature is not guaranteed to be identical. However,  $\mathbf{X}_\ell \rightarrow (1 + \lambda_j^H \lambda_1^A)^\ell s_{j,1} \mathbf{v}_1^A \mathbf{v}_j^{H^\top}$  is still a matrix of rank one. If instead multiple eigenvalue dominate and the geometric multiplicity of  $\lambda_1^A$  and  $\lambda_{j^*}^H$  are both greater than 1 then  $\mathbf{X}_\ell$  is a sum of at least 2 rank-1 matrices and so we do not have rank collapse.

Theorem 3 largely contradicts prior theoretical results on oversmoothing. We suspect a few reasons for this. First, if multiple types of analyses are used within one paper, and they give conflicting results, resolving this can be especially challenging (Wang et al., 2022). Second, certain assumptions may not always hold in practice, e.g., Noci et al. (2022) assume that  $\mathbf{A} = \frac{1}{n} \mathbf{1} \mathbf{1}^\top$  at initialization.

## 4. A Reparameterization that Influences Smoothing

**Corollary 3.** If the eigenvalues of  $\mathbf{H}$  fall within  $[-1, 0)$ , then  $(1 + \lambda_{j^*}^H \lambda_1^A)$  dominates. If the eigenvalues of  $\mathbf{H}$  fall within  $(0, \infty)$ , then  $(1 + \lambda_{j^*}^H \lambda_n^A)$  dominates.

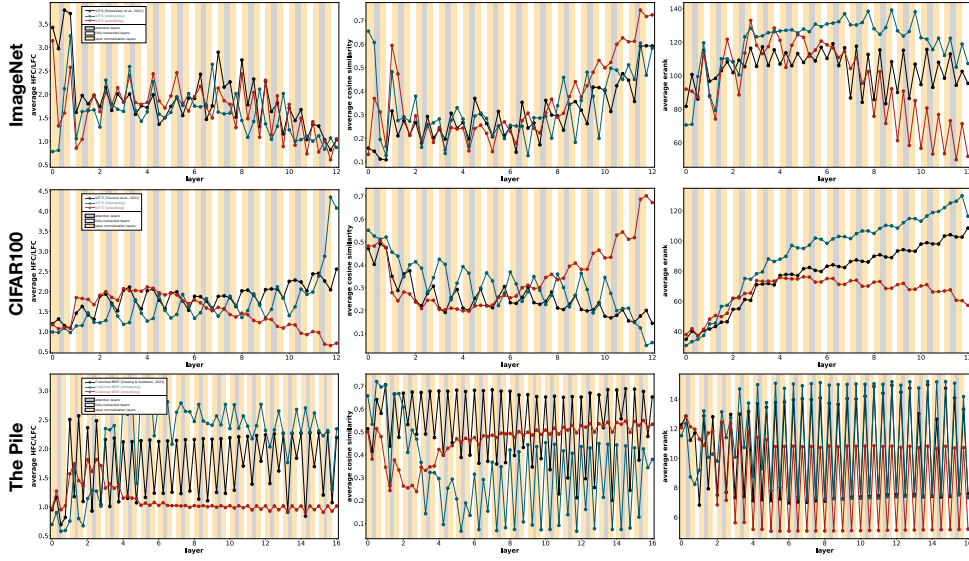


Figure 2. **Influencing smoothing.** The smoothing metrics defined in Definitions 1-3 for different models and datasets when  $\mathbf{H}$  is reparameterized as  $\mathbf{H} = \mathbf{V}_H \Lambda_H \mathbf{V}_H^{-1}$ . See text for details.

See the Appendix for a proof. To ensure that the eigenvalues of  $\mathbf{H}$  fall in these ranges, we propose to directly parameterize its eigendecomposition. Specifically, define  $\mathbf{H}$  as  $\mathbf{H} = \mathbf{V}_H \Lambda_H \mathbf{V}_H^{-1}$ , where  $\mathbf{V}_H$  is a full-rank matrix and  $\Lambda_H$  is diagonal. We learn parameters  $\mathbf{V}_H$  by taking gradients in the standard way (i.e., directly and through the inversion). To learn the diagonal of  $\Lambda_H$ , i.e.,  $\text{diag}(\Lambda_H)$ , we parameterize the sharpening model as  $\text{diag}(\Lambda_H) := \text{clip}(\psi, [-1, 0])$ , where  $\psi$  are tunable parameters and  $\text{clip}(\psi, [l, u]) := \min(\max(\psi, l), u)$  forces all of  $\psi$  to lie in  $[l, u]$ . Similarly we parameterize the smoothing model as  $\text{diag}(\Lambda_H) := \text{clip}(\psi, [0, 1])$ .<sup>1</sup>

**Reparameterization results.** Figure 2 show the effect of reparameterizing  $\mathbf{H}$  and restricting the range of eigenvalues to encourage **sharpening** and **smoothing**. For ImageNet we see that only the effective rank is somewhat affected in later layers. For CIFAR100 the **sharpening** parameterization reduces smoothing in all metrics while the **smoothing** parameterization further increases smoothing. For The Pile the effect is once again limited.

**Impact of layer normalization.** The position and weights of the layer normalization layer can impact the filtering behavior of a layer. In Fig. 3 we parameterize two layers, one smoothing and one sharpening and apply it to an input image for 128 iterations in order to visualize its asymptotic behavior. We repeat the process with the two most common

<sup>1</sup>While we could have allowed the smoothing model to use the space of positive reals via  $\text{diag}(\Lambda_H) := |\psi|$ , we found that restricting the space of allowed eigenvalues stabilized training.

