

Supplement to “Elliptical Attention”

Table of Contents

A	Full Derivation of Self-Attention as Non-Parametric Regression	17
B	Technical Proofs	18
B.1	Proof of Lemma 1	18
B.2	Proof of Proposition 1	19
B.3	Proof of Proposition 2	21
B.4	Edge-preservation Perspective on Representation Collapse	22
B.5	Proof of Proposition 3	23
B.6	Lipschitz smoothness in (\mathcal{X}, d)	25
C	Additional Theorems	26
D	A Consistent Estimator	27
E	Implementation Procedure and Computational Efficiency	28
F	Experimental Details and Additional Experiments	28
F.1	Out-of-Distribution Robustness and Data Corruption on ImageNet-A,R,C	28
F.2	Representation Collapse	28
F.3	Head Redundancy	29
F.4	Efficiency Results	29
F.5	Elliptical Attention in Mixture of Expert Architectures	29
F.6	Additional Adversarial Attack Results on DeiT-Small Configuration	30
F.7	Wikitext-103 Language Modelling and Word Swap Attack	30
F.8	ImageNet Image Classification and Adversarial Attack	31
F.9	LRA Long Sequence Classification.	31
F.10	ADE20K Image Segmentation	32
F.11	Ablation Studies	33
F.12	Pseudocode	33
G	Broader Impacts	34

A Full Derivation of Self-Attention as Non-Parametric Regression

Recall NW estimator is a non-parametric estimator of the unknown f at any given query \mathbf{q} described by

$$f(\mathbf{k}) = \mathbb{E}[\mathbf{v}|\mathbf{k}] = \int_{\mathbb{R}^D} \mathbf{v} \cdot p(\mathbf{v}|\mathbf{k}) d\mathbf{v} = \int_{\mathbb{R}^D} \frac{\mathbf{v} \cdot p(\mathbf{v}, \mathbf{k})}{p(\mathbf{k})} d\mathbf{v},$$

where the first equality comes from the noise being zero mean, the second equality comes from the definition of conditional expectation and the final equality comes from the definition of conditional density. Eqn. 3 implies that if we can just obtain good estimates of the joint density $p(\mathbf{v}, \mathbf{k})$ and marginal density $p(\mathbf{k})$ then we can estimate the required $f(\mathbf{q})$. The Gaussian isotropic kernels with

bandwidth σ are given by

$$\hat{p}_\sigma(\mathbf{v}, \mathbf{k}) = \frac{1}{N} \sum_{j \in [N]} \varphi_\sigma(\mathbf{v} - \mathbf{v}_j) \varphi_\sigma(\mathbf{k} - \mathbf{k}_j), \quad \hat{p}_\sigma(\mathbf{k}) = \frac{1}{N} \sum_{j \in [N]} \varphi_\sigma(\mathbf{k} - \mathbf{k}_j), \quad (14)$$

where φ_σ is the multivariate Gaussian density function with diagonal covariance matrix $\sigma^2 \mathbf{I}_D$. Given the kernel density estimators in Eqn. 14, the unknown function can be estimated as

$$\begin{aligned} \hat{f}_\sigma(\mathbf{k}) &= \int_{\mathbb{R}^D} \frac{\mathbf{v} \cdot \hat{p}_\sigma(\mathbf{v}, \mathbf{k})}{\hat{p}_\sigma(\mathbf{k})} d\mathbf{v} = \int_{\mathbb{R}^D} \frac{\mathbf{v} \cdot \sum_{j \in [N]} \varphi_\sigma(\mathbf{v} - \mathbf{v}_j) \varphi_\sigma(\mathbf{k} - \mathbf{k}_j)}{\sum_{j \in [N]} \varphi_\sigma(\mathbf{k} - \mathbf{k}_j)} d\mathbf{v} \\ &= \frac{\sum_{j \in [N]} \varphi_\sigma(\mathbf{k} - \mathbf{k}_j) \int \mathbf{v} \cdot \varphi_\sigma(\mathbf{v} - \mathbf{v}_j) d\mathbf{v}}{\sum_{j \in [N]} \varphi_\sigma(\mathbf{k} - \mathbf{k}_j)} = \frac{\sum_{j \in [N]} \mathbf{v}_j \varphi_\sigma(\mathbf{k} - \mathbf{k}_j)}{\sum_{j \in [N]} \varphi_\sigma(\mathbf{k} - \mathbf{k}_j)}. \end{aligned}$$

Then, using the definition of the Gaussian isotropic kernel and evaluating the estimated function at \mathbf{q}_i we have

$$\begin{aligned} \hat{f}(\mathbf{q}_i) &= \frac{\sum_j^N \mathbf{v}_j \exp(-\|\mathbf{q}_i - \mathbf{k}_j\|^2/2\sigma^2)}{\sum_j^N \exp(-\|\mathbf{q}_i - \mathbf{k}_j\|^2/2\sigma^2)} \\ &= \frac{\sum_j^N \mathbf{v}_j \exp[-(\|\mathbf{q}_i\|^2 + \|\mathbf{k}_j\|^2)/2\sigma^2] \exp(\mathbf{q}_i^\top \mathbf{k}_j/\sigma^2)}{\sum_j^N \exp[-(\|\mathbf{q}_i\|^2 + \|\mathbf{k}_j\|^2)/2\sigma^2] \exp(\mathbf{q}_i^\top \mathbf{k}_j/\sigma^2)} \\ &= \frac{\sum_j^N \mathbf{v}_j \exp(\mathbf{q}_i^\top \mathbf{k}_j/\sigma^2)}{\sum_j^N \exp(\mathbf{q}_i^\top \mathbf{k}_j/\sigma^2)} = \sum_{j \in [N]} \text{softmax}(\mathbf{q}_i^\top \mathbf{k}_j/\sigma^2) \mathbf{v}_j. \end{aligned}$$

Remark 6 Note that relaxing the assumption of normalized keys, the standard unnormalized self-attention score can be written as

$$\begin{aligned} \exp(\mathbf{q}_i^\top \mathbf{k}_j/\sigma^2) &= \exp(-\|\mathbf{q}_i - \mathbf{k}_j\|^2/2\sigma^2) \exp((\|\mathbf{q}_i\|^2 + \|\mathbf{k}_j\|^2)/2\sigma^2) \\ &\propto \exp(-\|\mathbf{q}_i - \mathbf{k}_j\|^2/2\sigma^2), \end{aligned}$$

which shows that the dot-product self-attention scores are proportional to the NW kernel value with Euclidean distance. Hence the assumption of key normalization is sufficient to recover exactly the correspondence between self-attention and NW kernel regression, but not necessary. Analogously, the unnormalized Elliptical Attention score takes the following form:

$$\begin{aligned} \exp(\mathbf{q}_i^\top \mathbf{M} \mathbf{k}_j/\sigma^2) &= \exp(-d(\mathbf{q}_i, \mathbf{k}_j)^2/2\sigma^2) \exp((\|\mathbf{q}_i\|_M^2 + \|\mathbf{k}_j\|_M^2)/2\sigma^2) \\ &\propto \exp(-d(\mathbf{q}_i, \mathbf{k}_j)^2/2\sigma^2), \end{aligned}$$

where $d(\cdot, \cdot)$ is the Mahalanobis distance used in Eqn. 7 and $\|\cdot\|_M$ is the norm in the transformed space with metric d . This observation justifies the use of the transformed dot product instead of the full Mahalanobis distance metric in Eqn. 12 as it preserves the proportionality relationship between the attention computation and the corresponding nonparametric regression estimator with chosen distance metric.

B Technical Proofs

In this section, we present the omitted theorem statements and technical proofs in the main body of the paper.

B.1 Proof of Lemma 1

Let $\mathcal{M} : \mathbb{R}^D \rightarrow \mathbb{R}^N$ be the transformed softmax operator as defined in Lemma 1. We wish to find its Jacobian matrix given by

$$\mathbf{J}_{\mathcal{M}}(\mathbf{q}) = \begin{bmatrix} \frac{\partial \mathcal{M}_1(\mathbf{q})}{\partial q^1} & \frac{\partial \mathcal{M}_1(\mathbf{q})}{\partial q^2} & \cdots & \frac{\partial \mathcal{M}_1(\mathbf{q})}{\partial q^D} \\ \frac{\partial \mathcal{M}_2(\mathbf{q})}{\partial q^1} & \frac{\partial \mathcal{M}_2(\mathbf{q})}{\partial q^2} & \cdots & \frac{\partial \mathcal{M}_2(\mathbf{q})}{\partial q^D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial \mathcal{M}_N(\mathbf{q})}{\partial q^1} & \frac{\partial \mathcal{M}_N(\mathbf{q})}{\partial q^2} & \cdots & \frac{\partial \mathcal{M}_N(\mathbf{q})}{\partial q^D} \end{bmatrix},$$

to measure the sensitivity of each output dimension to a change in each input dimension. Let $\mathcal{M}_j : \mathbb{R}^D \rightarrow \mathbb{R}$ denote the j^{th} component of the output vector for $j \in [N]$, that is, for a vector $\mathbf{q} \in \mathbb{R}^D$,

$$\mathcal{M}_j(\mathbf{q}) = \frac{\exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_j)}{\sum_{s \in [N]} \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_s)}. \quad (16)$$

Let q^i and k_j^i denote the i^{th} coordinates of vectors \mathbf{q} and \mathbf{k}_j , respectively. Then,

$$\begin{aligned} \frac{\partial}{\partial q^i} \ln(\mathcal{M}_j(\mathbf{q})) &= \frac{\partial}{\partial q^i} \left(\mathbf{q}^\top \mathbf{M} \mathbf{k}_j - \ln \left(\sum_{s \in [N]} \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_s) \right) \right) \\ &= m_i k_j^i - \frac{\sum_{s \in [N]} \frac{\partial}{\partial q^i} \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_s)}{\sum_{s \in [N]} \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_s)} \\ &= m_i k_j^i - m_i \sum_{s \in [N]} \frac{k_s^i \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_s)}{\sum_{s' \in [N]} \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_{s'})} \\ &= m_i \left(k_j^i - \sum_{s \in [N]} k_s^i \mathcal{M}_s(\mathbf{q}) \right). \end{aligned}$$

Since the output of Eqn. 16 consists of only positive components, we have

$$\begin{aligned} \frac{\partial}{\partial q^i} \mathcal{M}_j(\mathbf{q}) &= \frac{\partial}{\partial q^i} \ln(\mathcal{M}_j(\mathbf{q})) \cdot \mathcal{M}_j(\mathbf{q}) \\ &= m_i \left(k_j^i - \sum_{s \in [N]} k_s^i \mathcal{M}_s(\mathbf{q}) \right) \mathcal{M}_j(\mathbf{q}). \end{aligned}$$

