What Does It Mean To Be a Transformer?

Insights from a Theoretical Hessian Analysis

Weronika Ormaniec

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@wormaniec

Overview

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2. Motivation:
   - Why do we care about the loss Hessian?
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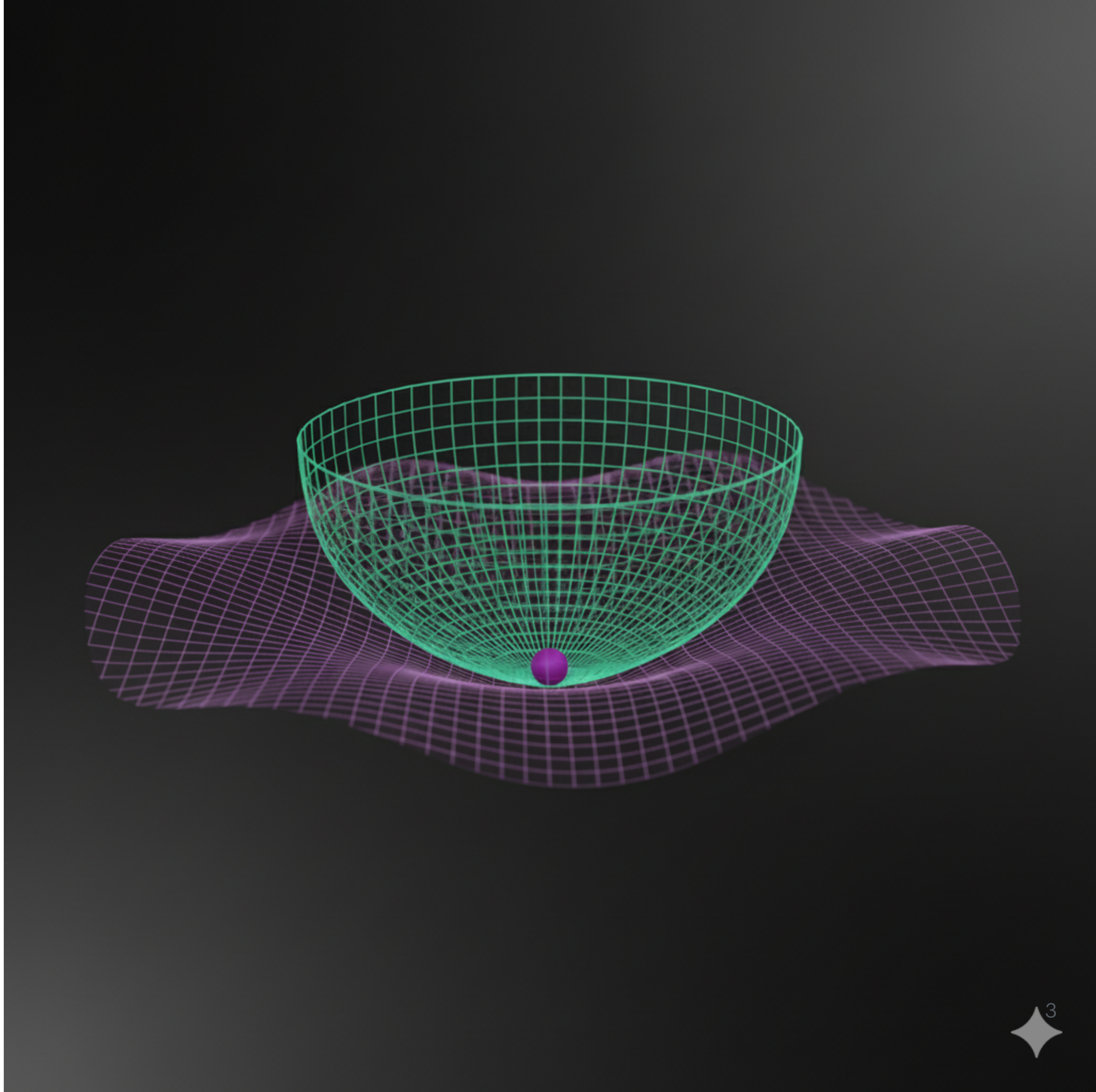
3. Results:
   - Hessian block-heterogeneity
   - Comparison of loss Hessian for Transformers and MLPs
   - Outlook: Primer on Transformer loss Hessian spectra

Neural Network Loss Hessian



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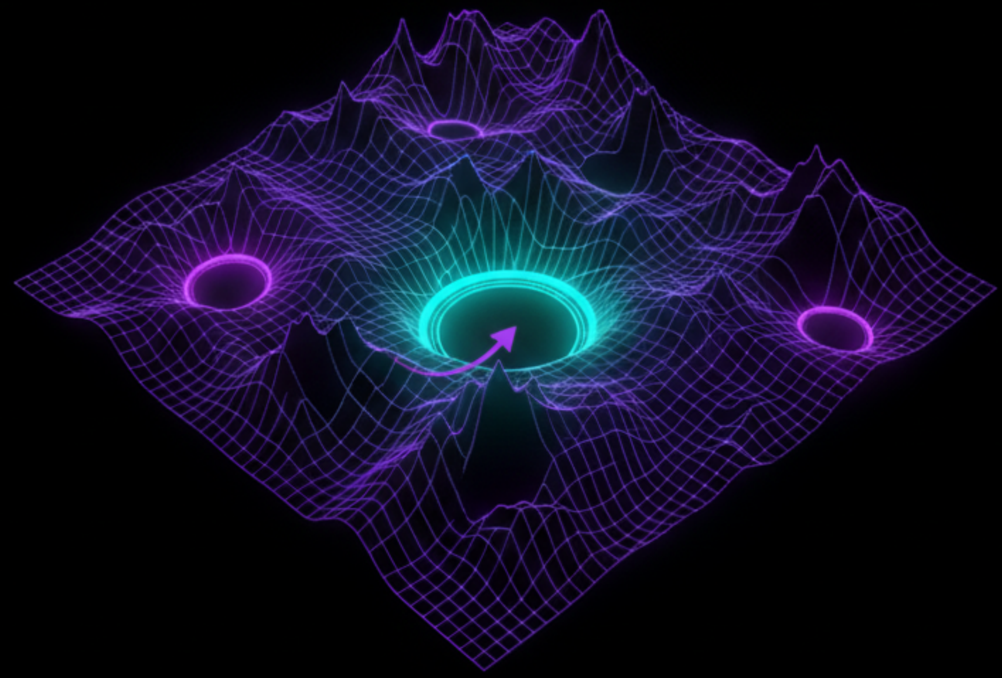
$$\mathbf{H} \in \mathbb{R}^{d_1 \times d_1} \qquad \mathbf{H}_{i,j} = \frac{\partial^2 \left(\ell \circ \mathbf{F}\left(\theta\right)\right)}{\partial \theta_i \partial \theta_j}$$

Motivation



Loss Approximation

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We can approximate the loss around any point with a polynomial defined with gradient and Hessian

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Taylor expansion $$\mathcal{L}(\theta + \Delta\theta) \approx \mathcal{L}(\theta) + \Delta\theta^\top \nabla\mathcal{L}(\theta) + \frac{1}{2}\Delta\theta^\top \mathbf{H}(\theta)\Delta\theta$$

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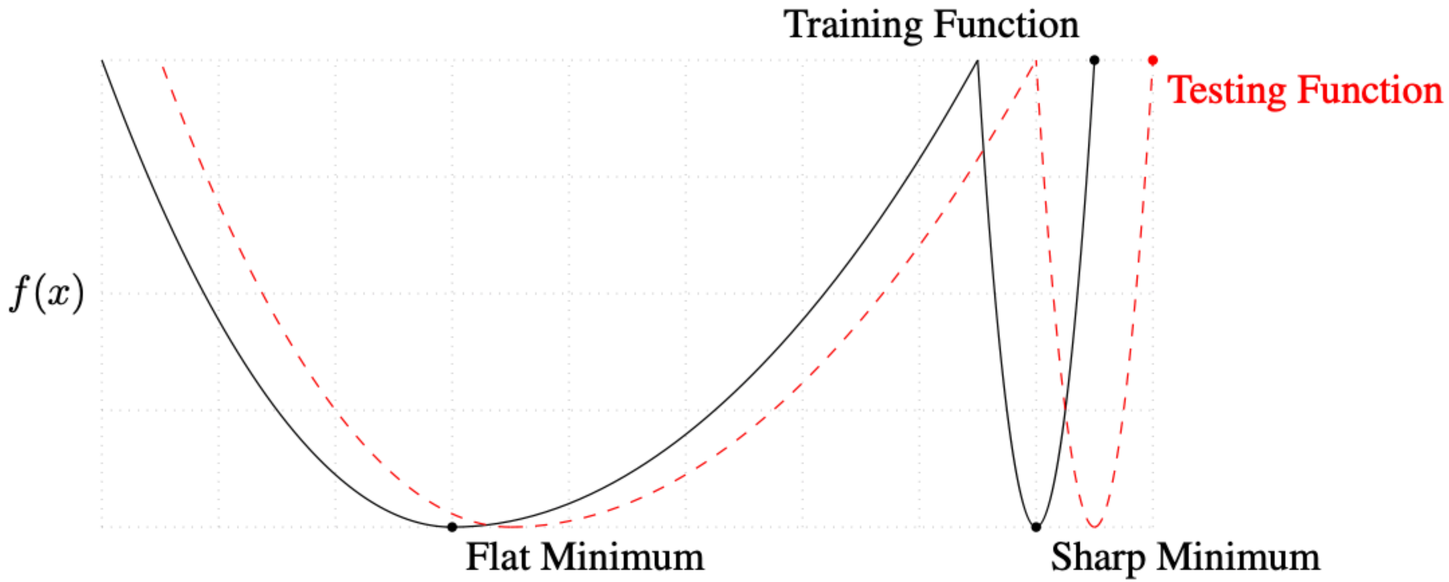
The Hessian...