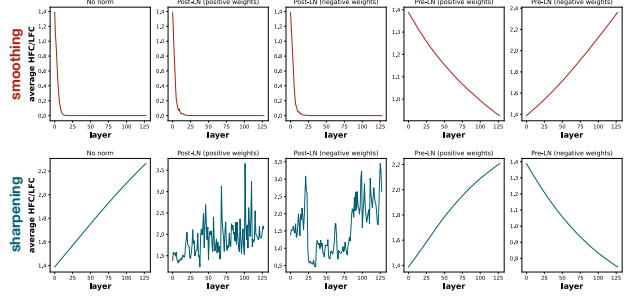


Figure 3. **Impact of Layer Normalization.** The average HFC/LFC for the Transformer update with repeated layers eq. (2) and different types of layer normalization (Post-LN (Vaswani et al., 2017), Pre-LN (Baevski & Auli, 2018)) where the weights of the layer normalization are fixed to be positive or negative.

layer normalization implementations: Pre-LN and Post-LN (Xiong et al., 2020), each with a positive then negative weight matrix sampled randomly. We do not use a bias since our focus is showing the impact of the normalization weight. When the weights are negative, Pre-LN reverses the expected filtering behavior of the layer.

## 5. Limitations

One limitation of the current theoretical analysis is that the results are asymptotic, applying in the limit as  $\ell \rightarrow \infty$ . We would like to expand the theoretical analysis to account for layer normalization and feed forward layers. Special

conditions will likely need to be placed on  $\mathbf{H}$  to enable this analysis, such as symmetric  $\mathbf{A}$ ,  $\mathbf{H}$  (Sander et al., 2022).

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## Setting the Record Straight on Transformer Oversmoothing

layer	CIFAR100			ImageNet						The Pile			
	ViT-Ti	ViT-Ti (sharpening)	ViT-Ti (smoothing)	ViT-S	ViT-S (sharpening)	ViT-S (smoothing)	ViT-B	DeiT-B	ViT-L	DeiT3-L	Cram. Bert	Cram. Bert (sharpening)	Cram. Bert (smoothing)
LayerNorm	-0.073	+0.011	-0.043	-0.126	+0.276	-0.244	+0.157	+0.338	-0.364	+0.811	-0.915	-0.086	-0.019
Attention	-0.165	+0.418	-0.121	-0.123	-0.048	+0.043	-0.535	-0.961	+0.008	-1.012	+0.994	-0.042	-0.003
MLP	+0.425	+0.418	+0.168	+0.175	-0.496	+0.270	+0.061	+0.258	+0.624	-0.604	+0.914	+0.316	+0.043

Table 1. Change in HFC/LFC for each layer type, across all models.

Layer type	CIFAR100			ImageNet						The Pile			
	ViT-Ti	ViT-Ti (sharpening)	ViT-Ti (smoothing)	ViT-S	ViT-S (sharpening)	ViT-S (smoothing)	ViT-B	DeiT-B	ViT-L	DeiT3-L	Cram. Bert	Cram. Bert (sharpening)	Cram. Bert (smoothing)
LayerNorm	+0.573	+1.304	+0.684	+14.975	+9.447	+2.628	+10.436	+12.41	+17.746	+19.18	+6.088	+6.084	+5.027
Attention	-0.171	+4.754	-2.870	-15.454	-5.185	+6.203	-10.247	-14.301	-18.671	-16.939	-5.927	-6.338	-5.002
MLP	+5.171	-0.217	+3.118	-13.352	-17.056	-8.405	-10.298	-8.821	-17.308	-21.052	-6.541	-6.093	-5.481

Table 2. Change in effective rank for each layer type, across all models.

## Appendix

### A. Implementation Details

Crucially, even though our theoretical analysis applies for fixed attention  $\mathbf{A}$  and weights  $\mathbf{H}$ , we use existing model architectures throughout, i.e., including different attention/weights each layer, multi-head attention, layer normalization (arranged in the pre-LN format (Xiong et al., 2020)), and fully-connected layers.<sup>2</sup>

**Initialization.** We initialize  $\mathbf{H} = \mathbf{V}_H \Lambda_H \mathbf{V}_H^{-1}$  to mimic the initializations used in the ViT-Ti and Bert baselines, which are initialized using He initialization (He et al., 2015). Specifically, we first initialize  $\mathbf{V}_H$  using He initialization. To initialize  $\text{diag}(\Lambda_H)$  we sample from a normal distribution with mean 0, as randomly initialized matrices will typically have normally distributed eigenvalues centered at 0. We noticed that if we set the standard deviation of this normal distribution to 1, the sampled values of  $\text{diag}(\Lambda_H)$  are often too large and lead to training instability. To stabilize training, we set the standard deviation to 0.1. All other training and architecture details are in the Appendix.

**Image Classification: Training & Architecture Details.** We base our image classification experiments on the ViT model (Dosovitskiy et al., 2020) and training recipe introduced in (Touvron et al., 2021). On CIFAR100 for 300 epochs using the cross-entropy loss and the AdamW optimizer (Loshchilov & Hutter, 2019). Our setup is the one used in (Park & Kim, 2022) which itself follows the DeiT training recipe (Touvron et al., 2021). We use a cosine annealing schedule with an initial learning rate of  $1.25 \times 10^{-4}$  and weight decay of  $5 \times 10^{-2}$ . We use a batch size of 96. We use data augmentation including RandAugment (Cubuk et al., 2019), CutMix (Yun et al., 2019), Mixup (Zhang et al., 2018), and label smoothing (Touvron et al., 2021). The models were trained on two Nvidia RTX 2080 Ti GPUs. On ImageNet, we use the original DeiT code and training recipe described above. Changes from CIFAR100 are that we use a batch size of 512 and train on a single Nvidia RTX 4090 GPU.