Therefore, the triangle inequality gives

$$\begin{aligned} \left| \frac{\partial}{\partial q^i} \mathcal{M}_j(\mathbf{q}) \right| &= \left| m_i \left(k_j^i - \sum_{s \in [N]} k_s^i \mathcal{M}_s(\mathbf{q}) \right) \mathcal{M}_j(\mathbf{q}) \right| \\ &\leq m_i \left(|k_j^i (1 - \mathcal{M}_j(\mathbf{q})) \mathcal{M}_j(\mathbf{q})| + \sum_{s \in [N] \setminus \{j\}} |k_s^i \mathcal{M}_s(\mathbf{q}) \mathcal{M}_j(\mathbf{q})| \right). \end{aligned} \quad (17)$$

We now bound each term individually. Consider the terms $j \neq s$ first. Since $0 \leq \mathcal{M}_s(\mathbf{q}) \leq 1$, we can bound them as

$$|k_s^i \mathcal{M}_s(\mathbf{q}) \mathcal{M}_j(\mathbf{q})| \leq |k_s^i|. \quad (18)$$

Now recall that the inequality $ab \leq (a+b)^2/4$ holds for any real numbers a and b with equality holding at $a = b$. Therefore, for the first term, we obtain

$$|k_j^i (1 - \mathcal{M}_j(\mathbf{q})) \mathcal{M}_j(\mathbf{q})| \leq |k_j^i| \frac{(1 - \mathcal{M}_j(\mathbf{q}) + \mathcal{M}_j(\mathbf{q}))^2}{4} = \frac{|k_j^i|}{4}. \quad (19)$$

Combining inequalities 17, 18 and 19, we finally arrive at

$$|\mathcal{J}_{\mathcal{M}}(\mathbf{q})_{ji}| = \left| \frac{\partial}{\partial q^i} \mathcal{M}_j(\mathbf{q}) \right| \leq m_i \left(\frac{|k_j^i|}{4} + \sum_{s \in [N] \setminus \{j\}} |k_s^i| \right) = \kappa_{ij} m_i \quad (20)$$

for all $i \in [D]$ and $j \in [N]$, where $\kappa_{ij} \geq 0$ denotes the coefficient in the bracket. \square

B.2 Proof of Proposition 1

Let us estimate the distance between two output vectors of Elliptical attention mechanism corresponding to clean and contaminated query inputs, namely:

$$\begin{aligned} \mathbf{h} &= \sum_{j \in [N]} \text{softmax}(\mathbf{q}^\top \mathbf{M} \mathbf{k}_j / \sigma^2) \mathbf{v}_j = \sum_{j \in [N]} \mathcal{M}_j(\mathbf{q}) \mathbf{v}_j \\ \mathbf{h}_\epsilon &= \sum_{j \in [N]} \text{softmax}((\mathbf{q} + \epsilon)^\top \mathbf{M} \mathbf{k}_j / \sigma^2) \mathbf{v}_j = \sum_{j \in [N]} \mathcal{M}_j(\mathbf{q} + \epsilon) \mathbf{v}_j, \end{aligned}$$

where \mathcal{M} is defined as in Lemma 1. We omit the keys and scaling parameter for convenience since they do not affect the analysis. Then,

$$\begin{aligned}\|\mathbf{h} - \mathbf{h}_\epsilon\| &= \left\| \sum_{j \in [N]} (\mathcal{M}_j(\mathbf{q}) - \mathcal{M}_j(\mathbf{q} + \boldsymbol{\epsilon})) \mathbf{v}_j \right\| \\ &\leq \sum_{j \in [N]} |\mathcal{M}_j(\mathbf{q}) - \mathcal{M}_j(\mathbf{q} + \boldsymbol{\epsilon})| \|\mathbf{v}_j\| \\ &\leq \sum_{j \in [N]} \|\nabla \mathcal{M}_j(\hat{\mathbf{q}})\| \|\boldsymbol{\epsilon}\| \|\mathbf{v}_j\| \end{aligned} \quad (21)$$

$$\begin{aligned} &= \sum_{j \in [N]} \sqrt{\sum_{i \in [D]} (\mathbf{J}_{\mathcal{M}}(\hat{\mathbf{q}})_{ji})^2} \|\mathbf{v}_j\| \|\boldsymbol{\epsilon}\| \\ &\leq \sum_{j \in [N]} \sqrt{\sum_{i \in [D]} \kappa_{ij}^2 m_i^2} \|\mathbf{v}_j\| \|\boldsymbol{\epsilon}\| \\ &= \sum_{j \in [N]} \sqrt{\text{tr}(\mathbf{K}_j^2 \mathbf{M}^2)} \|\mathbf{v}_j\| \|\boldsymbol{\epsilon}\|, \end{aligned} \quad (22)$$

where $\mathbf{K}_j := \text{diag}(\kappa_{1j}, \kappa_{2j}, \dots, \kappa_{Dj})$ and κ_{ij} is defined as in Eqn. 20. Note that 21 follows from mean value theorem for some $\beta \in [0, 1]$ and $\hat{\mathbf{q}} := \mathbf{q} + \beta \boldsymbol{\epsilon}$ while 22 follows from Lemma 1. \square

It should be noted that Proposition 1 addresses the impact of noise exclusively on the query vectors. However, the resulting bound can be extended to account for noise in all tokens by employing the same technique utilized in the proof. For completeness, we also provide the extension. Let $\mathcal{M} : \mathbb{R}^D \times \underbrace{\mathbb{R}^D \times \dots \times \mathbb{R}^D}_N \rightarrow \mathbb{R}^N$ be the Elliptical Softmax function defined as

$$\mathcal{M}(\mathbf{q}, \mathbf{k}_1, \dots, \mathbf{k}_N) = \frac{1}{\sum_{j \in [N]} \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_j)} \begin{bmatrix} \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_1) \\ \vdots \\ \exp(\mathbf{q}^\top \mathbf{M} \mathbf{k}_N) \end{bmatrix}. \quad (23)$$

Again, take the difference between output vectors calculated from clean and noisy tokens as follows

$$\mathbf{h}_\epsilon = \sum_{j \in [N]} \mathcal{M}_j(\mathbf{q} + \boldsymbol{\epsilon}_q, \mathbf{k}_1 + \boldsymbol{\epsilon}_k, \dots, \mathbf{k}_N + \boldsymbol{\epsilon}_k) (\mathbf{v}_j + \boldsymbol{\epsilon}_v), \quad (24)$$

$$\mathbf{h} = \sum_{j \in [N]} \mathcal{M}_j(\mathbf{q}, \mathbf{k}_1, \dots, \mathbf{k}_N) \mathbf{v}_j. \quad (25)$$

Let $\|\bar{\boldsymbol{\epsilon}}\| := \max\{\|\boldsymbol{\epsilon}_q\|, \|\boldsymbol{\epsilon}_k\|, \|\boldsymbol{\epsilon}_v\|\}$ denote the noise with the largest norm among query, key and value noises. Then,

$$\begin{aligned}\|\mathbf{h}_\epsilon - \mathbf{h}\| &\leq \sum_{j \in [N]} |\mathcal{M}_j(\mathbf{q} + \boldsymbol{\epsilon}_q, \mathbf{k}_1 + \boldsymbol{\epsilon}_k, \dots, \mathbf{k}_N + \boldsymbol{\epsilon}_k) - \mathcal{M}_j(\mathbf{q}, \mathbf{k}_1, \dots, \mathbf{k}_N)| \|\mathbf{v}_j\| \\ &\quad + \sum_{j \in [N]} \mathcal{M}_j(\mathbf{q} + \boldsymbol{\epsilon}_q, \mathbf{k}_1 + \boldsymbol{\epsilon}_k, \dots, \mathbf{k}_N + \boldsymbol{\epsilon}_k) \|\boldsymbol{\epsilon}_v\| \end{aligned} \quad (26)$$

$$\leq \sum_{j \in [N]} \left(\|\nabla_{\mathbf{q}} \mathcal{M}_j(\bar{\mathbf{q}})\| + \sum_{s \in [N]} \|\nabla_{\mathbf{k}_s} \mathcal{M}_j(\bar{\mathbf{k}}_s)\| \right) \|\bar{\boldsymbol{\epsilon}}\| \|\mathbf{v}_j\| + \|\bar{\boldsymbol{\epsilon}}\|. \quad (27)$$

Following the same steps as Lemma 1, one can derive the bound

$$\left| \frac{\partial}{\partial k_s^i} \mathcal{M}_j \right| \leq m_i \cdot |q^i| \left(1 - \frac{3\delta_{sj}}{4} \right) \propto m_i \quad (28)$$

for $s, j \in [N]$. Therefore, we obtain

$$\|\mathbf{h}_\epsilon - \mathbf{h}\| \leq \left(1 + \sum_{j \in [N]} \sum_{s \in [N+1]} \sqrt{\text{tr}(\mathbf{C}_{s,j}^2 \mathbf{M}^2)} \|\mathbf{v}_j\| \right) \|\bar{\boldsymbol{\epsilon}}\|, \quad (29)$$

where $\mathbf{C}_{s,j}$ are the diagonal matrices whose elements are the proportionality coefficients in the derived upper bounds.

B.3 Proof of Proposition 2

There are two avenues through which to see resistance to representation collapse. In this section, we provide a proof based on noise propagation through layers, which decreases representation capacity as representations in deeper layers are increasingly composed of uninformative noise. We refer the reader to Appendix B.4 for an additional lens on representation collapse, where we show that Elliptical Attention is more sensitive to the variation and local features of the underlying function.

Let the output at layer ℓ be denoted as h^ℓ , the standard self-attention estimator and Elliptical estimator fitted at layer ℓ be denoted \hat{f}^ℓ and \hat{f}_d^ℓ respectively, where d is the Mahalanobis metric described in Eqn. 7, and f be the true underlying function described in Eqn. 3. By assumption, \hat{f} is a higher variance estimator than \hat{f}_d for any layer. The output for either estimator at layer ℓ can be decomposed into ground truth and noise as follows:

$$h^\ell = \hat{f}^\ell(q^\ell) = f(q^\ell) + \epsilon^\ell \quad (30)$$

$$h_d^\ell = \hat{f}_d^\ell(q^\ell) = f(q^\ell) + \eta^\ell, \quad (31)$$

where $\eta^\ell \sim \gamma(\mathbf{0}, V_\eta)$, $\epsilon^\ell \sim \gamma(\mathbf{0}, V_\epsilon)$ are the noise components of the estimate at q^ℓ and $f(q^\ell)$ is the ground truth. By assumption of \hat{f}_d being lower variance, $V_\epsilon - V_\eta$ is a positive semi-definite matrix.

