Demystifying Attention Sink in LLMs and its Applications to Architecture Design

Presenter: **Xiangming Gu**

Affiliation: Google Deepmind, National University of Singapore

I am attempting to answer ...

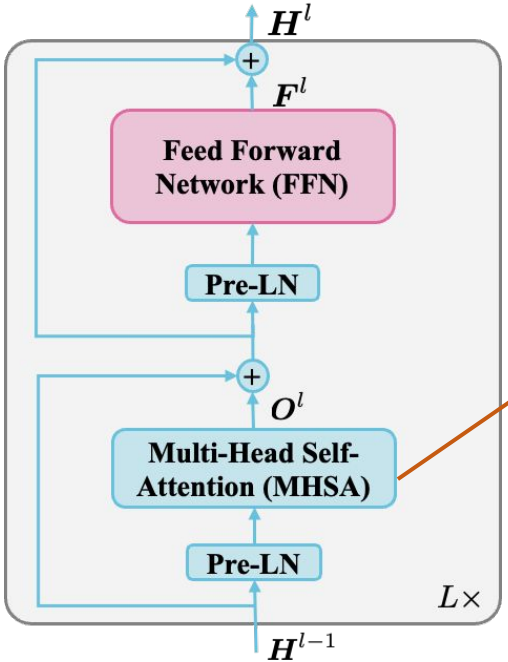
- Mechanism understanding of Attention Sink?
- When Attention Sink Emerges in LLMs?
- Why LLMs need Attention Sink?
- Why GPT-OSS and Qwen3-Next consider Attention Sink in the Model Design?

Covered the following two papers

- When Attention Sink Emerges in Language Models: An Empirical View. ICLR 2025
- Why Do LLMs Attend to the First Token? COLM 2025

What is Attention Sink?

- Decoder-only Transformer



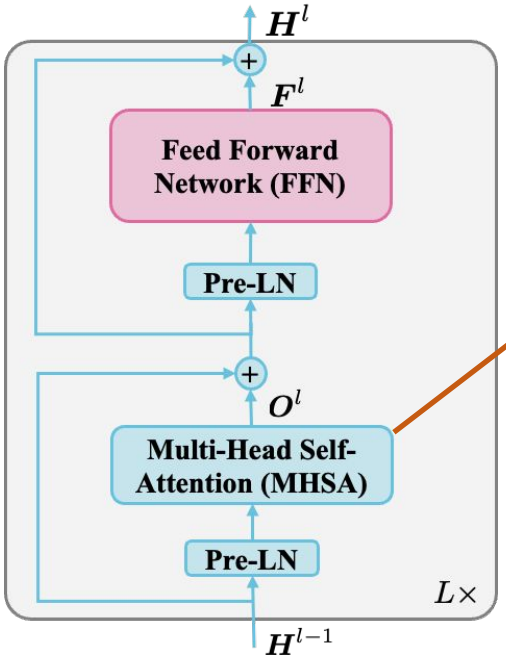
Self-attention is one of the most important parts

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}$$

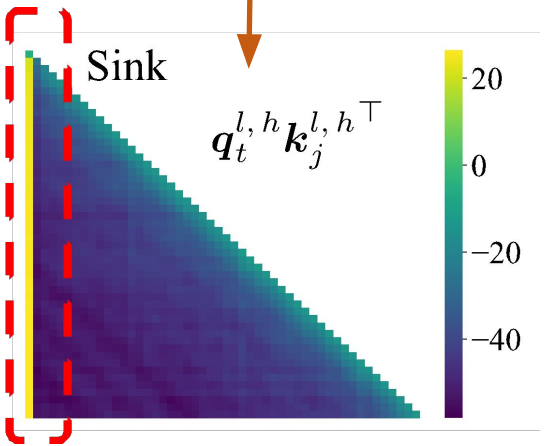
queries keys values

Casual mask

What is Attention Sink?