**Text Generation: Training & Architecture Details.** We base our NLP experiments on Geiping & Goldstein (2023), using their code-base. Following this work we pre-train encoder-only ‘Crammed’ Bert models with a maximum budget of 24 hours. We use a masked language modeling objective and train on the Pile dataset (Gao et al., 2020). The batch size is 8192 and the sequence length is 128. We evaluate models on SuperGLUE (Wang et al., 2020) after fine-tuning for each task. In order to ensure a fair comparison, all models are trained on a reference system with an RTX 4090 GPU. We use mixed precision training with bfloat16 as we found it to be the most stable (Kaddour et al., 2023).

### B. Do Transformers Oversmooth

Given the current theory on Transformer oversmoothing, how are Transformer models so successful for vision and NLP applications (Kenton & Toutanova, 2019; Liu et al., 2019; Lan et al., 2019; Brown et al., 2020; Dosovitskiy et al., 2020; Chowdhery et al., 2023)? To investigate this, we computed the above three metrics in Definitions 1-3 on a set of pre-trained

<sup>2</sup>If a model has multiple heads we will define  $\mathbf{W}_V = \mathbf{V}_H$  and  $\mathbf{W}_{\text{proj}} = \Lambda_H \mathbf{V}_H^T$ .

# Setting the Record Straight on Transformer Oversmoothing

Layer type	CIFAR100			ImageNet						The Pile			
	ViT-Ti	ViT-Ti (sharpening)	ViT-Ti (smoothing)	ViT-S	ViT-S (sharpening)	ViT-S (smoothing)	ViT-B	DeiT-B	ViT-L	DeiT3-L	Cram. Bert	Cram. Bert (sharpening)	Cram. Bert (smoothing)
LayerNorm	+0.006	-0.004	+0.001	-0.057	-0.013	-0.056	-0.061	-0.064	+0.002	-0.166	-0.274	-0.232	-0.025
Attention	+0.04	-0.086	+0.052	+0.129	+0.054	-0.005	+0.163	+0.192	+0.072	+0.211	+0.263	+0.258	+0.035
MLP	-0.078	+0.054	-0.038	+0.258	+0.021	+0.021	+0.005	-0.052	-0.058	+0.117	+0.111	+0.188	+0.016

Table 3. Change in cosine similarity for each layer type, across all models.

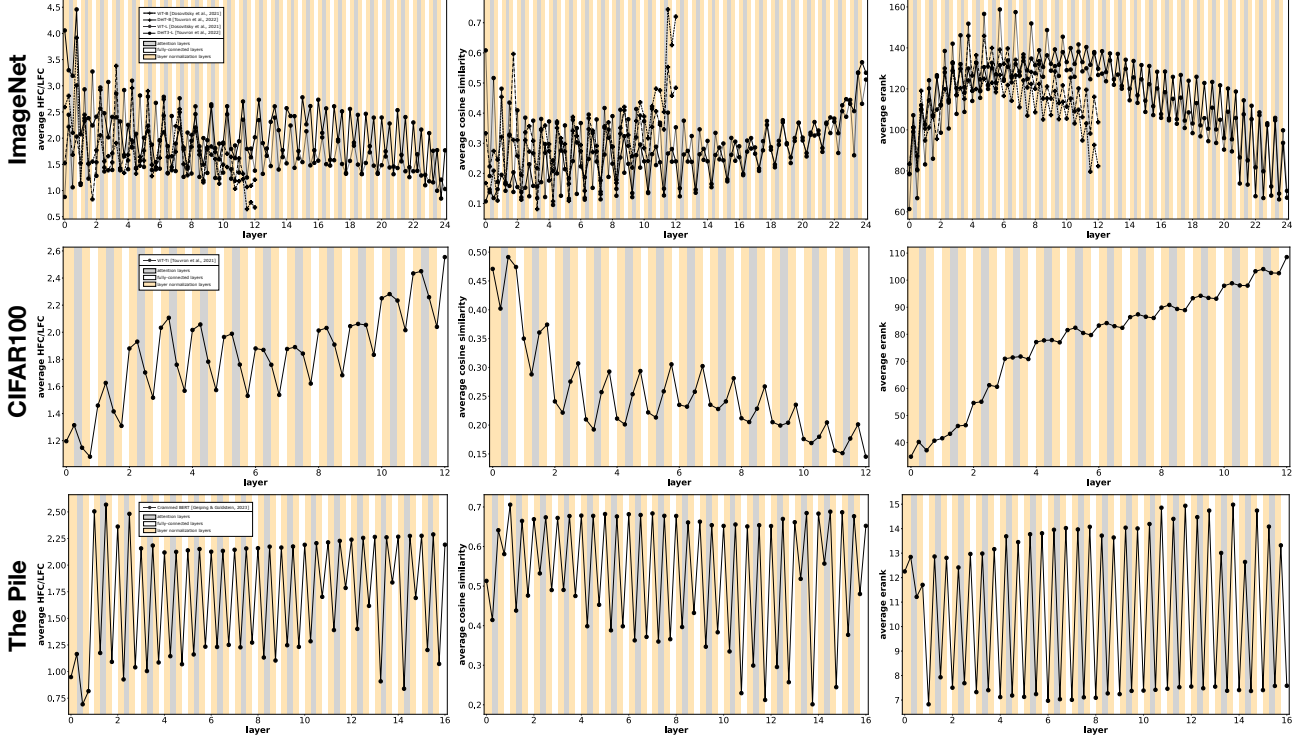


Figure 4. **Smoothing behavior.** The smoothing metrics defined in Definitions 1-3 for different models and datasets in vision and NLP. See text for details.