We first require the following Assumption 1, which is described as:

Assumption 1 (Random Input Noise Causes Estimator Attenuation) . Let \hat{f} be any estimator of true function f and let the input $x \sim \mu$ drawn from marginal μ be randomly corrupted by random noise $\epsilon \sim (0, \mathbf{V})$ of some unknown distribution and covariance matrix \mathbf{V} . Let c be some constant. Then, random input noise attenuates the estimator as follows:

$$\mathbb{E}_{x, \epsilon} \|\hat{f}(x + \epsilon) - c\| \leq \mathbb{E}_x \|\hat{f}(x) - c\| \quad (32)$$

Assumption 1 is a well-studied phenomenon in parametric regression, often referred to as attenuation bias [69], regression dilution [19], or errors-in-variables [34]. In parametric regression, it can be shown to have an exact form where the estimated gradients of the model are attenuated towards 0 proportional to the variance of the noise ϵ . In non-parametric regression, addition of input noise is often referred to as random smoothing or random input smoothing [46, 10], and is well known to be used as regularization technique to introduce bias into the model. In non-parametric models, no exact closed forms exist to express the attenuation bias, but for our purposes we only note the attenuation exists and provide a general form of it in Assumption 1.

The outputs of 30 and 31 then become the inputs to the following layer after being self-added, normalized, projected, and linearly transformed. For notational simplicity and because these operations do not change the analysis, we denote the input at the next layer as the previous layer output $q^{\ell+1} = h^\ell$. We therefore have the following process:

$$h^{\ell+1} = \hat{f}^{\ell+1}(q^{\ell+1}) = \hat{f}^{\ell+1}(h^\ell) = \hat{f}^{\ell+1}(\underbrace{f(q^\ell) + \epsilon^\ell}_{z^\ell}), \quad (33)$$

where we see the output $h^{\ell+1}$ is obtained by fitting $\hat{f}^{\ell+1}$ to input z^ℓ which is composed of ground truth $f(q^\ell)$ and noise ϵ^ℓ passed through from the previous layer.

The result then follows directly from the fact that in any given layer, the standard self-attention estimator produces noisier estimates, where that noise is then passed into the subsequent layer as input noise. This is

$$\mathbb{E} \|h^{\ell+1} - c\| = \mathbb{E} \|\hat{f}^{\ell+1}(q^{\ell+1}) - c\| = \mathbb{E} \|\hat{f}^{\ell+1}(f(q^\ell) + \epsilon^\ell) - c\| \quad (34)$$

$$\leq \mathbb{E} \|\hat{f}^{\ell+1}(f(q^\ell) + \eta^\ell) - c\| \quad (35)$$

$$\approx \mathbb{E} \|\hat{f}_d^{\ell+1}(f(q^\ell) + \eta^\ell) - c\| \quad (36)$$

$$= \mathbb{E} \|\hat{f}_d^{\ell+1}(f(q^{\ell+1}) - c\| = \mathbb{E} \|h_d^{\ell+1} - c\|, \quad (37)$$

where line 35 follows from combining the fact that η^ℓ is lower variance with Assumption 1 and line 36 follows from the fact that $\mathbb{E} \|X\| \approx \mathbb{E} \|Y\|$ when X, Y have the same mean and roughly similar distribution.

Therefore we obtain at any layer ℓ the following

$$\mathbb{E}\|\mathbf{h}^{\ell+1} - \mathbf{c}\| \leq \mathbb{E}\|\mathbf{h}_d^{\ell+1} - \mathbf{c}\|, \quad (38)$$

as required. \square

B.4 Edge-preservation Perspective on Representation Collapse

To further substantiate our findings on the mitigation of representation collapse in transformers, we now present an additional proposition that examines this phenomenon from a different perspective. In Proposition 4, we show that Elliptical attention reduces representation collapse by retaining the important local features (bumps etc.) better than the standard self-attention in the case of sparse piece-wise constant functions.

Proposition 4 (Representation Collapse) *Let $f : A \rightarrow \mathbb{R}^D$ for $A \subseteq \mathbb{R}^D$ be a piece-wise constant function with $f|_{A_i}(\mathbf{q}) = \mathbf{f}_i \in \mathbb{R}^D$ where $A = \bigcup_{i \in I} A_i$ for some (possibly infinite) index I . Let \mathbf{q}_1 and \mathbf{q}_2 be the queries lying in any of the adjacent domain pieces with distant function values. Then, the Elliptical estimates at these queries retain the distance better than the standard self-attention estimates which is formulated as*

$$\mathbb{E}\|\hat{f}_d(\mathbf{q}_2) - \hat{f}_d(\mathbf{q}_1)\| \geq \mathbb{E}\|\hat{f}(\mathbf{q}_2) - \hat{f}(\mathbf{q}_1)\|. \quad (39)$$

Proof. Assume all output vectors are normalized. Then, the Euclidean distance between two vectors is determined by their dot product since

$$\|\mathbf{a} - \mathbf{b}\|^2 = \|\mathbf{a}\|^2 + \|\mathbf{b}\|^2 - 2\mathbf{a}^\top \mathbf{b}. \quad (40)$$

Without loss of generality, we take A_1 and A_2 to be the two adjacent pieces so that $f(\mathbf{q}_i) = \mathbf{f}_i$ for $i = 1, 2$. Denote $\hat{f}(\mathbf{q}_i) = \mathbf{h}_i$ and $\hat{f}_d(\mathbf{q}_i) = \mathbf{h}_{id}$. Then, Eqn. 39 is equivalent to proving

$$\mathbb{E}_{\mathcal{D}}[\mathbf{h}_{1d}^\top \mathbf{h}_{2d}] \leq \mathbb{E}_{\mathcal{D}}[\mathbf{h}_1^\top \mathbf{h}_2], \quad (41)$$

where the expectation is taken over the whole sampling distribution \mathcal{D} but the points $\mathbf{q}_1 \in A_1$ and $\mathbf{q}_2 \in A_2$ are fixed as described in the definition. We drop the subscript \mathcal{D} as this will be the default distribution for computing expectation unless specified otherwise. Let $r_S = \text{cossim}(\mathbf{f}_1, \mathbf{f}_2) = \mathbf{f}_1^\top \mathbf{f}_2$ be the cosine similarity of the two piece-wise values. By definition of \mathbf{q}_1 and \mathbf{q}_2 and since the estimates work by averaging the output vectors with a small amount of noise, we have $r_S \leq \min \left\{ \mathbb{E}[\mathbf{h}_{1d}^\top \mathbf{h}_{2d}], \mathbb{E}[\mathbf{h}_1^\top \mathbf{h}_2] \right\}$. We now decompose \mathbf{h}_{1d} and \mathbf{h}_{2d} in terms of components along and orthogonal to \mathbf{f}_1 and \mathbf{f}_2 , respectively:

$$\mathbf{h}_{1d} = (\mathbf{h}_{1d}^\top \mathbf{f}_1) \mathbf{f}_1 + \mathbf{f}_1^\perp, \quad \mathbf{h}_{2d} = (\mathbf{h}_{2d}^\top \mathbf{f}_2) \mathbf{f}_2 + \mathbf{f}_2^\perp, \quad (42)$$

where $\mathbf{f}_i^\top \mathbf{f}_i^\perp = 0$. Then, for their dot product, we have

$$\begin{aligned} \mathbf{h}_{1d}^\top \mathbf{h}_{2d} &= \left[(\mathbf{h}_{1d}^\top \mathbf{f}_1) \mathbf{f}_1 + \mathbf{f}_1^\perp \right]^\top \left[(\mathbf{h}_{2d}^\top \mathbf{f}_2) \mathbf{f}_2 + \mathbf{f}_2^\perp \right] \\ &= (\mathbf{h}_{1d}^\top \mathbf{f}_1)(\mathbf{h}_{2d}^\top \mathbf{f}_2) \mathbf{f}_1^\top \mathbf{f}_2 + (\mathbf{h}_{1d}^\top \mathbf{f}_1) \mathbf{f}_1^\top \mathbf{f}_2^\perp \\ &\quad + (\mathbf{h}_{2d}^\top \mathbf{f}_2) \mathbf{f}_2^\top \mathbf{f}_1^\perp + (\mathbf{f}_1^\perp)^\top \mathbf{f}_2^\perp. \end{aligned} \quad (43)$$

The analogous decomposition of $\mathbf{h}_1^\top \mathbf{h}_2$ can be obtained. By Theorem 2 we have that the Elliptical estimator is lower variance and so we have $\mathbb{E}\|\mathbf{f}_i - \mathbf{h}_{id}\|^2 \leq \mathbb{E}\|\mathbf{f}_i - \mathbf{h}_i\|^2$. This has the following implications:

1. $1 \geq \mathbb{E}[\mathbf{h}_{id}^\top \mathbf{f}_i] \geq \mathbb{E}[\mathbf{h}_i^\top \mathbf{f}_i]$ i.e. the component of \mathbf{h}_{id} along \mathbf{f}_i is larger than that of \mathbf{h}_i , and hence $\mathbf{h}_{id}^\top \mathbf{f}_i$ is closer to 1.
2. Due to the first implication above, the orthogonal component \mathbf{f}_i^\perp becomes smaller in terms of magnitude so that $\mathbf{f}_j^\top \mathbf{f}_i^\perp$ and $(\mathbf{f}_i^\perp)^\top \mathbf{f}_j^\perp$ are closer to 0 for Elliptical compared to the standard self-attention.

These two arguments, combined with Eqn. 43, imply that in expectation $\mathbf{h}_{1d}^\top \mathbf{h}_{2d}$ is closer to $1 \cdot (\mathbf{f}_1^\top \mathbf{f}_2) + 0 = \mathbf{f}_1^\top \mathbf{f}_2 = r_S$ which, by definition, is the smallest dot product over S , and hence, $r_S \leq \mathbb{E}[\mathbf{h}_{1d}^\top \mathbf{h}_{2d}] \leq \mathbb{E}[\mathbf{h}_1^\top \mathbf{h}_2]$ as desired. \square

B.5 Proof of Proposition 3

The lemma below encapsulates the necessary calculations that will then be used in the following proofs.