- Locally characterises the curvature of the loss
- Eigenvectors and eigenvalues $\Longrightarrow$ in which directions the loss is locally flat, convex or concave
- Specifies the nature of critical points

Generalisation

Generalisation



Source: On Large-Batch Training for Deep Learning: Generalization Gap and Sharp Minima. Keskar et al. (2017)

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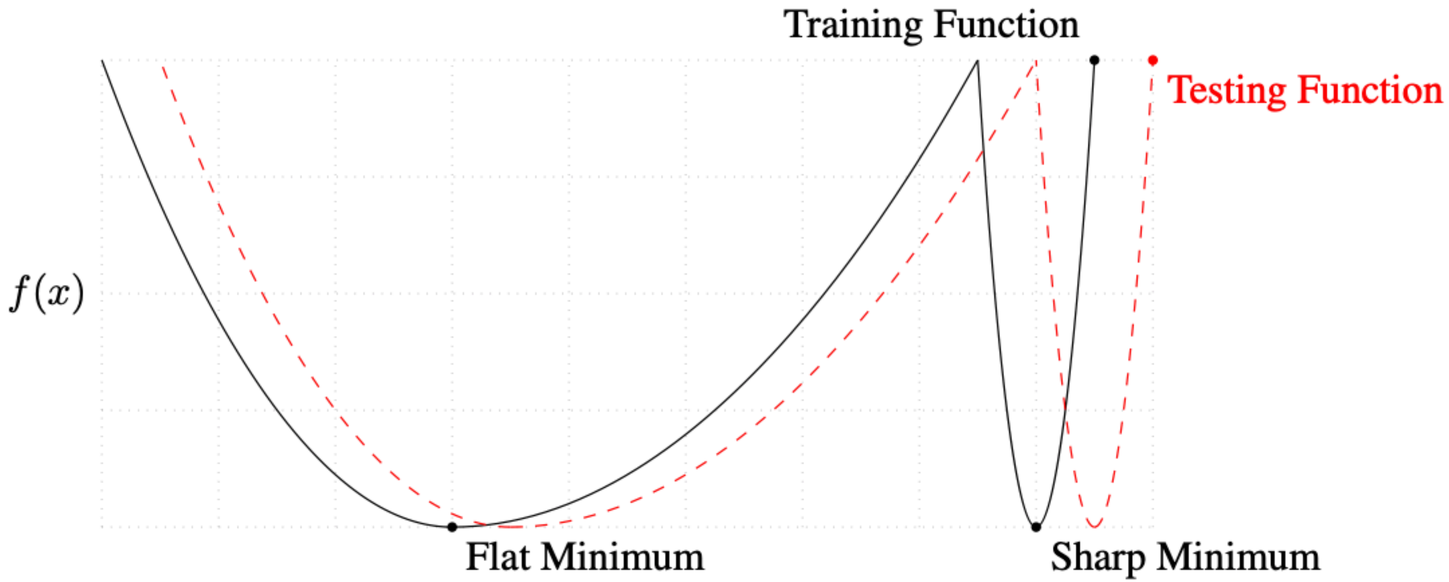

Loss Hessian properties at minima are used as a measure of flatness

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Many other block-diagonal approximations: KFAC, Shampoo, PSGD, etc.

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The loss should decrease for $\eta \in (0, \frac{2}{\lambda_{\max}(\mathbf{H}(\theta))})$

Pruning & Quantisation

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Optimal Brain Surgeon Framework

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$$\min_{q} \min_{\delta \mathbf{w}^\top} \frac{1}{2} \delta \mathbf{w}^\top \mathbf{H} \delta \mathbf{w}, \; s.t. \; \mathbf{e}_q^\top \delta \mathbf{w} + \mathbf{w}_q = 0$$

$$\delta \mathbf{w} = -\frac{w_q^2}{[\mathbf{H}_{qq}^{-1}]} \mathbf{H}^{-1} \mathbf{e}_q$$

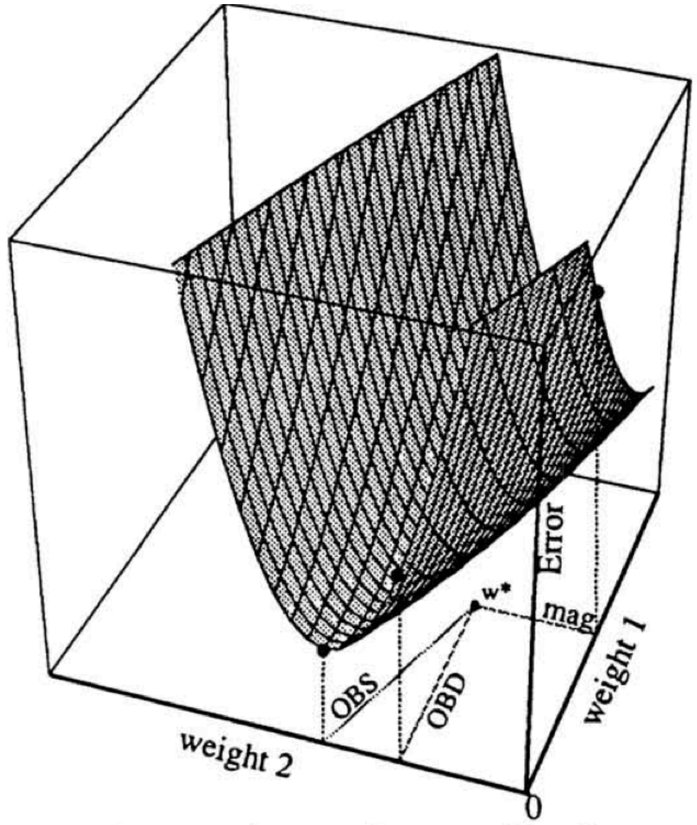

Figure 1: Error as a function of two weights in a network. The (local) minimum occurs at weight w*, found by gradient descent or other learning method. In this illustration, a magnitude based pruning technique (mag) then removes the smallest weight, weight 2; Optimal Brain Damage before retraining (OBD) removes weight 1. In contrast, our Optimal Brain Surgeon method (OBS) not only removes weight 1, but *also* automatically adjusts the value of weight 2 to minimize the error, without retraining.

Source:

Second order derivatives for network pruning: Optimal Brain Surgeon. Hassibi and Stork (1992)

Why study the loss Hessian for Transformers?