models for vision and NLP that have been used in prior work on oversmoothing (Wang et al., 2022; Choi et al., 2023) in Figure 4. We notice that for all ImageNet models (ViT-B, ViT-L (Dosovitskiy et al., 2020), DeiT-B (Touvron et al., 2021), DeiT3-L (Touvron et al., 2022)), as depth increases, we do see the metrics approaching their oversmoothing values as described in Definitions 1-3. Rank (Definition 3) does not consistently decrease and stays relatively high for 12 layer models, but continues to drop as depth is increased. However, we see something completely unexpected from the CIFAR model (ViT-Ti (Touvron et al., 2021)). All of the metrics *show reduction in smoothing behavior* as depth increases. Similarly, for The Pile model (Crammed BERT (Geiping & Goldstein, 2023)) we see behavior that appears to oscillate between more and less smoothing. These behaviors motivate us to further investigate the Transformer update.

## C. Proofs

**Proposition 1** ((Meyer & Stewart, 2023)). *Given Assumption 1, all eigenvalues of  $\mathbf{A}$  lie within  $(-1, 1]$ . There is one largest eigenvalue that is equal to 1, with corresponding unique eigenvector  $\mathbf{1}$ .*

*Proof.* First, because  $\mathbf{A}$  is positive, by the Perron-Frobenius Theorem (Meyer & Stewart, 2023) all eigenvalues of  $\mathbf{A}$  are in  $\mathbb{R}$  (and so there exist associated eigenvectors that are also in  $\mathbb{R}$ ). Next, recall the definition of an eigenvalue  $\lambda$  and



eigenvector  $\mathbf{v}$ :  $\mathbf{A}\mathbf{v} = \lambda\mathbf{v}$ . Let us write the equation for any row  $i \in \{1, \dots, n\}$  explicitly:

$$a_{i1}v_1 + \dots + a_{in}v_n = \lambda v_i.$$

Further let,

$$v_{\max} := \max\{|v_1|, \dots, |v_n|\} \quad (3)$$

Note that  $v_{\max} > 0$ , otherwise it is not a valid eigenvector. Further let  $k_{\max}$  be the index of  $\mathbf{v}$  corresponding to  $v_{\max}$ . Then we have,

$$\begin{aligned} |\lambda|v_{\max} &= |a_{k_{\max}1}v_1 + \dots + a_{k_{\max}n}v_n| \\ &\leq a_{k_{\max}1}|v_1| + \dots + a_{k_{\max}n}|v_n| \\ &\leq a_{k_{\max}1}|v_{k_{\max}}| + \dots + a_{k_{\max}n}|v_{k_{\max}}| \\ &= (a_{k_{\max}1} + \dots + a_{k_{\max}n})|v_{k_{\max}}| = |v_{\max}| \end{aligned}$$

The first inequality is given by the triangle inequality and because  $a_{ij} > 0$ . The second is given by the definition of  $v_{\max}$  as the maximal element in  $\mathbf{v}$ . The final inequality is given by the definition of  $\mathbf{A}$  in eq. (??) as right stochastic (i.e., all rows of  $\mathbf{A}$  sum to 1) and because  $|v_{k_{\max}}| = |v_{\max}|$ . Next, note that because  $v_{\max} > 0$ , it must be that  $\lambda \leq 1$ . Finally, to show that the one largest eigenvalue is equal to 1, recall by the definition of  $\mathbf{A}$  in eq. (??) that  $\mathbf{A}\mathbf{1} = \mathbf{1}$ , where  $\mathbf{1}$  is the vector of all ones. So  $\mathbf{1}$  is an eigenvector of  $\mathbf{A}$ , with eigenvalue  $\lambda^* = 1$ . Because  $a_{ij} > 0$ , and we showed above that all eigenvalues must lie in in  $[-1, 1]$ , by the Perron-Frobenius theorem (Meyer & Stewart, 2023)  $\lambda^* = 1$  is the Perron root. This means that all other eigenvalues  $\lambda_i$  satisfy the following inequality  $|\lambda_i| < \lambda^*$ . Further  $\mathbf{1}$  is the Perron eigenvector, and all other eigenvectors have at least one negative component, making  $\mathbf{1}$  unique. Finally, because  $\mathbf{A}$  is diagonalizable it has  $n$  linearly independent eigenvectors.  $\square$

**Lemma 1.** Let  $\lambda_1^A, \dots, \lambda_n^A$  be the eigenvalues of  $\mathbf{A}$  and let  $\lambda_1^H, \dots, \lambda_r^H$  for  $r \leq d$  be the eigenvalues of  $\mathbf{H}$ . The eigenvalues of  $(\mathbf{I} + \mathbf{H} \otimes \mathbf{A})^\ell$  are equal to  $(1 + \lambda_j^H \lambda_i^A)^\ell$  for  $j \in \{1, \dots, r\}$  and  $i \in \{1, \dots, n\}$ .