Lemma 2 *Given a normally distributed zero mean random variable $\xi \sim \mathcal{N}(0, \sigma^2)$, the expectation of a random variable obtained by its absolute value is $\mathbb{E}|\xi| = \sqrt{2\sigma^2/\pi}$.*

Proof. Since $\xi \sim \mathcal{N}(0, \sigma^2)$, by definition of expectation, we have

$$\begin{aligned} \mathbb{E}|\xi| &= \int_{-\infty}^{\infty} \frac{|x|}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) dx \\ &= \int_{-\infty}^0 \frac{-x}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) dx + \int_0^{\infty} \frac{x}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{x^2}{2\sigma^2}\right) dx \end{aligned} \quad (44)$$

$$\begin{aligned} &= \frac{2}{\sqrt{2\pi\sigma^2}} \int_0^{\infty} x \exp\left(-\frac{x^2}{2\sigma^2}\right) dx \\ &= \sqrt{\frac{2}{\pi\sigma^2}} \left[-\sigma^2 \exp\left(-\frac{x^2}{2\sigma^2}\right) \right]_0^{\infty} \\ &= \sqrt{\frac{2\sigma^2}{\pi}}, \end{aligned} \quad (45)$$

where we used the variable change $x \leftarrow (-x)$ in the first integral of 44 to obtain 45. \square

We derive the bounds for the impact of noise in 3, with respect to its variance, on our estimator 10 in Lemma 3. Henceforth, we omit the factor δ in Eqn. 10 since it does not affect the further analysis.

Lemma 3 *Given that the noise term in 3 follows a normal distribution with zero mean and variance σ^2 , the following inequality*

$$\left| m_i - \mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^{\ell})| \right| \leq \frac{2}{\sqrt{\pi}} \sigma \quad (46)$$

holds for all $i \in [D]$, where f_i denotes the i^{th} component of $f(\mathbf{k}^{\ell}) = (f_1(\mathbf{k}), f_2(\mathbf{k}), \dots, f_D(\mathbf{k}))^{\top}$.

Proof. Since all value vectors are taken from the data generating process 3, we have

$$\begin{aligned} m_i &= \mathbb{E}_{(\mathbf{v}^{\ell}, \mathbf{v}^{\ell+1}) \in \mathcal{X}_v^{\ell, \ell+1}} |\mathbf{v}_i^{\ell+1} - \mathbf{v}_i^{\ell}| \\ &= \mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^{\ell}) + \epsilon_i^{\ell+1} - \epsilon_i^{\ell}|, \end{aligned} \quad (47)$$

where ϵ_i^{ℓ} and $\epsilon_i^{\ell+1}$ denote the i^{th} components of the noise terms ϵ^{ℓ} and $\epsilon^{\ell+1}$, respectively. Note that for real numbers a and b , we have by triangle inequality that $|a + b| \leq |a| + |b|$ and $|a + b| = |a - (-b)| \geq ||a| - |-b|| \geq |a| - |b|$. Applying these and the linearity of expectation to 47, we obtain

$$\mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^{\ell})| - \mathbb{E}|\epsilon_i^{\ell+1} - \epsilon_i^{\ell}| \leq m_i \leq \mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^{\ell})| + \mathbb{E}|\epsilon_i^{\ell+1} - \epsilon_i^{\ell}| \quad (48)$$

Recall that $\epsilon_i^{\ell} \sim \mathcal{N}(0, \sigma^2)$ and independent. Now we have that $\epsilon_i^{\ell+1} - \epsilon_i^{\ell} \sim \mathcal{N}(0, 2\sigma^2)$ as the mean value does not change while variance accumulates when subtracting two zero-mean normal variables. Therefore, the Lemma 2 gives that

$$\mathbb{E}|\epsilon_i^{\ell+1} - \epsilon_i^{\ell}| = \frac{2}{\sqrt{\pi}} \sigma.$$

Plugging this back into the inequalities 48, we get

$$\mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^{\ell})| - \frac{2}{\sqrt{\pi}} \sigma \leq m_i \leq \mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^{\ell})| + \frac{2}{\sqrt{\pi}} \sigma,$$

which is equivalent to 46 as desired. \square

Remark 7 *Note that in Lemma 3, we may also take into account the possible noise in the value vectors. Let $\epsilon_{i,v}^{\ell} \sim \mathcal{N}(0, \sigma_v^2)$ be the noise in the values vectors as $m_i^{\epsilon} = \mathbb{E}|\mathbf{v}_i^{\ell+1} - \mathbf{v}_i^{\ell} + \epsilon_{i,v}^{\ell+1} - \epsilon_{i,v}^{\ell}|$. Then, applying the triangle inequality, we obtain*

$$\mathbb{E}|\mathbf{v}^{\ell+1} - \mathbf{v}^{\ell}| - \mathbb{E}|\epsilon_{i,v}^{\ell+1} - \epsilon_{i,v}^{\ell}| \leq m_i^{\epsilon} \leq \mathbb{E}|\mathbf{v}^{\ell+1} - \mathbf{v}^{\ell}| + \mathbb{E}|\epsilon_{i,v}^{\ell+1} - \epsilon_{i,v}^{\ell}|.$$

Now applying Lemma 2 and Lemma 3, we arrive at

$$\left| m_i^{\epsilon} - \mathbb{E}|f(\mathbf{k}^{\ell+1}) - f(\mathbf{k}^{\ell})| \right| \leq \frac{2}{\sqrt{\pi}} (\sigma + \sigma_v).$$

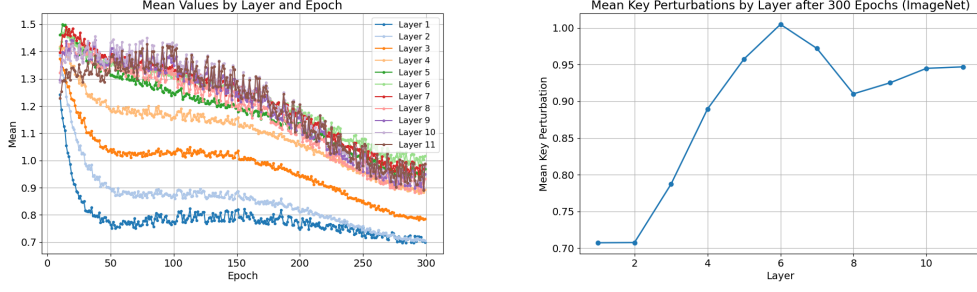


Figure 5: **Left:** Evolution of mean values of key perturbations over successive layers. **Right:** Mean key perturbations at different layers after 300 epochs. The figures show that as the number of layers increases, mean key perturbations over layers stabilize around a constant value.

Proof of Proposition 3. We shall first make the following assumptions on the data generating process 3:

Assumption 2 The underlying coordinate system in the feature space \mathcal{X}_k is independent, implying that the function $f : \mathbb{R}^D \rightarrow \mathbb{R}^D$ in Eqn. 3 can be separated as $f(\mathbf{k}) = (f_1(k_1), \dots, f_D(k_D))^T$

Assumption 3 The noise term in Eqn. 3 has independent components with each component ϵ_j^ℓ following a normal distribution $\mathcal{N}(0, \sigma^2)$ for small σ , for all $j \in [D]$ and $\ell \in \mathbb{N}$

Assumption 4 The magnitude of each component of key perturbations across consecutive layers, defined as $|k_i^{\ell+1} - k_i^\ell|$, follows a distribution with small, layer-independent mean (δ) and variance (ν)

Remark 8 The assumption of layer-independence in Assumption 4, especially for deeper layers, is supported well empirically, as shown in Figure 5. Given the over-smoothing observed in transformers [24], where token representations stabilize after initial few layers, it is also practical to assume that key perturbations across layers have relatively small mean and variance when modelled as a random process.

Proof. Under the Assumptions 2, 3, 4, we show that $\|f'_i\|_{1,\mu} \geq \|f'_j\|_{1,\mu}$ implies $m_i \geq m_j$ with high probability where m_i is defined as in (10).

Directly from the Lemma 3, we have

$$|m_i - \mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^\ell)|| \leq \frac{2}{\sqrt{\pi}}\sigma.$$

Letting $\sigma \rightarrow 0$ in this inequality, which is feasible under the Assumption 3, one can get with a small error that

$$m_i \approx \mathbb{E}|f_i(\mathbf{k}^{\ell+1}) - f_i(\mathbf{k}^\ell)|, \quad (49)$$

which in turn implies that the impact of the noise in (10) is negligible and the error of ignoring them can be controlled by the bounds given by (46). Now according to the theorem statement,

$$\begin{aligned} \|f'_i\|_{1,\mu} \geq \|f'_j\|_{1,\mu} &\iff \mathbb{E}\|\mathbf{J}_f(\mathbf{k})\mathbf{e}_i\|_1 \geq \mathbb{E}\|\mathbf{J}_f(\mathbf{k})\mathbf{e}_j\|_1 \\ &\iff \mathbb{E}\left[\sum_{s \in [D]} \left|\frac{\partial f_s(\mathbf{k})}{\partial k_i}\right|\right] \geq \mathbb{E}\left[\sum_{s \in [D]} \left|\frac{\partial f_s(\mathbf{k})}{\partial k_j}\right|\right] \\ &\iff \mathbb{E}|f'_i(k_i)| \geq \mathbb{E}|f'_j(k_j)| \end{aligned} \quad (50)$$

where we used the separability of f as given in Assumption 2 which simplifies the Jacobian matrix as

$$\begin{aligned} \mathbf{J}_f(\mathbf{k}) &= \begin{bmatrix} \frac{\partial f_1(\mathbf{k})}{\partial k_1} & \frac{\partial f_1(\mathbf{k})}{\partial k_2} & \cdots & \frac{\partial f_1(\mathbf{k})}{\partial k_D} \\ \frac{\partial f_2(\mathbf{k})}{\partial k_1} & \frac{\partial f_2(\mathbf{k})}{\partial k_2} & \cdots & \frac{\partial f_2(\mathbf{k})}{\partial k_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_D(\mathbf{k})}{\partial k_1} & \frac{\partial f_D(\mathbf{k})}{\partial k_2} & \cdots & \frac{\partial f_D(\mathbf{k})}{\partial k_D} \end{bmatrix} = \begin{bmatrix} \frac{\partial f_1(k_1)}{\partial k_1} & \frac{\partial f_1(k_1)}{\partial k_2} & \cdots & \frac{\partial f_1(k_1)}{\partial k_D} \\ \frac{\partial f_2(k_2)}{\partial k_1} & \frac{\partial f_2(k_2)}{\partial k_2} & \cdots & \frac{\partial f_2(k_2)}{\partial k_D} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial f_D(k_D)}{\partial k_1} & \frac{\partial f_D(k_D)}{\partial k_2} & \cdots & \frac{\partial f_D(k_D)}{\partial k_D} \end{bmatrix} \\ &= \begin{bmatrix} f'_1(k_1) & 0 & \cdots & 0 \\ 0 & f'_2(k_2) & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & f'_D(k_D) \end{bmatrix}, \end{aligned}$$

so that $[\mathbf{J}_f(\mathbf{k})]_{ii} = f'_i(k_i)$. Using the definition of derivative, the inequality 50 is equivalent to

$$\mathbb{E} \left| \lim_{\tau \rightarrow 0} \frac{f^i(k_i^\ell + \tau) - f^i(k_i^\ell)}{\tau} \right| \geq \mathbb{E} \left| \lim_{\tau \rightarrow 0} \frac{f^j(k_j^\ell + \tau) - f^j(k_j^\ell)}{\tau} \right|. \quad (51)$$