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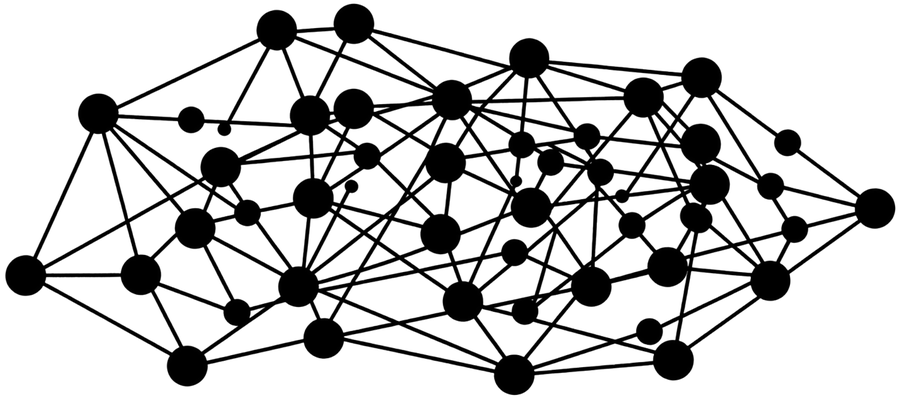

Unique architecture

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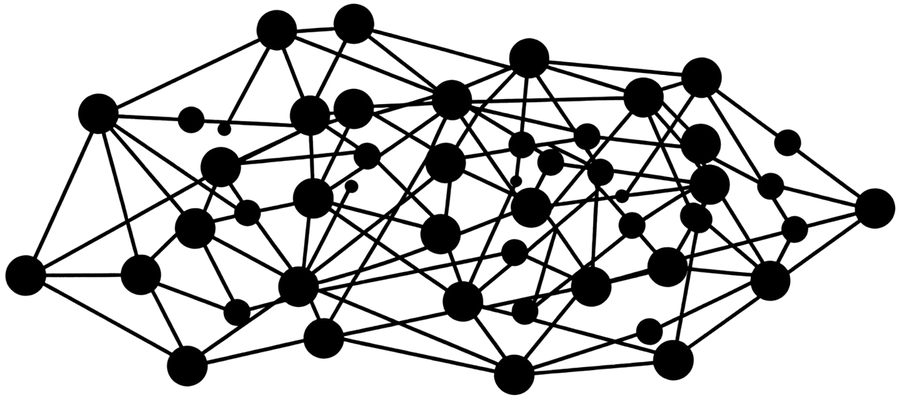

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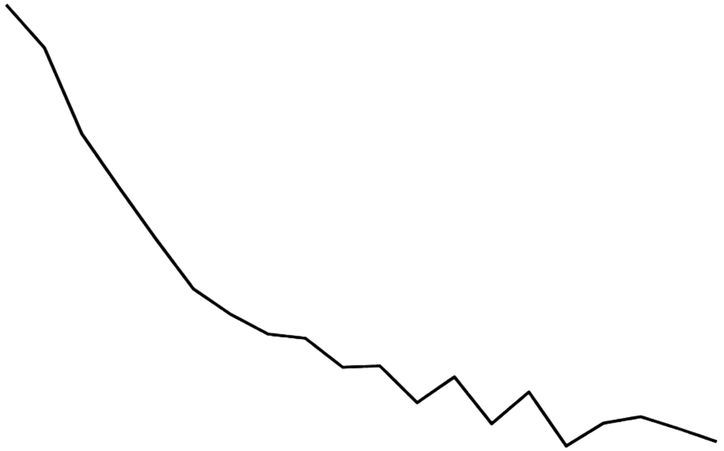

Tricky optimisation

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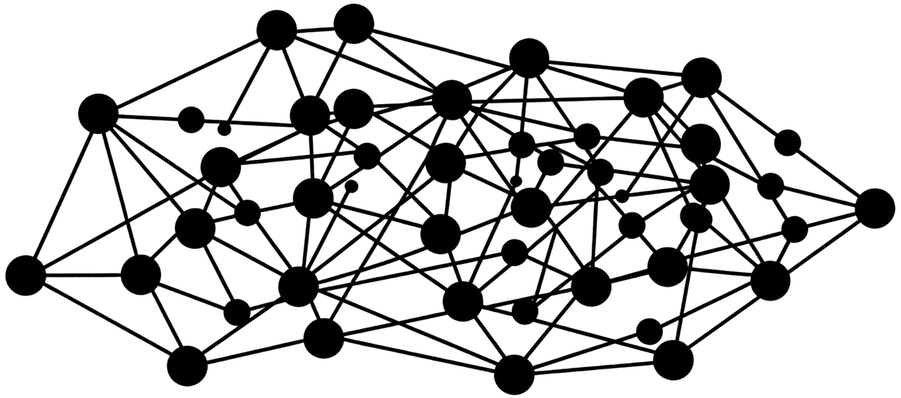

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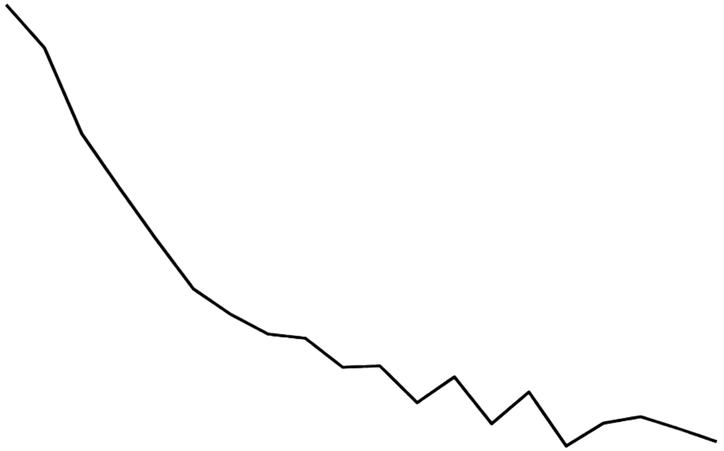

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Objective:

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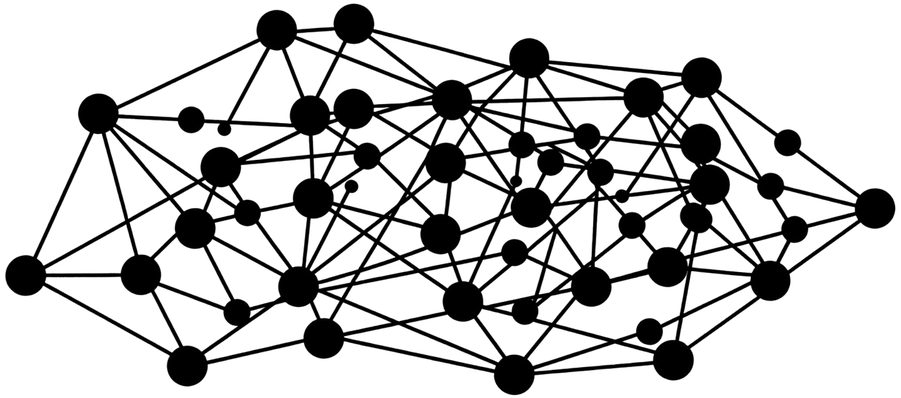

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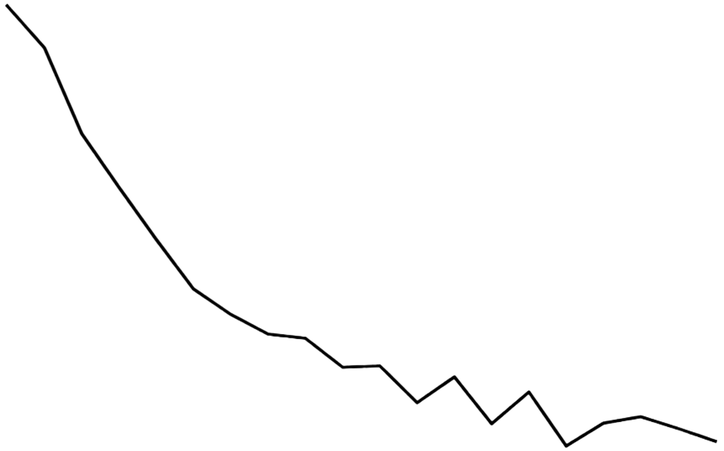

Tricky optimisation

Objective:

Analytically characterise the influence of self-attention on the loss Hessian and contrast it with classical architectures

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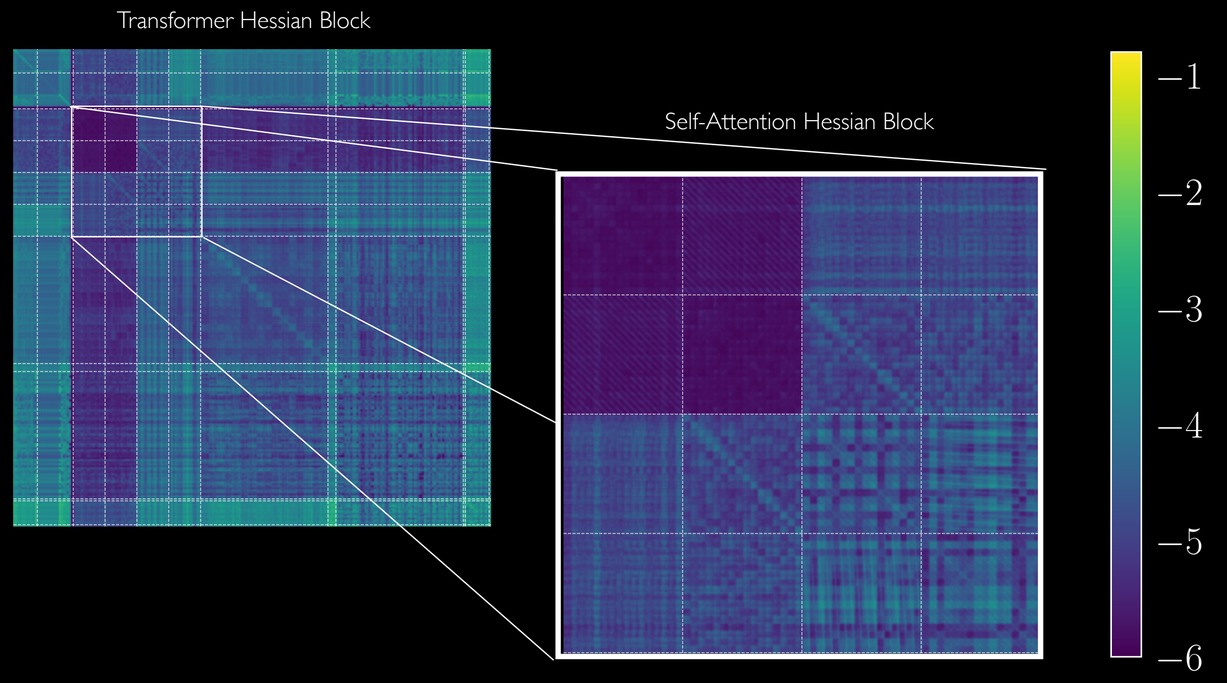
Insights from the Hessian