The proof can be derived from Theorem 2.3 of (Schacke, 2004). We now prove a lemma that will allow us to prove Theorem 1.

**Lemma 2.** Consider the Transformer update in eq. (2). Let  $\{\lambda_i^A, \mathbf{v}_i^A\}_{i=1}^n$  and  $\{\lambda_j^H, \mathbf{v}_j^H\}_{j=1}^r$  for  $r \leq d$  be the eigenvalue and eigenvectors of  $\mathbf{A}$  and  $\mathbf{H}$ . Let the eigenvalues (and associated eigenvectors) be sorted as follows,  $\lambda_1^A \leq \dots \leq \lambda_n^A$  and  $|1 + \lambda_1^H| \leq \dots \leq |1 + \lambda_r^H|$ . Let  $\varphi_1^H, \dots, \varphi_r^H$  be the phases of  $\lambda_1^H, \dots, \lambda_r^H$ . As the number of layers  $L \rightarrow \infty$ , one eigenvalue dominates the rest (multiple dominate if there are ties):

$$\left\{ \begin{array}{ll} \left( \begin{array}{ll} (1 + \lambda_r^H \lambda_n^A) & \text{if } |1 + \lambda_r^H \lambda_n^A| \geq 1 \\ (1 + \lambda_{\min}^H \lambda_1^A) & \text{if } |1 + \lambda_r^H \lambda_n^A| < 1 \end{array} \right) & \text{if } \lambda_1^A > 0 \\ \left( \begin{array}{ll} (1 + \lambda_r^H \lambda_n^A) & \text{if } |1 + \lambda_r^H \lambda_n^A| > |1 + \lambda_k^H \lambda_1^A| \\ (1 + \lambda_k^H \lambda_1^A) & \text{if } |1 + \lambda_r^H \lambda_n^A| < |1 + \lambda_k^H \lambda_1^A| \end{array} \right) & \text{if } \lambda_1^A < 0, \varphi_r^H \in [-\frac{\pi}{2}, \frac{\pi}{2}] \\ \left( \begin{array}{ll} (1 + \lambda_r^H \lambda_n^A) & \text{if } |1 + \lambda_r^H \lambda_n^A| > |1 + \lambda_r^H \lambda_1^A| \\ (1 + \lambda_r^H \lambda_1^A) & \text{if } |1 + \lambda_r^H \lambda_n^A| < |1 + \lambda_r^H \lambda_1^A| \end{array} \right) & \text{if } \lambda_1^A < 0, \varphi_r^H \in (\frac{\pi}{2}, \pi] \cup [-\pi, -\frac{\pi}{2}) \end{array} \right.$$

where  $\lambda_{\min}^H$  be the eigenvalue of  $\mathbf{H}$  with smallest magnitude and  $\lambda_k^H$  is the eigenvalue with the largest index  $k$  such that  $\varphi_k^H \in (\pi/2, \pi] \cup [-\pi, -\pi/2)$ .

*Proof.* Given Lemma 1, the eigenvalues and eigenvectors of  $(\mathbf{I} + \mathbf{H} \otimes \mathbf{A})$  are equal to  $(1 + \lambda_j^H \lambda_i^A)$  and  $\mathbf{v}_j^H \otimes \mathbf{v}_i^A$  for all  $j \in \{1, \dots, d\}$  and  $i \in \{1, \dots, n\}$ . Recall that eigenvalues (and associated eigenvectors) are sorted in the following order  $\lambda_1^A \leq \dots \leq \lambda_n^A$  and  $|1 + \lambda_1^H| \leq \dots \leq |1 + \lambda_d^H|$ . Our goal is to understand the identity of the dominating eigenvalue(s)  $\lambda_j^H \lambda_i^A$  for all possible values of  $\lambda_H, \lambda_A$ .

First recall that  $\lambda_i^A \in (-1, 1]$  and  $\lambda_n^A = 1$ . A useful way to view selecting  $\lambda_j^H \lambda_i^A$  to maximize  $|1 + \lambda_j^H \lambda_i^A|$  is as maximizing distance to  $-1$ . If (i),  $\lambda_1^A > 0$  then  $\lambda_i^A$ , for all  $i \in \{1, \dots, n-1\}$  always shrinks  $\lambda_j^H$  to the origin and  $\lambda_n^A$  leaves it unchanged. Because of how the eigenvalues are ordered we must have that  $|1 + \lambda_r^H| = |1 + \lambda_j^H \lambda_n^A| \leq |1 + \lambda_r^H \lambda_n^A| = |1 + \lambda_r^H|$ . If  $|1 + \lambda_r^H \lambda_n^A| \geq 1$  then shrinking any  $\lambda_i^H$  to the origin will also move it closer to  $-1$ . However, if  $|1 + \lambda_r^H \lambda_n^A| < 1$  then shrinking to the origin can move  $\lambda_i^H$  farther from  $-1$  than  $|1 + \lambda_r^H \lambda_n^A|$ . The eigenvalue of  $\mathbf{H}$  that can be moved farthest is the one with the smallest overall magnitude, defined as  $\lambda_{\min}^H$ . The eigenvalue of  $\mathbf{A}$  that can shrink it the most is  $\lambda_1^A$ . This completes the first two cases.