Next, we note that for a small δ , the limits in (51) can be approximated with $\frac{f^s(k_s^\ell + \delta) - f^s(k_s^\ell)}{\delta}$ for $s \in \{i, j\}$:

$$\frac{\mathbb{E}|f^i(k_i^\ell + \delta) - f^i(k_i^\ell)|}{\delta} \geq \frac{\mathbb{E}|f^j(k_j^\ell + \delta) - f^j(k_j^\ell)|}{\delta}. \quad (52)$$

Let us choose $\delta = \mathbb{E}|k_i^{\ell+1} - k_i^\ell|$. Then, by Chebyshev's inequality, we have for any $\varepsilon > 0$ that

$$\begin{aligned} 1 - \frac{\nu^2}{\varepsilon^2} &\leq \mathbb{P}(|k_i^{\ell+1} - k_i^\ell| - \delta \leq \varepsilon) \\ &= \mathbb{P}(\delta - \varepsilon \leq |k_i^{\ell+1} - k_i^\ell| \leq \delta + \varepsilon). \end{aligned} \quad (53)$$

Given that the variance ν is sufficiently small as in the Assumption 4, the inequality (53) implies that $k_i^{\ell+1} \approx k_i^\ell \pm \delta$ with high probability. Therefore, it follows from (52) with high probability that

$$\frac{\mathbb{E}|f^i(k_i^{\ell+1}) - f^i(k_i^\ell)|}{\delta} \geq \frac{\mathbb{E}|f^j(k_j^{\ell+1}) - f^j(k_j^\ell)|}{\delta},$$

which, due to 49, is equivalent to $m_i \geq m_j$ as desired. \square

B.6 Lipschitz smoothness in (\mathcal{X}, d)

Below we show how Lipschitz smoothness of f changes when moving from Euclidean to the Mahalanobis transformed space. We shall follow similar steps to [29] and [30] but for a more general class of functions.

Proposition 5 (Change in Lipschitz smoothness for f) *Suppose there exists a positive constant G_i such that $\|\nabla f_i(\mathbf{k})\| \leq G_i$ for any $\mathbf{k} \in \mathcal{X}_{\mathbf{k}}$ and $m_i > 0$ for all $i \in [D]$. Then for any $\mathbf{q}, \mathbf{k} \in \mathcal{X}_{\mathbf{k}}$, the following inequality holds:*

$$\|f(\mathbf{q}) - f(\mathbf{k})\| \leq \left(\sum_{i \in [D]} \frac{G_i}{\sqrt{m_i}} \right) d(\mathbf{q}, \mathbf{k}).$$

Proof. Let $\boldsymbol{\omega} := \frac{\mathbf{q} - \mathbf{k}}{\|\mathbf{q} - \mathbf{k}\|}$ denote the unit vector pointing from \mathbf{k} to \mathbf{q} . The fundamental theorem of calculus implies that

$$f(\mathbf{q}) - f(\mathbf{k}) = \int_0^{\|\mathbf{q} - \mathbf{k}\|} \frac{d}{dt} f(\mathbf{k} + t\boldsymbol{\omega}) dt = \int_0^{\|\mathbf{q} - \mathbf{k}\|} \boldsymbol{\omega}^\top \mathbf{J}_f(\mathbf{k} + t\boldsymbol{\omega}) dt,$$

where \mathbf{J}_f is the Jacobian matrix of f as usual. Starting with the distance between outputs $f(\mathbf{q})$ and $f(\mathbf{k})$ we have

$$\begin{aligned} \|f(\mathbf{q}) - f(\mathbf{k})\| &= \left\| \int_0^{\|\mathbf{q} - \mathbf{k}\|} \boldsymbol{\omega}^\top \mathbf{J}_f(\mathbf{k} + t\boldsymbol{\omega}) dt \right\| \leq \int_0^{\|\mathbf{q} - \mathbf{k}\|} \left\| \sum_{i \in [D]} \omega_i \nabla f_i(\mathbf{k} + t\boldsymbol{\omega}) \right\| dt \\ &\leq \int_0^{\|\mathbf{q} - \mathbf{k}\|} \sum_{i \in [D]} |\omega_i| \|\nabla f_i(\mathbf{k} + t\boldsymbol{\omega})\| dt \leq \sum_{i \in [D]} G_i |\omega_i| \int_0^{\|\mathbf{q} - \mathbf{k}\|} dt \\ &= \sum_{i \in [D]} G_i |q_i - k_i|, \end{aligned} \quad (54)$$

where, as for all other vectors, q_i denotes the i^{th} component of vector \mathbf{q} . Now note that

$$|q_i - k_i| \leq \sqrt{(q_i - k_i)^2 + \sum_{j \neq i} \frac{m_j}{m_i} (q_j - k_j)^2} = \sqrt{\frac{(\mathbf{q} - \mathbf{k})^\top \mathbf{M}(\mathbf{q} - \mathbf{k})}{m_i}} = \frac{d(\mathbf{q}, \mathbf{k})}{\sqrt{m_i}}. \quad (55)$$

Combining 54 and 55, we finally attain

$$\|f(\mathbf{q}) - f(\mathbf{k})\| \leq \sum_{i \in [D]} \frac{G_i}{\sqrt{m_i}} d(\mathbf{q}, \mathbf{k}), \quad (56)$$

which completes the proof. \square

C Additional Theorems

The following Theorem 1 is a classic result from [70]. We refer the reader to their work for details.

Theorem 1 (Minimax rate for functions of bounded variability [70]) *Let F_λ denote the class of distributions $P_{X,Y}$ on $\mathcal{X} \times [0, 1]$ such that $\forall i \in [d]$, the directional derivatives of $f(x) := \mathbb{E}[Y|X = x]$ satisfy $|f'_i|_{\sup} := \sup_{\mathbf{q} \in \mathcal{X}_k} \|\nabla f_i(\mathbf{q})\|_{\sup} \leq \lambda$. Then for any $f \in F_\lambda$, estimator \hat{f} , sample size $n \in \mathbb{N}$, there exists a $\tilde{c} \leq 1$ independent of n satisfying*

$$\inf_{f_n} \sup_{f \in F_\lambda} \mathbb{E}_{X^n, Y^n} \|\hat{f} - f\|^2 \geq 2\tilde{c}^{2/(2+d)} (d\lambda)^{2d/(2+d)} n^{-2/(2+d)} \quad (57)$$

Theorem 2 (Improvement in MSE for approximately sparse functions [30]) *Let the norm of the largest gradient be $\lambda := \sup_{i \in [D]} \|\nabla f_i(\mathbf{q})\|_{\sup}$ and \hat{f}_d be an estimator in metric space (\mathcal{X}_q, d) where d is defined as Eqn. 7. Then,*

$$\mathbb{E} \|\hat{f}_d - f\|_2^2 < \inf_{\tilde{f}} \sup_{\mathcal{F}_\lambda} \mathbb{E} \|\tilde{f} - f\|_2^2. \quad (58)$$

Proof. We provide an abridged proof for completeness. We refer the reader to [30] for the full details.

First, the full bound is described as follows:

$$\mathbb{E} \|\hat{f}_d - f\|_2^2 \leq 2C_{\kappa_R}^{2/2+r} (CD\lambda_d d(\mathcal{X}))^{2r/2+r} n^{-2/2+r} < \inf_{\tilde{f}} \sup_{\mathcal{F}_\lambda} \mathbb{E} \|\tilde{f} - f\|_2^2, \quad (59)$$

where $d(\mathcal{X})$ is the d-diameter of \mathcal{X} defined as $\sup_{x, x' \in \mathcal{X}} d(x, x')$, $R \subset [D]$, $1 \leq C_{\kappa_R} \leq C'(4\kappa_R)^{|R|}$, C and C_1 are universal constants and $\lambda_d \geq \sup_i \|f'_i\|_{\sup} / \sqrt{m_i}$. Let

$$r(\epsilon) \leq \begin{cases} |R| & \text{if } \epsilon \geq \epsilon_R/d(\mathcal{X}) \\ D - (D - |R|) \frac{\log(d(\mathcal{X})/\epsilon_R)}{\log(1/\epsilon)} & \text{if } \epsilon < \epsilon_R/d(\mathcal{X}) \end{cases}.$$

For bandwidth ϵ_n , $r = r(\epsilon_n)$ and let $|R| \leq r \leq D$. Let $\epsilon > 0$, \tilde{c} be defined as the same \tilde{c} in Theorem 1, and $n \in \mathbb{N}$, define the function $\psi_{n,d} = C\epsilon^{-r(\epsilon)}/n$ and $\psi_{n,\mathcal{A}}(\epsilon) = C'_1\epsilon^{-D}/n$ where $C_1 = \tilde{c}(\lambda/C\lambda_d d(\mathcal{X}))^D$. Also define $\phi(\epsilon) = C^2 D^2 \lambda_d^2 d(\mathcal{X})^2 \cdot \epsilon^2$.

For any fixed n , let $\epsilon_{n,\mathcal{A}}$ be a solution to $\psi_{n,\mathcal{A}}(\epsilon) = \phi(\epsilon)$. Solving for $\epsilon_{n,\mathcal{A}}$ obtains the following lower bound on the minmax rate of

$$2\phi(\epsilon_{n,\mathcal{A}}) = 2\tilde{c}^{2/(2+D)} (D\lambda)^{2d/(2+d)} n^{-2/(2+d)}. \quad (60)$$

For any $n \in \mathbb{N}$ there exists a solution $\epsilon_{n,d}$ to the equation $\psi_{n,d}(\epsilon) = \phi(\epsilon)$ since $r(\epsilon)$ is nondecreasing. Therefore it is possible to obtain the following:

$$\mathbb{E}_{X^n, Y^n} \|f_{n,\epsilon,d} - f\|_2^2 \leq 2\phi(\epsilon_{n,d}). \quad (61)$$

Since ϕ is independent of n , and both $\psi_{n,d}$ and $\psi_{n,\mathcal{A}}$ are strictly decreasing functions of n , we have that $\epsilon_{n,d}$ and $\epsilon_{n,\mathcal{A}}$ both tend to 0 as $n \rightarrow \infty$. Therefore we can define n_0 such that, for all $n \geq n_0$, both $\epsilon_{n,d}$ and $\epsilon_{n,\mathcal{A}}$ are less than $\epsilon_R/d(\mathcal{X})$.