Collaborators

Felix Dangel

Sidak Pal Singh

Thomas Hofmann

Problem setup

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Model consisting of a single self-attention layer

$$\mathbf{F}(\mathbf{X}) = \mathbf{A}(\mathbf{X})\mathbf{X}\mathbf{W}_{\mathrm{V}}$$

where

$$\mathbf{A}(\mathbf{X}) = \mathrm{softmax}\left(\mathbf{X}\mathbf{W}_{\mathrm{Q}}\mathbf{W}_{\mathrm{K}}^{\top}\mathbf{X}^{\top} / \sqrt{d_K}\right)$$

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MSE loss

$$\ell(\mathbf{F}(\mathbf{X}), \mathbf{Y}) = \|\mathbf{F}(\mathbf{X}) - \mathbf{Y}\|_{\mathrm{F}}^2 / (Ld_V)$$

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$$\frac{\partial^2 (\ell \circ \mathbf{F})}{\partial \mathbf{W}_i \partial \mathbf{W}_j}(\cdot) = \underbrace{\frac{\partial \mathbf{F}}{\partial \mathbf{W}_i}(\cdot)^\top \frac{\partial^2 \ell}{\partial \mathbf{F}^2}(\mathbf{F}(\cdot)) \frac{\partial \mathbf{F}}{\partial \mathbf{W}_j}(\cdot)}_{\text{Outer-product Hessian}} + \underbrace{\left(\frac{\partial \ell}{\partial \mathbf{F}}(\mathbf{F}(\cdot)) \otimes \mathbf{I}_{p_i q_i} \right) \frac{\partial^2 \mathbf{F}}{\partial \mathbf{W}_i \partial \mathbf{W}_j}(\cdot)}_{\text{Functional Hessian}}$$

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$$\mathbf{H}_\bullet = \begin{bmatrix} \mathbf{H}_\bullet(\mathbf{W}_\mathrm{Q}, \mathbf{W}_\mathrm{Q}) & \mathbf{H}_\bullet(\mathbf{W}_\mathrm{Q}, \mathbf{W}_\mathrm{K}) & \mathbf{H}_\bullet(\mathbf{W}_\mathrm{Q}, \mathbf{W}_\mathrm{V}) \\ \mathbf{H}_\bullet(\mathbf{W}_\mathrm{K}, \mathbf{W}_\mathrm{Q}) & \mathbf{H}_\bullet(\mathbf{W}_\mathrm{K}, \mathbf{W}_\mathrm{K}) & \mathbf{H}_\bullet(\mathbf{W}_\mathrm{K}, \mathbf{W}_\mathrm{V}) \\ \mathbf{H}_\bullet(\mathbf{W}_\mathrm{V}, \mathbf{W}_\mathrm{Q}) & \mathbf{H}_\bullet(\mathbf{W}_\mathrm{V}, \mathbf{W}_\mathrm{K}) & \mathbf{H}_\bullet(\mathbf{W}_\mathrm{V}, \mathbf{W}_\mathrm{V}) \end{bmatrix}$$

$$\bullet \in \{\mathrm{o}, \mathrm{f}\}$$

Main Result — Outer-Product Hessian

Theorem 3.1. Outer-product Hessian $\mathbf{H}_o$. For a single self-attention layer, the blocks of $\mathbf{H}_o$ are

$$\mathbf{H}_o(\mathbf{W}_V, \mathbf{W}_V) = \frac{2}{Ld_V}\mathbf{M}_1^\top \mathbf{M}_1 \otimes \mathbf{I}_{d_V},$$

$$\mathbf{H}_o(\mathbf{W}_Q, \mathbf{W}_Q) = \frac{2}{Ld_V d_K}\left(\mathbf{I}_{d_V} \otimes \mathbf{W}_K^\top\right)\mathbf{Z}_1^\top\left(\mathbf{I}_L \otimes \mathbf{W}_V\mathbf{W}_V^\top\right)\mathbf{Z}_1\left(\mathbf{I}_{d_V} \otimes \mathbf{W}_K\right),$$

$$\mathbf{H}_o(\mathbf{W}_V, \mathbf{W}_Q) = \frac{2}{Ld_V\sqrt{d_K}}\left(\mathbf{M}_1^\top \otimes \mathbf{W}_V^\top\right)\mathbf{Z}_1\left(\mathbf{I}_{d_V} \otimes \mathbf{W}_K\right),$$

$$\mathbf{H}_o(\mathbf{W}_Q, \mathbf{W}_K) = \frac{2}{Ld_V d_K}\left(\mathbf{I}_{d_V} \otimes \mathbf{W}_K^\top\right)\mathbf{Z}_1^\top\left(\mathbf{I}_L \otimes \mathbf{W}_V\mathbf{W}_V^\top\right)\mathbf{Z}_1\left(\mathbf{W}_Q \otimes \mathbf{I}_{d_V}\right)\mathbf{K}_{d_K,d_V},$$

where $\mathbf{Z}_1 = \mathbf{X} * \mathbf{M}_2 \in \mathbb{R}^{Ld_V \times d_V^2}$ with $\mathbf{M}_1$ and $\mathbf{M}_2$ containing moments of the distributions given by self-attention scores.

Main Result — Functional Hessian

Theorem 3.2. Functional Hessian $\mathbf{H}_\mathrm{f}$. For a single self-attention layer, the functional Hessian w.r.t. the value weight matrix $\mathbf{H}_\mathrm{f}\left(\mathbf{W}_\mathrm{V}, \mathbf{W}_\mathrm{V}\right)$ is zero and the remaining blocks are given by

$$\mathbf{H}_\mathrm{f}\left(\mathbf{W}_\mathrm{Q}, \mathbf{W}_\mathrm{Q}\right) = \frac{2}{L d_V d_K} \mathbf{R}_{d_V d_K} \left(\mathbf{I}_L \otimes \mathbf{W}_\mathrm{V}^\top \otimes \mathbf{I}_{d_V} \otimes \mathbf{W}_\mathrm{K}^\top\right) \mathbf{Z}_2 \left(\mathbf{I}_{d_V} \otimes \mathbf{W}_\mathrm{K}\right),$$

$$\mathbf{H}_\mathrm{f}\left(\mathbf{W}_\mathrm{V}, \mathbf{W}_\mathrm{Q}\right) = \frac{2}{L d_V \sqrt{d_K}} \mathbf{R}_{d_V^2} \left(\mathbf{I}_L \otimes \mathbf{S}\right) \mathbf{Z}_1 \left(\mathbf{I}_{d_V} \otimes \mathbf{W}_\mathrm{K}\right),$$

$$\begin{aligned}\mathbf{H}_\mathrm{f}\left(\mathbf{W}_\mathrm{Q}, \mathbf{W}_\mathrm{K}\right) = &\frac{2}{L d_V d_K} \mathbf{R}_{d_V d_K} \left(\mathbf{I}_L \otimes \mathbf{W}_\mathrm{V}^\top \otimes \mathbf{I}_{d_V} \otimes \mathbf{W}_\mathrm{K}^\top\right) \mathbf{Z}_2 \left(\mathbf{W}_\mathrm{Q} \otimes \mathbf{I}_{d_V}\right) \mathbf{K}_{d_K, d_V} \\ &+ \frac{2}{L d_V \sqrt{d_K}} \mathbf{R}_{d_V} \left(\mathbf{I}_L \otimes \mathbf{W}_\mathrm{V}^\top \otimes \mathbf{I}_{d_V}\right) \left(\mathbf{Z}_1 \otimes \mathbf{I}_{d_V}\right) \mathbf{S} \otimes \mathbf{I}_{d_K},\end{aligned}$$

with the residual $\mathbf{R}_m := \mathrm{vec}_r\left(\mathbf{F}(\mathbf{X}) - \mathbf{Y}\right)^\top \otimes \mathbf{I}_m \in \mathbb{R}^{m \times m L d_V}$,
a shuffling matrix $\mathbf{S} := \left(\mathbf{I}_{d_V} \otimes \mathbf{K}_{d_V, d_V}\right)\left(\mathrm{vec}_r\, \mathbf{I}_{d_V} \otimes \mathbf{I}_{d_V}\right) \in \mathbb{R}^{d_V^3 \times d_V}$,
and $\mathbf{Z}_2 := \left(\mathbf{I}_L \otimes \mathbf{K}_{d_V, d_V} \otimes \mathbf{I}_{d_V}\right)\left(\mathbf{X} * \mathbf{X}^\top * \mathbf{M}_3\right) \in \mathbb{R}^{L d_V^3 \times d_V^2}$ with $\mathbf{M}_2$ and $\mathbf{M}_3$ containing moments of the distributions given by self-attention scores.