If instead (ii),  $\lambda_1^A < 0$  then it is possible to ‘flip’  $\lambda_j^H$  across the origin, and so the maximizer depends on  $\varphi_r^H$ . If a)  $\varphi_r^H \in [-\pi/2, \pi/2]$  then let  $\lambda_k^H$  be the eigenvalue with the largest index  $k$  such that  $\varphi_k^H \in (\pi/2, \pi] \cup [-\pi, -\pi/2)$ . It is possible that ‘flipping’ this eigenvalue across the origin makes it farther away than  $\lambda_r^H$ , i.e.,  $|1 + \lambda_k^H \lambda_1^A| > |1 + \lambda_r^H \lambda_n^A|$ . In this case  $(1 + \lambda_k^H \lambda_1^A)$  dominates, otherwise  $(1 + \lambda_r^H \lambda_n^A)$  dominates. If they are equal then both dominate. If instead b)  $\varphi_r^H \in (\pi/2, \pi] \cup [-\pi, -\pi/2)$  then either  $|1 + \lambda_r^H \lambda_n^A| > |1 + \lambda_{j'}^H \lambda_{i'}^A|$  for all  $j' \neq d$  and  $i' \neq n$ , and so  $(1 + \lambda_r^H \lambda_n^A)$  dominates, or ‘flipping’  $\lambda_r^H$  increases its distance from  $-1$ , and so  $|1 + \lambda_r^H \lambda_1^A| > |1 + \lambda_{j'}^H \lambda_{i'}^A|$  for all  $j' \neq d$  and  $i' \neq n$ , and so  $(1 + \lambda_r^H \lambda_1^A)$  dominates. Because we cannot have that  $|1 + \lambda_r^H \lambda_n^A| = |1 + \lambda_r^H \lambda_1^A|$  as  $\lambda_1^A > -1$  this covers all cases.  $\square$

Now we can prove Theorem 1.

**Theorem 1.** *Given the Transformer update in eq. (2), let  $\{\lambda_i^A\}_{i=1}^n$  and  $\{\lambda_j^H\}_{j=1}^r$  for  $r \leq d$  be the eigenvalues of  $\mathbf{A}$  and  $\mathbf{H}$ . Let the eigenvalues be sorted as follows,  $\lambda_1^A \leq \dots \leq \lambda_n^A$  and  $|1 + \lambda_1^H| \leq \dots \leq |1 + \lambda_r^H|$ . As the number of layers  $\ell \rightarrow \infty$ , there are two types of dominating eigenvalues: (1)  $(1 + \lambda_{j^*}^H \lambda_n^A)$ , and (2)  $(1 + \lambda_j^H \lambda_1^A)$*

The proof follows immediately from Lemma 2.

**Theorem 2.** *Given the Transformer update in eq. (2), if a single eigenvalue dominates, as the number of total layers  $\ell \rightarrow \infty$ , the feature representation  $\mathbf{X}_\ell$  converges to one of two representations: (1) If  $(1 + \lambda_{j^*}^H \lambda_n^A)$  dominates then,*

$$\mathbf{X}_\ell \rightarrow (1 + \lambda_{j^*}^H \lambda_n^A)^\ell s_{j^*,n} \mathbf{1} \mathbf{v}_{j^*}^{H\top}, \quad (4)$$

(2) If  $(1 + \lambda_j^H \lambda_1^A)$  dominates then,

$$\mathbf{X}_\ell \rightarrow (1 + \lambda_j^H \lambda_1^A)^\ell s_{j,1} \mathbf{v}_1^A \mathbf{v}_j^{H\top} \quad (5)$$

where  $\mathbf{v}^H, \mathbf{v}^A$  are eigenvalues of  $\mathbf{H}, \mathbf{A}$  and  $s_{j,i} := \langle \mathbf{v}_{j,i}^{Q^{-1}}, \text{vec}(\mathbf{X}) \rangle$  and  $\mathbf{v}_{j,i}^{Q^{-1}}$  is row  $ji$  in the matrix  $\mathbf{Q}^{-1}$  (here  $\mathbf{Q}$  is the matrix of eigenvectors of  $(\mathbf{I} + \mathbf{H} \otimes \mathbf{A})$ ). (3) If multiple eigenvalues have the same dominating magnitude,  $\mathbf{X}_\ell$  converges to the sum of the dominating terms.

*Proof.* Recall that the eigenvalues and eigenvectors of  $(\mathbf{I} + \mathbf{H} \otimes \mathbf{A})$  are equal to  $(1 + \lambda_j^H \lambda_i^A)$  and  $\mathbf{v}_j^H \otimes \mathbf{v}_i^A$  for all  $j \in \{1, \dots, d\}$  and  $i \in \{1, \dots, n\}$ . This means,

$$\text{vec}(\mathbf{X}_\ell) = \sum_{i,j} (1 + \lambda_j^H \lambda_i^A)^\ell \langle \mathbf{v}_{j,i}^{Q^{-1}}, \text{vec}(\mathbf{X}) \rangle (\mathbf{v}_j^H \otimes \mathbf{v}_i^A).$$

Recall that  $\mathbf{v}_{j,i}^{Q^{-1}}$  is row  $ji$  in the matrix  $\mathbf{Q}^{-1}$ , where  $\mathbf{Q}$  is the matrix of eigenvectors  $\mathbf{v}_j^H \otimes \mathbf{v}_i^A$ . Further recall that  $\mathbf{v}_i^A = \mathbf{1}$ . As described in Theorem 1, as  $\ell \rightarrow \infty$  at least one of the eigenvalues pairs  $\lambda_j^H \lambda_i^A$  will dominate the expression  $(1 + \lambda_j^H \lambda_i^A)^\ell$ , which causes  $\text{vec}(\mathbf{X}_\ell)$  to converge to the dominating term. Finally, we can rewrite,  $\mathbf{v}_1 \otimes \mathbf{v}_2$  as  $\text{vec}(\mathbf{v}_2 \mathbf{v}_1^\top)$ . Now all non-scalar terms have  $\text{vec}(\cdot)$  applied, so we can remove this function everywhere to give the matrix form given in eq. (4) and eq. (5).  $\square$