Thus, $\forall n \geq n_0$, we have $\epsilon_{n,d} < \epsilon_{n,\mathcal{A}}$ if, for all $0 < \epsilon < \epsilon_R/d(\mathcal{X})$, $\psi_{n,d}(\epsilon) < \psi_{n,\mathcal{A}}(\epsilon)$, which completes the proof \square .

D A Consistent Estimator

In this section, we present a consistent centered difference-based quotient estimator of the coordinate-wise variability obtained by perturbing the estimated function in the i^{th} direction and measuring the L_1 norm of the difference. Similarly, this estimator requires no learnable parameters or gradients. The estimator is described in the following proposition.

Proposition 6 (Consistent Estimator) *Given a function $f : \mathbb{R}^D \rightarrow \mathbb{R}^{D_v}$ with i th directional variation $\|f'_i\|_{1,\mu}, i \in [D]$, the directional variation can be estimated by the quantity*

$$\hat{m}_i := \mathbb{E}_n \left[\frac{\|\bar{f}(\mathbf{k} + t\mathbf{e}_i) - \bar{f}(\mathbf{k} - t\mathbf{e}_i)\|_1}{2t} \right], \quad (62)$$

where t is a hyperparameter controlling the degree of locality of the estimator and \mathbb{E}_n denotes the empirical expectation for n samples.

Despite \hat{m}_i in proposition 6's simple formulation, it is nonetheless a consistent estimator of the coordinate-wise variation in the underlying function. We utilize a simplified version of a theorem from [30], adapted to suit our specific needs, as the original formulation is more detailed than necessary for our purposes.

Theorem 3 (Consistency of Centered Difference-based Estimator for Scalar Function [30])

Let $\varphi : \mathbb{R}^D \rightarrow \mathbb{R}$ be a smooth scalar function and $\|\varphi'_i\|_{1,\mu} := \mathbb{E}_{\mathbf{x} \sim \mu} |\mathbf{e}_i^\top \nabla \varphi|$ be the coordinate-wise variability for that scalar function. Then, for any direction i and any $0 < \delta < 1/2$, the following bound holds with probability of at least $1 - 2\delta$:

$$\left| \mathbb{E}_n \frac{|\bar{\varphi}(\mathbf{x} + t\mathbf{e}_i) - \bar{\varphi}(\mathbf{x} - t\mathbf{e}_i)|}{2t} - \|\varphi'_i\|_{1,\mu} \right| \leq \mathcal{O}(n^{-1/2}t^{-1} \ln(2D/\delta)^{1/2}). \quad (63)$$

Note that the Theorem 3 is different from our setting by studying a scalar function as opposed to a vector valued function. However, we show that the result can be generalized to the latter case in Corollary 1 below via the estimator 62.

Corollary 1 (Consistency of the Estimator (62) for Vector-valued Function) Let $f : \mathbb{R}^D \rightarrow \mathbb{R}^{D_v}$ be a vector valued function and $\|f'_i\|_{1,\mu}$ be defined as in Definition 1. Then, for any direction i and any $0 < \delta < 1/2$, the following bound holds with probability of at least $1 - 2\delta$:

$$|\hat{m}_i - \|f'_i\|_{1,\mu}| \leq \mathcal{O}(n^{-1/2}t^{-1} \ln(2D/\delta)^{1/2}). \quad (64)$$

Proof. We first derive the relation between the left hand side of 64 and its coordinate-wise differences as follows:

$$\begin{aligned} |\hat{m}_i - \|f'_i\|_{1,\mu}| &= \left| \mathbb{E}_n \left[\frac{\|\bar{f}(\mathbf{k} + t\mathbf{e}_i) - \bar{f}(\mathbf{k} - t\mathbf{e}_i)\|_1}{2t} \right] - \mathbb{E}_{\mathbf{k} \sim \mu} [\|\mathbf{J}_f(\mathbf{k})\mathbf{e}_i\|_1] \right| \\ &= \left| \mathbb{E}_n \left[\sum_{j \in [D]} \frac{|\bar{f}_j(\mathbf{k} + t\mathbf{e}_i) - \bar{f}_j(\mathbf{k} - t\mathbf{e}_i)|}{2t} \right] - \mathbb{E}_{\mathbf{k} \sim \mu} \left[\sum_{j \in [D]} |\mathbf{e}_i^\top \nabla f_j| \right] \right| \end{aligned} \quad (65)$$

$$= \left| \sum_{j \in [D]} \mathbb{E}_n \frac{|\bar{f}_j(\mathbf{k} + t\mathbf{e}_i) - \bar{f}_j(\mathbf{k} - t\mathbf{e}_i)|}{2t} - \sum_{j \in [D]} \mathbb{E}_{\mathbf{k} \sim \mu} |\mathbf{e}_i^\top \nabla f_j| \right| \quad (66)$$

$$= \left| \sum_{j \in [D]} \left(m_i^{(j)} - \|f'_i\|_{1,\mu}^{(j)} \right) \right| \quad (\text{definition of } m_i \text{ and } \|f'_i\|_{1,\mu} \text{ for components } f_j)$$

$$\leq \sum_{j \in [D]} \left| m_i^{(j)} - \|f'_i\|_{1,\mu}^{(j)} \right| \quad (\text{triangle inequality})$$

$$\leq \mathcal{O}(n^{-1/2}t^{-1} \ln(2D/\delta)^{1/2}), \quad (\text{Theorem 3})$$

where line 65 follows from the definition of the ℓ_1 norm, line 66 follows from the linearity of expectation, the superscript j indicates that the case is reduced to the scalar function case for each j^{th} summand individually. Note that the probability of the last bound is at least $(1 - 2\delta/D)^D$ since each component-wise bound holds with probability at least $1 - 2\delta/D$. However, since we can choose δ small enough such that $2\delta < 1$, by Bernoulli's inequality $(1 - 2\delta/D)^D \geq 1 - 2D\delta/D = 1 - 2\delta$. \square

Table 9: Evaluation of the performance of our model and DeiT across multiple robustness benchmarks, using appropriate evaluation metrics for each.

Dataset Metric	ImageNet-R Top-1	ImageNet-A Top-1	ImageNet-C mCE (\downarrow)	ImageNet-C (Extra) mCE (\downarrow)
<i>DeiT</i>	32.22	7.33	72.21	63.68
<i>DeiT-Elliptical</i>	32.66	7.63	73.59	65.71

Remark 9 *Despite the proven consistency of this estimator, we opt for the efficient estimator presented in our main body described in Eqn 10. This is because the consistent estimator requires materialising the prediction function – that is, computing a forward pass of the self-attention mechanism – twice per dimension. This makes the consistent estimator unusable in most problem settings. We present results for the consistent estimator in Appendix F.11.*

E Implementation Procedure and Computational Efficiency

Training and Inference. Given Elliptical Attention requires keys and values from the previous layer in order to compute the required transformation, we can only implement Elliptical Attention from the second layer on. We incorporate our Elliptical Attention into both training and inference stages. This is because, firstly, Elliptical Attention is designed to offer improvements to both clean and contaminated data, and so even in the presence of completely clean train and test data, it is advantageous to incorporate Elliptical Attention into both stages. Secondly, it is commonplace to encounter data contamination in test data and indeed also highly possible to encounter it in train data as well. Therefore, in the interest of robustness as well, we also incorporate Elliptical Attention into both stages.

Computational Efficiency. Computing the required transformation requires no learnable parameters and is obtained simply by averaging absolute differences in values over layers. These operations are therefore just of the order $\mathcal{O}(bhnD) = \mathcal{O}(n)$ for batch size b , head number h , key/value length n , and dimension D . Hence upper-bound time complexity of the overall Transformer is unaffected. We provide efficiency analysis in terms of computation speed and max GPU memory allocated (calculated by CUDA `max_memory_allocated` in Figure 4, which shows that compared with baseline robust models, Elliptical is the fastest and most memory efficient. Elliptical exhibits no perceptible slowdown versus DeiT of the same configuration and only a 0.99% increase in max memory allocated, which is why Elliptical and DeiT are shown as the same data point in the Figure 4.

F Experimental Details and Additional Experiments

F.1 Out-of-Distribution Robustness and Data Corruption on ImageNet-A,R,C

ImageNet-A,R,C are benchmarks capturing a range of out-of-distribution and corrupted samples. ImageNet-A contains real world adversarially filtered images that fool current ImageNet classifiers. ImageNet-R contains various artistic renditions of object classes from the original ImageNet. ImageNet-C consists of 15 types of algorithmically generated corruptions with 5 levels of severity (e.g blurring, pixelation, speckle noise etc). Given that Elliptical Attention learns attention weights dependant on the transformation M , which is itself dependant on the train data distribution, our proposed model is not designed for situations in which the test distribution is substantially different from the train distribution. This then includes OOD robustness and robustness to heavy corruption to the point where the underlying data distribution is fundamentally different. We nonetheless evaluate Elliptical Attention on ImageNet-A,R,C to assess these important forms of robustness as well. Table 9 shows that Elliptical Attention is still able to offer improvements over baseline *DeiT* in terms of OOD robustness, while maintaining approximately the same performance as the baseline for ImageNet-C. Figure 7 shows for *Fog* and *Pixelate* corruptions how Elliptical compares with DeiT over the 5 severity levels, where we see that at low severity levels Elliptical improves over DeiT, however as the severity level gets too high Elliptical falls behind. This agrees with our expectation that as the severity level grows, the distribution is further shifted relative to the train distribution and so Elliptical Attention is unable to improve performance.

F.2 Representation Collapse

We provide in Figure 6 additional representation collapse results for ImageNet and ADE20K, showing that across modalities Elliptical Attention resists representation collapse.