Let’s simplify with big O notation

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We summarise the dependencies using big O notation

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Definition

For matrices $\mathbf{A}, \mathbf{B}$ *,* $f \in \mathcal{O}(\mathbf{AB})$ *means that all entries of* f *are* $\mathcal{O}(A_{i,j}B_{k,l})$ *for any* i, j, k, l

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We omit the softmax expressions as they are bounded to [0,1]

Heterogeneity in big O notation

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- Self-attention Hessian shows heterogeneous dependence on data

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Predicted growth rates generalise to deeper Transformers

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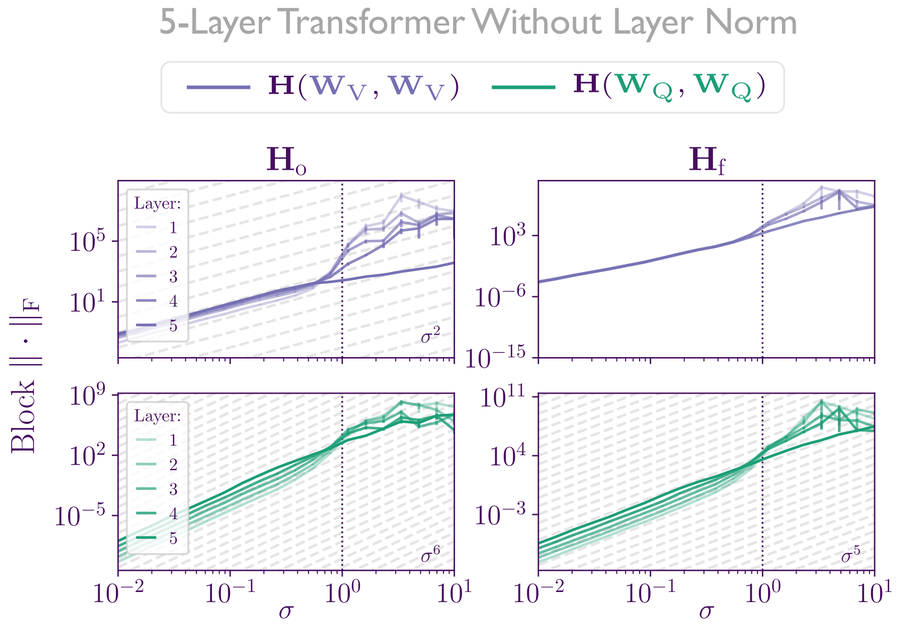

Heterogeneity in big O notation

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Self-attention Hessian shows heterogeneous dependence on data

$$\mathbf{H}_{\mathrm{o}} \in \begin{array}{c} \\ \mathrm{Q} \\ \mathrm{K} \\ \mathrm{V} \end{array} \begin{array}{c} \begin{array}{ccc} \mathrm{Q} & \mathrm{K} & \mathrm{V} \end{array} \\ \begin{bmatrix} \mathcal{O}(\mathbf{X}^6) & \mathcal{O}(\mathbf{X}^6) & \mathcal{O}(\mathbf{X}^4) \\ \cdot & \mathcal{O}(\mathbf{X}^6) & \mathcal{O}(\mathbf{X}^4) \\ \cdot & \cdot & \mathcal{O}(\mathbf{X}^2) \end{bmatrix} \end{array}$$

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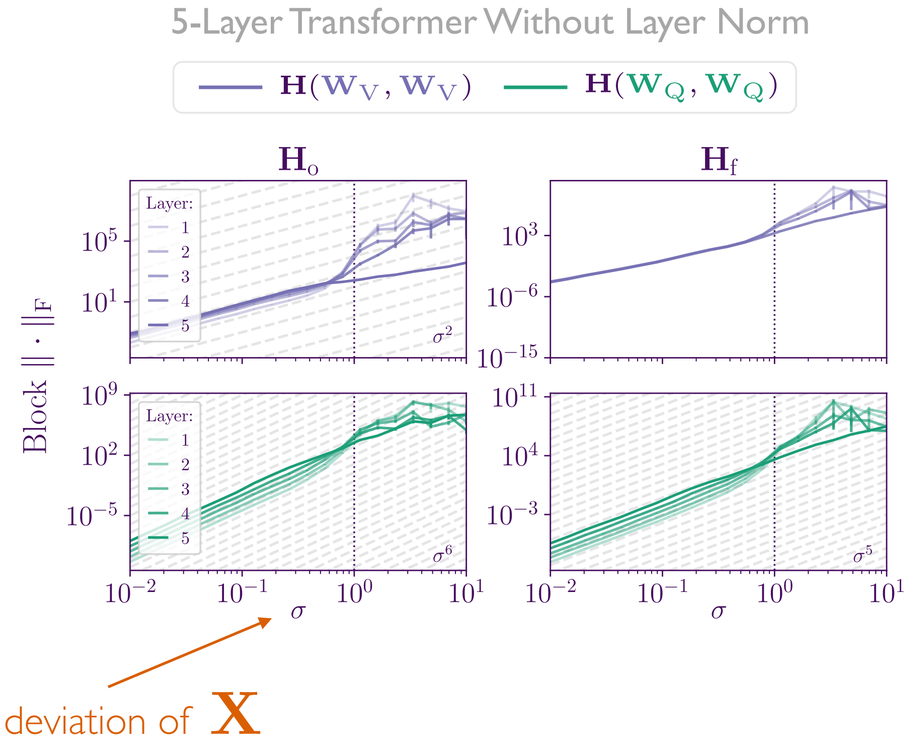
Predicted growth rates generalise to deeper Transformers



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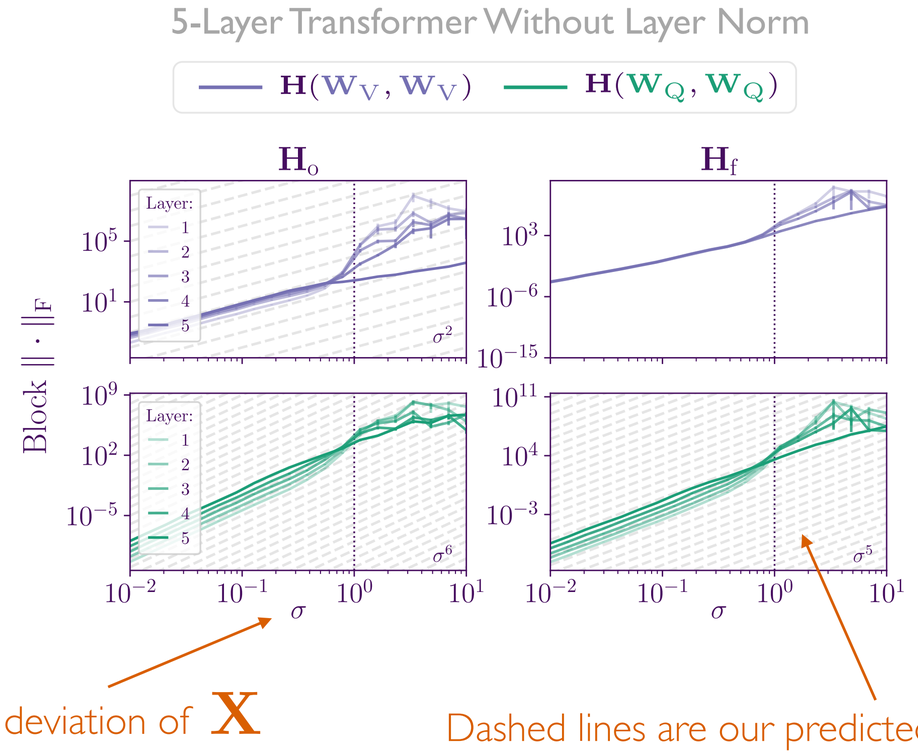