**Corollary 1.** *If the residual connection is removed in the Transformer update, then the eigenvalues are of the form  $(\lambda_j^H \lambda_i^A)$ . Further,  $(\lambda_{j^*}^H \lambda_n^A)$  is always a dominating eigenvalue, and  $\mathbf{X}_\ell \rightarrow (\lambda_{j^*}^H \lambda_n^A)^\ell s_{j^*,n} \bar{\mathbf{v}}_{j^*}^{H\top}$  as  $\ell \rightarrow \infty$ , where  $\bar{\mathbf{v}}_{j^*}^H$  is the sum of all eigenvectors with eigenvalue equal to the dominating eigenvalue  $\lambda_{j^*}^H$ .*

*Proof.* The eigendecomposition of the Transformer update without the residual connection is:

$$\text{vec}(\mathbf{X}_\ell) = \sum_{i,j} (\lambda_j^H \lambda_i^A)^\ell \langle \mathbf{v}_{j,i}^{Q-1}, \text{vec}(\mathbf{X}) \rangle (\mathbf{v}_j^H \otimes \mathbf{v}_i^A).$$

In this case,  $(\lambda_{j^*}^H \lambda_n^A)$  is always a dominating eigenvalue because  $|\lambda_n^A| > |\lambda_i^A|$  for any  $i \in \{1, \dots, n-1\}$ . This and the above eigendecomposition yields  $\mathbf{X}_\ell \rightarrow (\lambda_{j^*}^H \lambda_n^A)^\ell s_{j,n} \mathbf{1} \bar{\mathbf{v}}_{j^*}^H{}^\top$  as  $\ell \rightarrow \infty$ .  $\square$

**Theorem 3.** *Given the Transformer update eq. (2), as the number of total layers  $\ell \rightarrow \infty$ , if (1) one eigenvalue  $(1 + \lambda_j^H \lambda_n^A)$  dominates, we have input convergence, angle convergence, and rank collapse. If (2) one eigenvalue  $(1 + \lambda_j^H \lambda_1^A)$  dominates, we do not have input convergence or angle convergence, but we do have rank collapse. If (3) multiple eigenvalues have the same dominating magnitude and: (a) there is at least one dominating eigenvalue  $(1 + \lambda_{j^*}^H \lambda_{i^*}^A)$  where  $\lambda_{i^*}^A \neq \lambda_n^A$ , then we do not have input convergence or angle convergence, or (b) the geometric multiplicity of  $\lambda_1^A$  and  $\lambda_{j^*}^H$  are both greater than 1, then we also do not have rank collapse.*

*Proof.* If (1) one eigenvalue  $(1 + \lambda_j^H \lambda_n^A)$  dominates then we have that  $\mathbf{X}_\ell \rightarrow (1 + \lambda_j^H \lambda_n^A)^\ell s_{j,n} \mathbf{1} \bar{\mathbf{v}}_j^H{}^\top$ . Therefore,  $\mathbf{X}_\ell$  has all the same inputs which also implies angle convergence and rank collapse. If (2) one eigenvalue  $(1 + \lambda_j^H \lambda_1^A)$  dominates then we have that  $\mathbf{X}_\ell \rightarrow (1 + \lambda_j^H \lambda_1^A)^\ell s_{j,1} \mathbf{v}_1^A \bar{\mathbf{v}}_j^H{}^\top$ . Therefore, we do not have input convergence. Further as  $\mathbf{v}_1^A$  can contain both positive and negative components we do not have angle convergence. However,  $\mathbf{X}_\ell$  is rank one so we do have rank collapse. If (3) multiple eigenvalues have the same dominating magnitude and: (a) there is at least one dominating eigenvalue  $(1 + \lambda_{j^*}^H \lambda_{i^*}^A)$  where  $\lambda_{i^*}^A \neq \lambda_n^A$  then we do not have input convergence or rank convergence, as shown for case (2); if (b) the geometric multiplicity of  $\lambda_1^A$  and  $\lambda_{j^*}^H$  are both greater than 1, then  $\mathbf{X}_\ell$  converges to the sum of at least 2 rank-1 matrices which are not themselves linear combinations of each other. Therefore,  $\text{rank}(\mathbf{X}_\ell) \geq 2$ .  $\square$

**Corollary 2.** *If the residual connection is removed in the Transformer update, input convergence, angle convergence, and rank collapse are guaranteed.*

*Proof.* Corollary 1 tells us that in this case  $\mathbf{X}_\ell \rightarrow (\lambda_{j^*}^H \lambda_n^A)^\ell s_{j,n} \mathbf{1} \bar{\mathbf{v}}_{j^*}^H{}^\top$  as  $\ell \rightarrow \infty$ , where  $\bar{\mathbf{v}}_{j^*}^H$  is the sum of all eigenvectors with eigenvalue equal to the dominating eigenvalue  $\lambda_{j^*}^H$ . This matrix has all the same features and so we have input convergence, angle convergence, and rank collapse.  $\square$