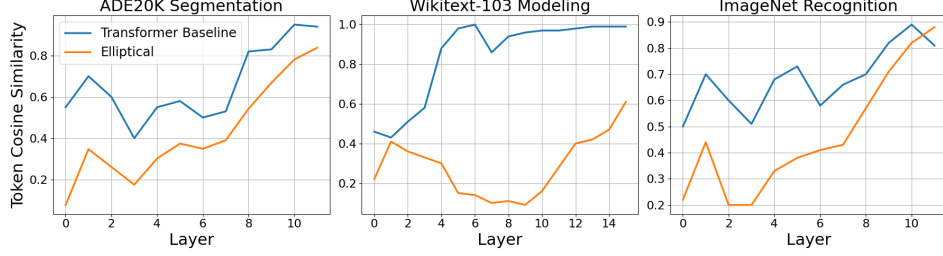


Figure 6: Additional Representation Collapse Results on ADE20K, WikiText-103 and ImageNet. Elliptical reduces token similarity over layers across a range of modalities

Table 10: Additional Results on Imagenet Increasing Heads But Maintaining Overall Embedding Dimension

Model	Num. Heads	Head Dim.	#Params.	Top-1 Accuracy	Top-5 Accuracy
<i>DeiT</i>	3	64	5M	72.23	91.13
<i>Elliptical</i>	3	64	5M	72.36	91.33
<i>DeiT-6head</i>	6	32	5M	72.34	91.22
<i>Elliptical-6head</i>	6	32	5M	73.00	91.77

F.3 Head Redundancy

We present in Table 18 head redundancy results on the two large-scale tasks, WikiText-103 language modelling and ImageNet-1K object classification. Mean \mathcal{L}_2 distance between vectorized attention heads, with the mean taken over a batch of size 1000 and averaged layer-wise. We see that Elliptical improves head redundancy on WikiText-103 versus the baseline transformer while performing approximately equally to the DeiT baseline on ImageNet.

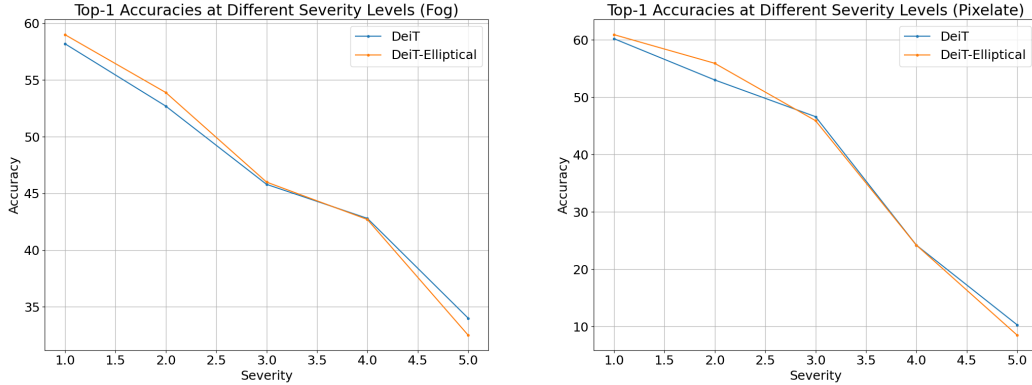


Figure 7: Comparison of *DeiT* versus *DeiT-Elliptical* accuracies on two types of ImageNet-C corruptions, namely, Fog (left) and Pixelate (right). The figures show two out of many cases where *DeiT-Elliptical* outperforms its counterpart while vanilla *DeiT* manages to exceed only at higher severity levels.

F.4 Efficiency Results

We present here the comparative efficiency results for DeiT and DeiT-Elliptical in a side-by-side comparison at tiny, small, and base sizes, along with DeiT-Elliptical compared with other robust baselines.

F.5 Elliptical Attention in Mixture of Expert Architectures

We additionally evaluate Elliptical Attention within Mixture of Expert architectures. Specifically, we show in Tables 13, 14, and 15 the performance of Elliptical Attention within the Switch Transformer [18] and Generalized Language Model (GLaM) backbones [17].

Table 11: Side-by-side Efficiency comparison of DeiT and DeiT-Elliptical

Model	Compute Speed (it/s)	Max Memory (K)	FLOPs / sample	#Params (M)
<i>Tiny</i>				
DeiT	0.347	2.08	1.77	5.7
DeiT-Elliptical	0.342	2.12	1.79	5.7
% Change	-1.44%	1.92%	1.12%	-
<i>Small</i>				
DeiT	0.297	4.89	6.91	22.1
DeiT-Elliptical	0.289	4.96	6.99	22.1
% Change	-2.69%	1.43%	1.16%	-
<i>Base</i>				
DeiT	0.132	10.27	26.37	86.6
DeiT-Elliptical	0.130	10.54	26.63	86.6
% Change	-1.52%	2.63%	0.98%	-
Avg. % Change	1.88%	1.99%	1.09%	-

Table 12: Efficiency Comparison between Elliptical and baseline robust models

Model	Compute Speed (it/s)	Max Memory (K)	FLOPs / sample	#Params (M)
DeiT-MoM	0.331	2.24	1.74	5.7
DeiT-RKDE	0.271	3.12	1.77	5.7
DeiT-SPKDE	0.168	3.35	1.75	5.7
DeiT-RVT	0.292	3.91	1.89	7.1
DeiT-Elliptical	0.342	2.12	1.79	5.7

F.6 Additional Adversarial Attack Results on DeiT-Small Configuration

We present here additional results for DeiT and DeiT-Elliptical at the Small configuration [78] (22.1M parameters) under adversarial attack. Table 16 shows the result of Elliptical against PGD, FGSM, and SPSA. Table 17 shows the results of Elliptical against Auto Attack. Given the larger model size, we attack with a perturbation budget of 3/255.

F.7 Wikitext-103 Language Modelling and Word Swap Attack

Dataset. The WikiText-103² dataset contains around 268K words and its training set consists of about 28K articles with 103M tokens. This corresponds to text blocks of about 3600 words. The validation set and test sets consist of 60 articles with 218K and 246K tokens respectively.

Corruption. Word Swap Text Attack³ corrupts the data by substituting random words with a generic token 'AAA'. We follow the setup of [23] and assess models by training them on clean data before attacking only the evaluation set using a substitution rate of 2.5%.

Model, Optimizer & Train Specification. We adopt the training regime of [54]. To this end, the small backbone uses 16 layers, 8 heads of dimension 16, a feedforward layer of size 2048 and an embedding dimension of 128. We use a dropout rate of 0.1. We trained with Adam using a starting learning rate of 0.00025 and cosine scheduling under default PyTorch settings. We used a batch size of 96 and trained for 120 epochs and 2000 warmup steps. The train and evaluation target lengths were set to 256.

The medium backbone uses 16 layers, 8 heads of dimension 32, a feedforward layer of size 2048 and embedding dimension of 256. We use a dropout rate of 0.1. We trained with Adam using a starting

²www.salesforce.com/products/einstein/ai-research/the-wikitext-dependency-language-modeling-dataset/

³Implementation available at github.com/QData/TextAttack

Table 13: Elliptical Switch Transformers Pretrained on WikiText-103 and Finetuned on Stanford Sentiment Treebank 2 (SST-2)

Model	Test PPL (\downarrow)	Finetune Test Acc. (\uparrow)
<i>Switch Transformer-medium</i>	35.33	76.27
Switch Elliptical-medium	34.67	77.32
<i>Switch Transformer-large</i>	31.18	76.79
Switch Elliptical-large	30.56	78.08

Table 14: Elliptical Switch Transformers Pretrained on EnWik8 and Finetuned on Stanford Sentiment Treebank 2 (SST-2)

Model	Test BPC (\downarrow)	Finetune Test Acc. (\uparrow)
<i>Switch Transformer</i>	1.153	63.27
Switch Elliptical	1.142	67.75

learning rate 0.00025 and cosine scheduling under default PyTorch settings. We used a batch size of 56 and trained for 100 epochs and 2000 warmup steps. The train and evaluation target lengths were set to 384.

For Elliptical Attention, we use an Elliptical layer on all possible layers 2 through 16. We use a constant delta of 1.

Compute Resources. All models are trained and evaluated on two NVIDIA A100 SXM4 40GB GPUs.

F.8 ImageNet Image Classification and Adversarial Attack

Dataset. We use the full ImageNet dataset that contains 1.28M training images and 50K validation images. The model learns to predict the class of the input image among 1000 categories. We report the top-1 and top-5 accuracy on all experiments.

Corruption. We use attacks FGSM [22], PGD [42], and Auto Attack [11] with perturbation budget $1/255$ while SPSA [81] uses a perturbation budget 0.1. All attacks perturb under l_∞ norm. PGD attack uses 20 steps with step size of 0.15.

Model, Optimizer & Train Specification. The configuration follows the default DeiT tiny configuration [78]. In particular, we follow the experimental setup of [23, 54]. To this end, the DeiT backbone uses 12 layers, 3 heads of dimension 64, patch size 16, feedforward layer of size 768 and embedding dimension of 192. We train using Adam with a starting learning rate of 0.0005 using cosine scheduling under default PyTorch settings, momentum of 0.9, batch size of 256, 5 warmup epochs starting from 0.000001 and 10 cooldown epochs, for an overall train run of 300 epochs. The input size is 224 and we follow the default AutoAugment policy and color jitter 0.4.

For Elliptical Attention, we use an Elliptical layer on all possible layers 2 through 12. We use a constant delta of 1.

Compute Resources. We train and evaluate all models on four NVIDIA A100 SXM4 40GB GPUs, with the exception of the robustness experiments on ImageNet-C which are conducted using four NVIDIA Tesla V100 SXM2 32GB GPUs.

F.9 LRA Long Sequence Classification.

Dataset. The LRA benchmark consists 5 tasks involving long range contexts of up to 4000 in sequence length. These tasks consist of equation calculation (ListOps) [50], review classification (Text) [41], document retrieval (Retrieval) [61], image classification (Image) [32] and image spatial dependencies (Pathfinder) [37].