Partial Fix: Pre-Layer Norm

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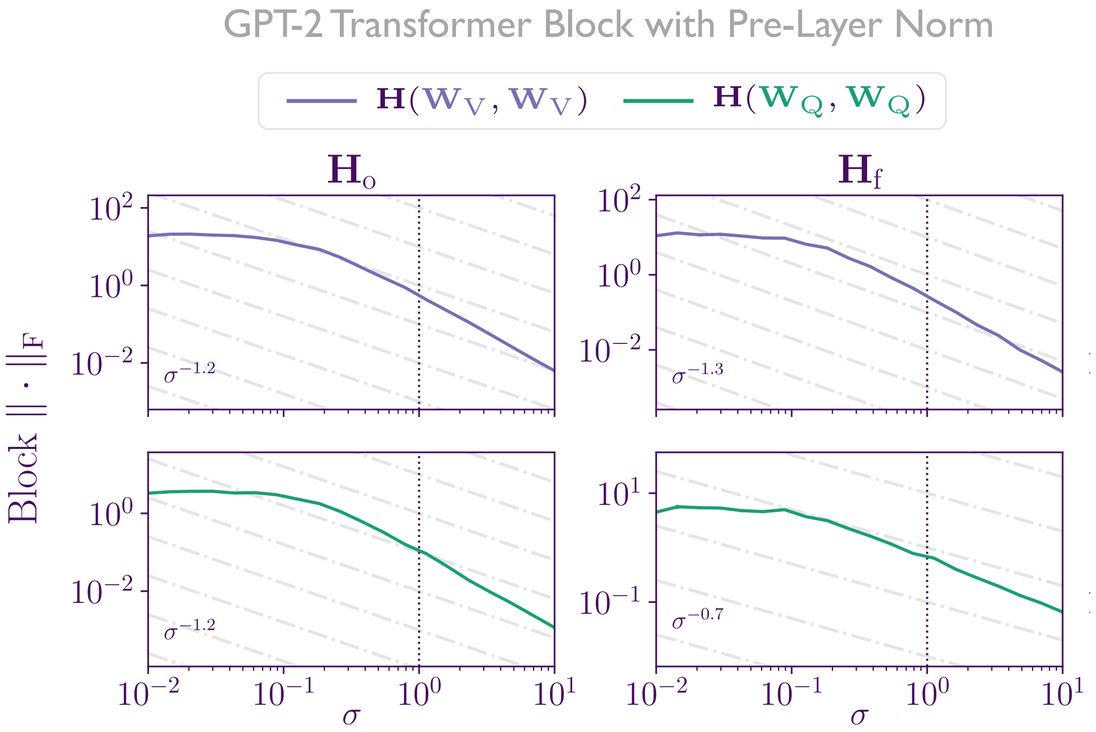

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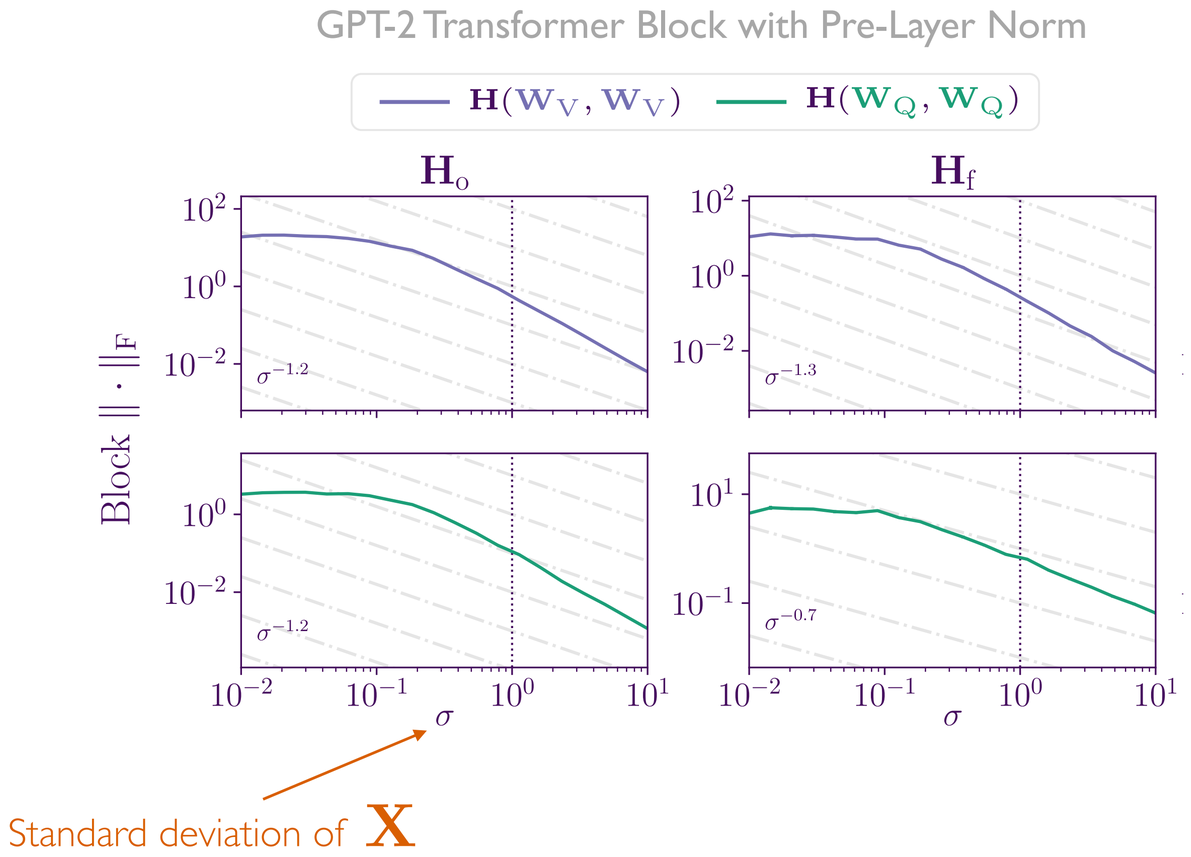

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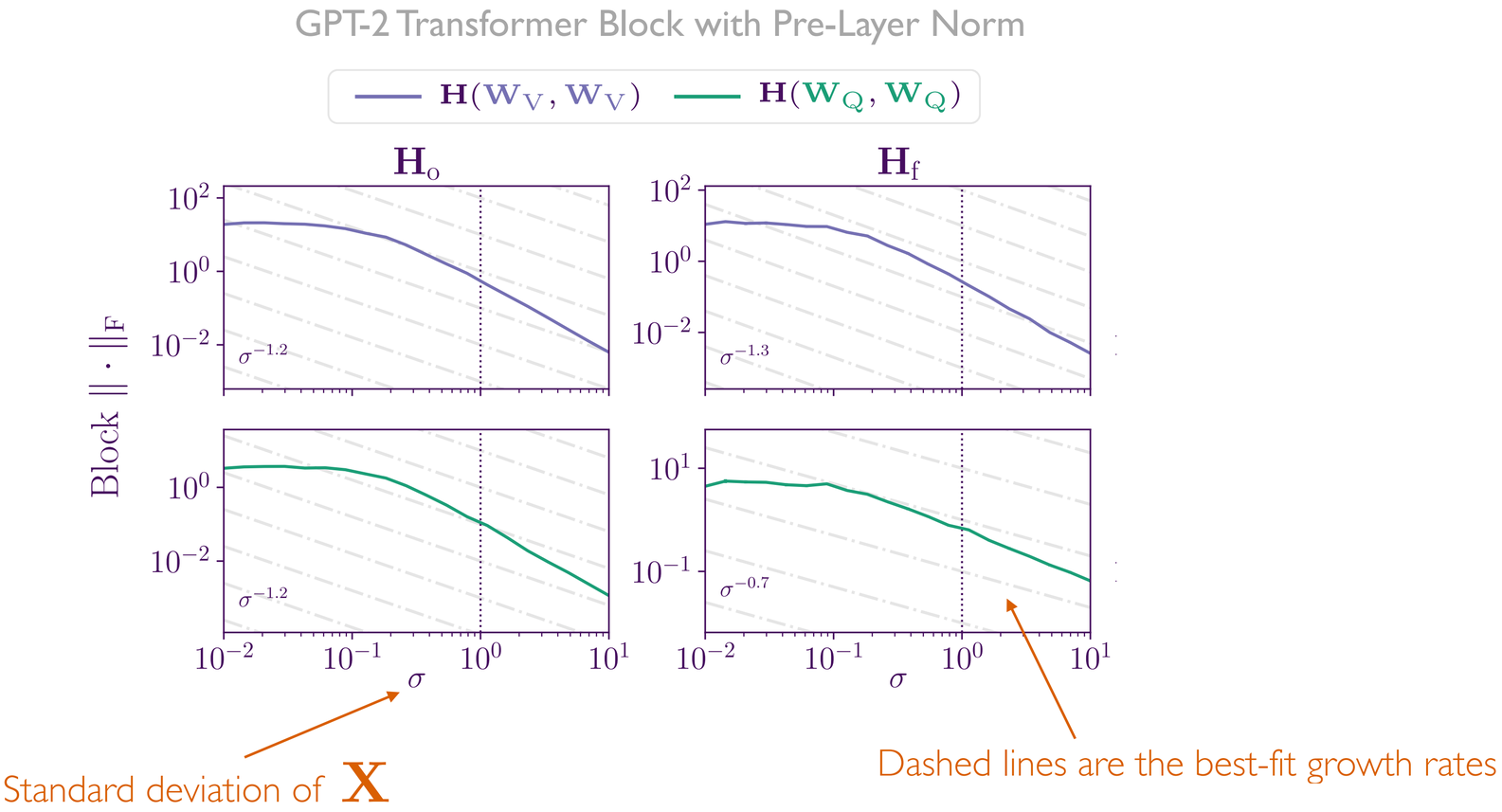