**Corollary 3.** *If the eigenvalues of  $\mathbf{H}$  fall within  $[-1, 0)$ , then  $(1 + \lambda_{j^*}^H \lambda_1^A)$  dominates. If the eigenvalues of  $\mathbf{H}$  fall within  $(0, \infty)$ , then  $(1 + \lambda_{j^*}^H \lambda_n^A)$  dominates.*

*Proof.* Let  $\lambda_1^H \leq \dots \leq \lambda_r^H$ . Again we can think of selecting  $\lambda_j^H \lambda_i^A$  that maximizes  $|1 + \lambda_j^H \lambda_i^A|$  as maximizing the distance of  $\lambda_j^H \lambda_i^A$  to  $-1$ . Consider the first case where  $\lambda_1^H, \dots, \lambda_r^H \in [-1, 0)$ , and so  $\lambda_1^H$  is the closest eigenvalue to  $-1$  and  $\lambda_r^H$  is the farthest. If  $\lambda_1^A > 0$  then all  $\lambda^A$  can do is shrink  $\lambda^H$  to the origin, where  $\lambda_1^A$  shrinks  $\lambda^H$  the most. The closest eigenvalue to the origin is  $\lambda_r^H$ , and so  $(1 + \lambda_r^H \lambda_1^A)$  dominates. If instead  $\lambda_1^A < 0$ , then we can ‘flip’  $\lambda_j^H$  over the origin, making it farther from  $-1$  than all other  $\lambda_{j'}^H$ . The eigenvalue that we can ‘flip’ the farthest from  $-1$  is  $\lambda_1^H$ , and so  $(1 + \lambda_1^H \lambda_1^A)$  dominates. If all eigenvalues of  $\mathbf{H}$  are equal, then both  $(1 + \lambda_r^H \lambda_1^A)$  and  $(1 + \lambda_1^H \lambda_1^A)$  dominate. For the second case where  $\lambda_1^H, \dots, \lambda_r^H \in (0, \infty)$ , we have that  $|1 + \lambda_r^H \lambda_n^A| > |1 + \lambda_{j'}^H \lambda_{i'}^A|$  for all  $j' \in \{1, \dots, d-1\}$  and  $i' \in \{1, \dots, n-1\}$ . This is because, by definition  $\lambda_r^H \lambda_n^A > \lambda_{j'}^H \lambda_{i'}^A$ . Further,  $1 + \lambda_r^H \lambda_n^A \geq |1 + \lambda_{j'}^H \lambda_{i'}^A|$  as the largest  $|1 + \lambda_{j'}^H \lambda_{i'}^A|$  can be is either (i)  $|1 - \epsilon \lambda_r^H|$  for  $0 < \epsilon < 1$  or (ii)  $|1 + \lambda_{r-1}^H \lambda_n^A|$  (i.e., in (i)  $\lambda_r^H$  is negated by  $\lambda_1^A$  and in (ii)  $\lambda_{r-1}^H$  is the next largest value of  $\lambda^H$ ). For (i), it must be that  $1 + \lambda_r^H \lambda_n^A \geq |1 - \epsilon \lambda_r^H|$  as  $\lambda_r^H > 0$ . For (ii)  $\lambda_r^H \geq \lambda_{r-1}^H > 0$ , and so  $|1 + \lambda_r^H \lambda_n^A| \geq |1 + \lambda_{r-1}^H \lambda_n^A|$ . Therefore  $\lambda_n^A$  dominates.  $\square$

## D. Distribution of the eigenvalues of $\mathbf{H}$ in trained models

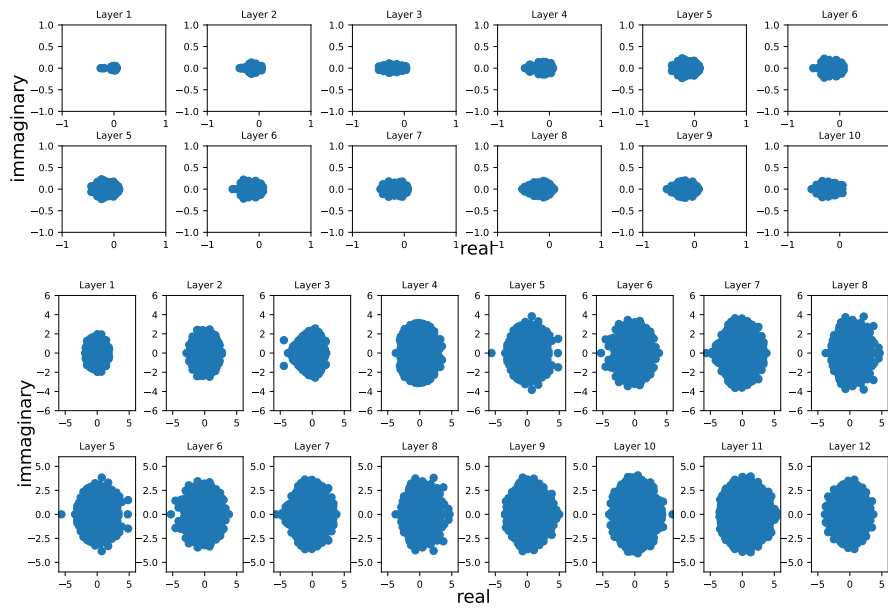


Figure 5. Distributions of eigenvalues of  $H$  (Top) Vision models have distributions skewing to the negatives; (Bottom) Language models have symmetrically distributed eigenvalues.