Model, Optimizer & Train Specification. We adopt the same experimental setup as [7]. To that end, the Transformer backbone is set with 2 layers, hidden dimension of 128, 2 attention heads

Table 15: Test Perplexity of Elliptical GLaM on WikiText-103 Modeling

Model	Test PPL
<i>GLAM-small</i>	58.27
GLAM-Elliptical-small	56.69
<i>GLAM-medium</i>	38.27
GLAM-Elliptical-medium	36.34

Table 16: DeiT and DeiT-Elliptical Accuracy on ImageNet Under Adversarial Attacks PGD, FGSM, and SPSA with Small Backbone Configuration

Method	Clean Data		PGD		FGSM		SPSA	
	Top 1	Top 5	Top 1	Top 5	Top 1	Top 5	Top 1	Top 5
<i>DeiT-small</i>	79.89	95.04	21.41	51.50	51.57	82.12	65.68	91.28
Elliptical-small	79.92	95.06	22.39	54.02	51.86	82.87	72.02	92.45

Table 17: DeiT and DeiT-Elliptical Accuracy on ImageNet under Auto Attack with Small Backbone Configuration

Method	Clean Data		APGD-CE		APGD-T		FAB-T		Square	
	Top 1	Top 5	Top 1	Top 5	Top 1	Top 5	Top 1	Top 5	Top 1	Top 5
<i>DeiT-small</i>	79.89	95.04	19.18	50.75	16.54	63.84	80.66	95.09	49.98	89.17
Elliptical-small	79.92	95.06	18.88	51.07	17.30	65.28	81.64	95.59	55.89	89.36

Table 18: Head Redundancy Results

Model	Num. Heads	Dim. Head	\mathcal{L}_2 Distance
<i>WikiText-103</i>			
<i>Transformer-Small</i>	8	16	5.40 ± 2.21
<i>Elliptical-Small</i>	8	16	6.45 ± 2.38
<i>ImageNet</i>			
<i>DeiT</i>	3	64	5.11 ± 1.67
<i>Elliptical</i>	3	64	4.98 ± 1.54

of dimension 32, and embedding dimension of 64. We use a dropout rate of 0.1. Built on top of the standard transformer backbone, Reformer uses 2 hashes, Performer has 256 random feature dimensions and Linformer uses a projection dimension of 256. We train with Adam using a learning rate of 0.0001 with linear decay. We use a batch size of 32 for ListOps, Retrieval, and Text and 256 for Image and Pathfinder32. We use 1000, 175, 312, 800, and 1000 warmup steps for ListOps, Image, Pathfinder32, Retrieval, and Text respectively.

Elliptical places the Elliptical Attention layer on the final layer (as the only one possible) and uses delta equal to 1.

Compute Resources. All models are trained and evaluated on a single NVIDIA A100 SXM4 40GB GPU.

F.10 ADE20K Image Segmentation

Dataset. ADE20K [88] contains challenging scenes with fine-grained labels and is one of the most challenging semantic segmentation datasets. The training set contains 20,210 images with 150 semantic classes. The validation and test set contain 2,000 and 3,352 images respectively.

Model, Optimizer & Train Specification. We follow the experimental setup as in [71]. The encoder is pretrained on ImageNet following the specification described in F.8 using the setup in [78, 54]. That is, the encoder is a DeiT backbone using 12 layers, 3 heads of dimension 64, patch

Table 19: Perplexity (PPL) of Elliptical and baselines on WikiText-103 under Word Swap data contamination. Best results are in bold. Our Elliptical method achieve substantially better robust PPL without compromising performance on clean data.

Model	Clean Test PPL (\downarrow)	Contaminated Test PPL (\downarrow)
<i>Transformer</i>	34.29	74.56
<i>Performer</i>	33.49	73.48
<i>Transformer-MGK</i>	33.21	71.03
<i>FourierFormer</i>	32.85	68.33
<i>Transformer-SPKDE</i>	32.18	54.97
<i>Transformer-MoM</i>	34.68	52.14
<i>Elliptical</i>	32.00	52.59
<i>Random Ablation</i>	37.84	46.82
<i>Elliptical-Consistent</i>	32.95	54.67
<i>Elliptical-Meanscale</i>	31.94	52.78

size 16, feedforward layer of size 768 and embedding dimension of 192. We train using Adam with a starting learning rate of 0.0005 using cosine scheduling under default PyTorch settings, momentum of 0.9, batch size of 256, 5 warmup epochs starting from 0.000001 and 10 cooldown epochs, for an overall train run of 300 epochs. The input size is 224 and we follow the default AutoAugment policy and color jitter 0.4. After pretraining the encoder, we then attach as decoder a masked transformer consisting of 2 layers. Each layer contains 3 heads of dimension 64, embedding dimension of 192 and feedforward dimension of 768. The decoder uses a dropout rate of 0.1. The full segmenter (encoder and decoder) is then finetuned using SGD with starting learning rate 0.001 and polynomial scheduling. The batch size is set to 8.

Compute Resources. All models are trained and evaluated on a single NVIDIA A100 SXM4 40GB GPU.

F.11 Ablation Studies

Ablation Models. We consider the following models in our ablation studies:

- *Random Ablation.* To validate the efficacy of our proposed estimator given in Eqn. 10, we consider an alternate model in which M is populated by weights uniformly drawn from the $[0, 1]$ interval followed by the same maxscaling as in *Elliptical*.
- *Elliptical-Meanscale.* We ablate the effect of maxscaling by considering meanscaling of the estimates m_i . That is, each $m_i \leftarrow m_i/\bar{m}$ is scaled by the mean variability estimate $\bar{m} = \mathbb{E}_D[m_i]$.
- *Elliptical-Consistent.* We consider also the performance of Elliptical when using the consistent estimator of $\|f'_i\|_{1,\mu}$ described by Equation 62.

Language Modelling. Results are shown in Table 19. Amazingly, the random ablation model performs extremely well on contaminated data. In general, this most likely suggests that training a model with randomness injected into the attention matrix can generate some robustness benefits, which is intuitive. It does, less surprisingly, come at the cost of clean data performance, where Random Ablation performs almost 10% worse than baseline transformer.

F.12 Pseudocode

Algorithm 1 presents a pseudocode for implementing Elliptical Attention as given by Eqn. 13 on top of conventional self-attention.

ImageNet Classification and Attack. Table 21 shows the ablation model’s performance on both clean ImageNet and under Auto Attack. The ablation model shows a slight improvement over the DeiT baseline in Top 1 accuracy, however Top 5 accuracy is substantially lower. Reasonable performance again Auto Attack is overall unsurprising given that the random Random Ablation model is essentially employing random defence. Nonetheless, it still does not surpass the performance of Elliptical.

Algorithm 1 Computation of Elliptical Attention

Require:

```
1: Tensor  $\mathbf{Q} \in \mathbb{R}^{N \times D}$   $\triangleright$  current layer queries
2: Tensor  $\mathbf{K} \in \mathbb{R}^{N \times D}$   $\triangleright$  current layer keys
3: Tensor  $\mathbf{V} \in \mathbb{R}^{N \times D}$   $\triangleright$  current layer values
4: Tensor  $\mathbf{V}^{\text{prev}} \in \mathbb{R}^{N \times D}$   $\triangleright$  previous layer values
5: float  $\delta \in \mathbb{R}_+$   $\triangleright$  step size
6: integer  $D \in \mathbb{N}$   $\triangleright$  head dimension

7: function ELLIPTICAL_ATTENTION( $\mathbf{Q}, \mathbf{K}, \mathbf{V}, \mathbf{V}^{\text{prev}}, \delta, D$ )
8:    $\mathbf{M} \leftarrow \text{ELLIPTICAL\_WEIGHTS}(\mathbf{V}, \mathbf{V}^{\text{prev}}, \delta)$   $\triangleright$  compute weight matrix  $\mathbf{M}$ 
9:    $\text{logits} \leftarrow \mathbf{Q} \times \mathbf{M} \times \mathbf{K}^\top \times \frac{1}{\sqrt{D}}$   $\triangleright$  modify the dot-product computation
10:   $\text{attention} \leftarrow \text{SOFTMAX}(\text{logits})$ 
11:   $\text{output} \leftarrow \text{attention} \times \mathbf{V}$ 
12:  return output
13: end function

14: function ELLIPTICAL_WEIGHTS( $\mathbf{V}, \mathbf{V}^{\text{prev}}, \delta$ )
15:  with torch.no_grad() do
16:     $N \leftarrow \mathbf{V}.\text{size}(0)$   $\triangleright$  sequence length
17:     $\text{value\_diff} \leftarrow (\mathbf{V} - \mathbf{V}^{\text{prev}}) / \delta$ 
18:     $\mathbf{M} \leftarrow \frac{1}{N} \times \text{NORM}(\text{value\_diff}, p = 1, \text{dim} = 0)$   $\triangleright$  column-wise average of  $\mathcal{L}_1$  norms
19:     $\mathbf{M} \leftarrow \text{DIAG\_EMBED}(\mathbf{M})$   $\triangleright$  embed the vector into a diagonal matrix
20:  return  $\mathbf{M}$ 
21: end function
```

Table 20: Evaluation of the performance of our model and DeiT across multiple robustness benchmarks, using appropriate evaluation metrics for each.

Dataset Metric	ImageNet-R Top-1	ImageNet-A Top-1	ImageNet-C mCE (\downarrow)	ImageNet-C (Extra) mCE (\downarrow)
<i>DeiT</i>	25.38	3.65	72.21	63.68
<i>Elliptical</i>	31.37	6.76	73.59	65.71
<i>Random Ablation</i>	30.87	5.85	74.02	65.90
<i>Elliptical-Consistent</i>	31.46	6.71	82.92	71.74
<i>Elliptical-Meanscale</i>	32.66	7.63	72.28	63.79

Table 21: Auto Attack Ablation Study: Top 1 and Top 5 test accuracies on clean ImageNet and under Auto Attack. The ablation model fails to fit the clean data well and is highly prone to adversarial attack.

Method	<i>DeiT</i> [78]		<i>DeiT-Elliptical</i>		<i>Random Ablation</i>	
	Top 1	Top 5	Top 1	Top 5	Top 1	Top 5
Clean Data	72.23	91.13	72.36	91.33	71.44	91.29
APGD-CE	27.75	66.48	31.27	68.28	27.85	61.74
APGD-T	27.74	73.37	29.69	74.39	28.60	68.72
FAB-T	71.61	90.54	71.74	90.81	68.54	89.43
Square	43.55	80.96	47.25	81.65	47.24	78.87
Average	42.66	77.84	45.00	78.78	43.06	74.69
Sequential Attack	26.08	64.18	27.45	67.77	26.33	60.85

G Broader Impacts

Our research offers benefits to both clean data and robust performance. We in particular show improved results in domains with wide social applicability. These include image segmentation, with benefits to self-driving cars, and language modeling, with benefits to AI chatbot assistants. We in particular show strong improvements against contamination by adversarial attack, which we hope can protect vital AI systems from malicious actors, and competitive performance in contaminated

language modeling, which we hope can improve language models evaluated on imperfect data as is often the case in the real world. There is always possibility of misuse of AI systems, however our research shows substantive improvements in fundamental architectures and theory which we hope can spur further socially beneficial outcomes.

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