Heterogeneity in big O notation

Moments of attention scores distribution

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Moments of attention scores distribution

Definition

Every row of the attention matrix is a normalised distribution over input tokens. We can compute their (centred) moments:

$$\mathbf{M}_1 := \mathbf{A}\mathbf{X} = \left[\mathbf{A}_{i,:}^\top \mathbf{X}\right]_{1 \le i \le L}$$

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$$\mathbf{H}_{\mathrm{o}} \in \mathcal{O}(\boldsymbol{\Sigma}_{\mathbf{XX}}^{3}) \quad \text{and} \quad \mathbf{H}_{\mathrm{f}} \in \mathcal{O}(\boldsymbol{\Omega}_{\mathbf{xy}}\boldsymbol{\Sigma}_{\mathbf{XX}})$$

where

$$\boldsymbol{\Sigma}_{\mathbf{XX}} := \mathbf{X}^{\top}\mathbf{X} / L \quad \text{and} \quad \boldsymbol{\Omega}_{\mathbf{xy}} := \mathbf{X}^{\top}(\mathbf{F}(\mathbf{X}) - \mathbf{Y}) / L$$

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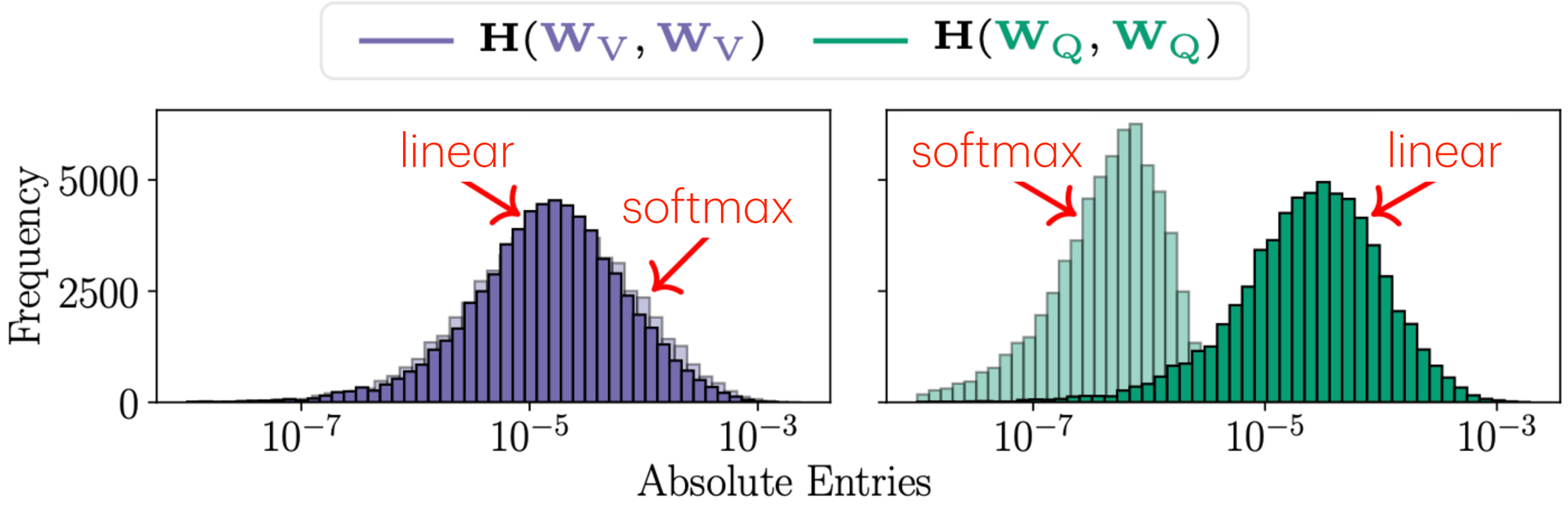

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We showed that for self-attention

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From Singh et al. (2023) we know that for a linear MLP of any depth

$$\mathbf{H}_{\mathrm{o}} \in \mathcal{O}(\boldsymbol{\Sigma}_{\mathbf{XX}}) \quad \text{and} \quad \mathbf{H}_{\mathrm{f}} \in \mathcal{O}(\boldsymbol{\Omega}_{\mathbf{xy}})$$

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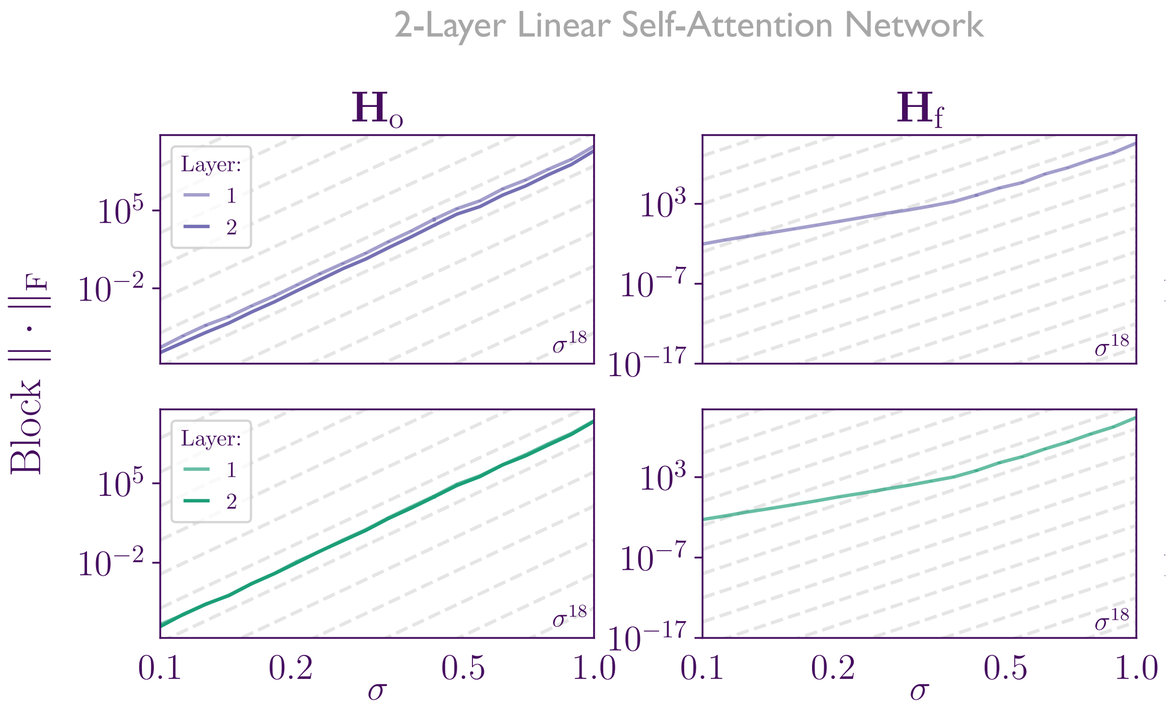

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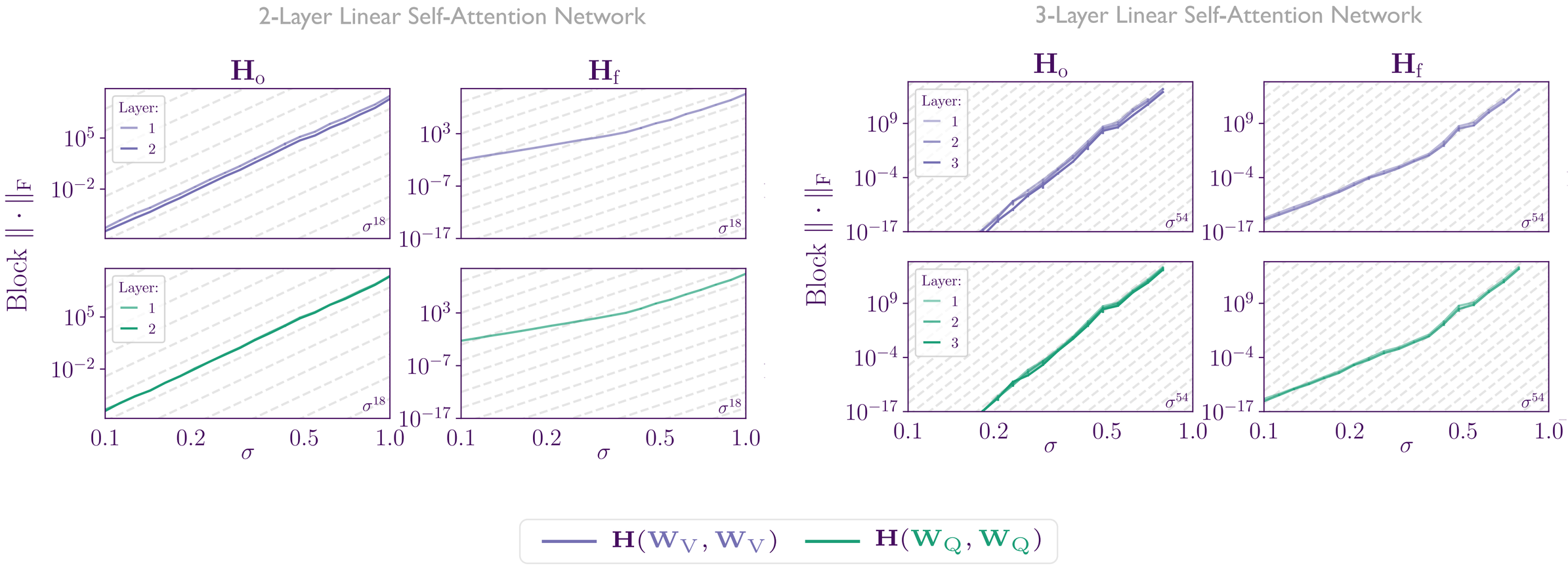

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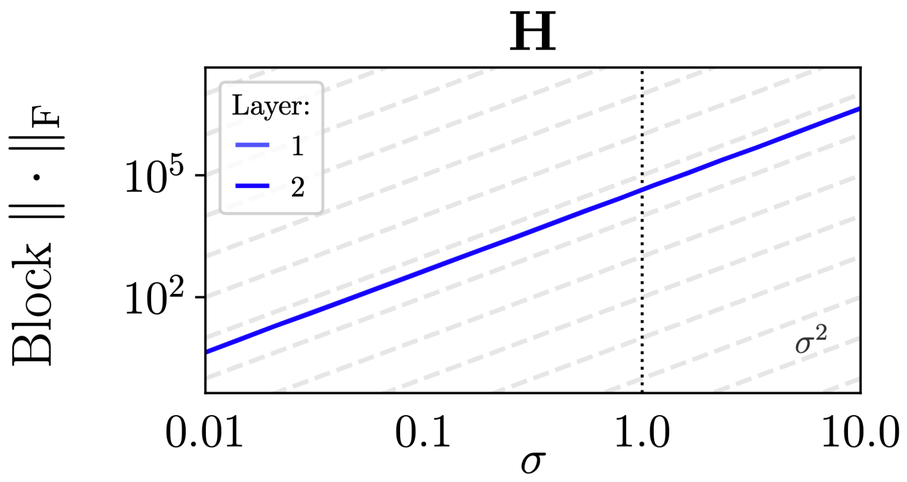
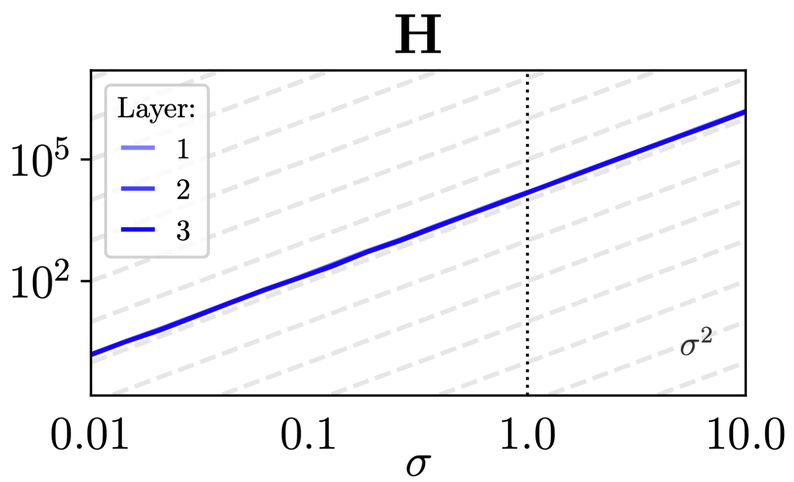
2-Layer Linear MLP



3-Layer Linear MLP



What about Hessian eigenvalues?

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Assume the following model:

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In this model we can derive all loss Hessian eigenvalues in closed form!

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- GGN-based approximations of the largest eigenvalue are worse for Transformers than for MLPs
- The Hessian spectrum is sensitive to the outlier activations and attention sinks

Outliers in activations and the spectrum

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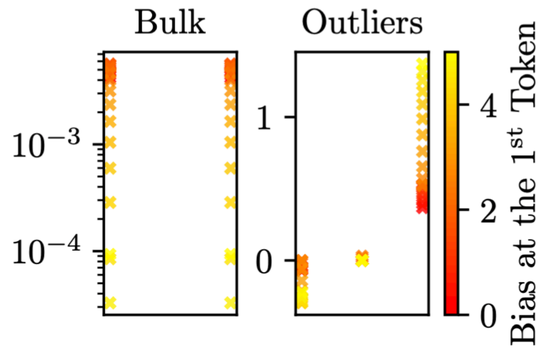

(c) Larger bias at the first token (an attention sink) shrinks the bulk and grows the outliers.

Source:
Sidak Pal Singh, Weronika Ormaniec, Thomas Hofmann. *Cracking the Hessian: Closed-Form Hessian Spectra for Fundamental Neural Networks*. 2025 (Preprint)

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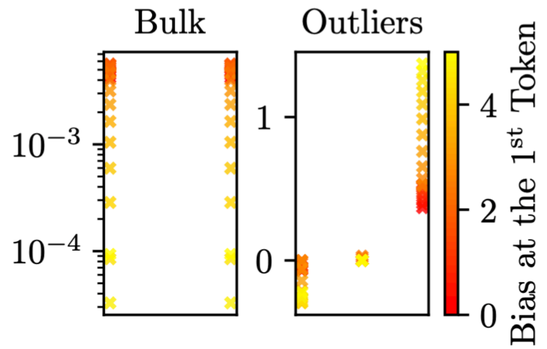

(c) Larger bias at the first token (an attention sink) shrinks the bulk and grows the outliers.

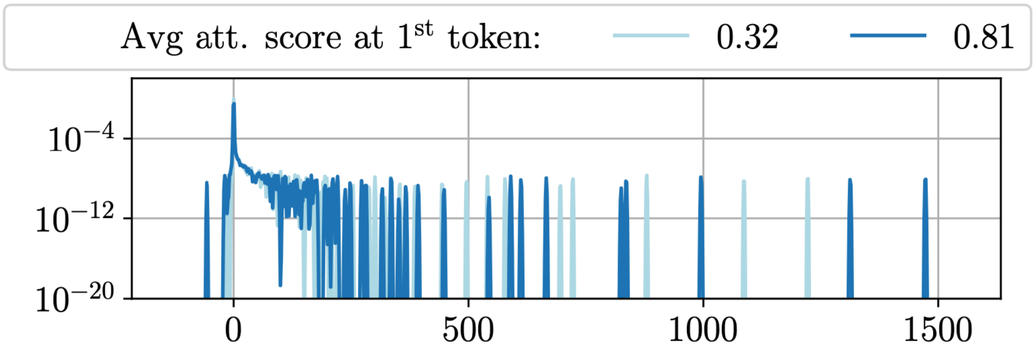

Figure 6: Hessian spectra in the GPT2 model for different magnitudes of attention sinks. Larger attention sinks stretch the spectrum.

Source:
Sidak Pal Singh, Weronika Ormaniec, Thomas Hofmann. *Cracking the Hessian: Closed-Form Hessian Spectra for Fundamental Neural Networks*. 2025 (Preprint)

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3. The outliers in self-attention scores have a direct impact on the self-attention Hessian spectrum.

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Thank you!

Questions?

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