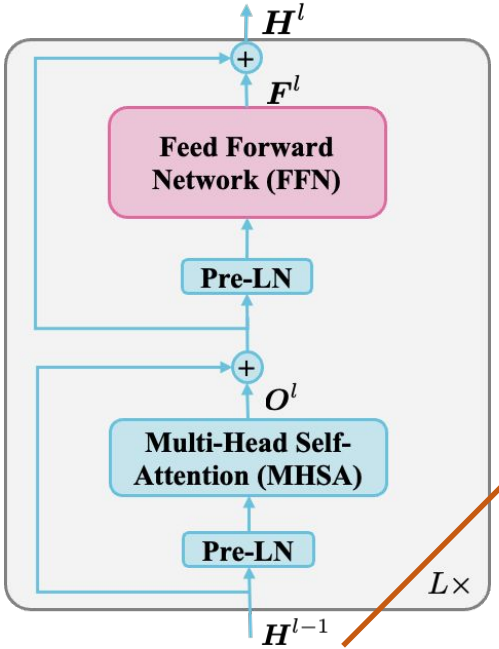
$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}$$

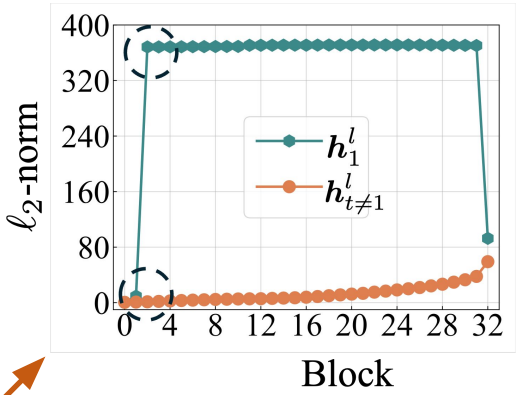


Xiao et al. Efficient Streaming Language Models with Attention Sinks. ICLR 2024

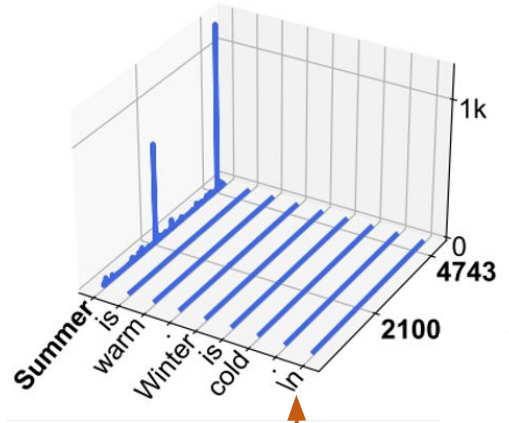
Phenomenons associated to Attention Sink

- Massive Activations





Activations extremely large

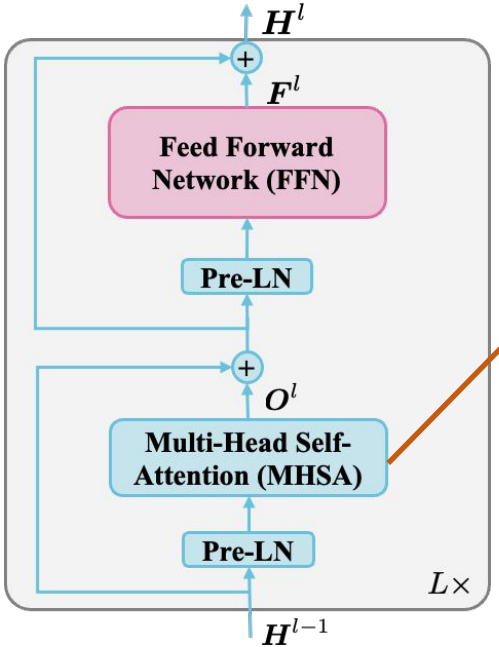


Few dimensions have spikes/outliers

Sun et al. Massive activations in large language models. COLM 2024

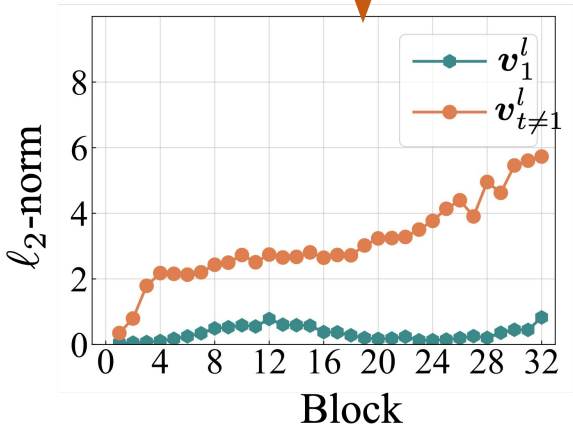
Phenomenons associated to Attention Sink

- Value Drains



$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}$$

Values extremely small

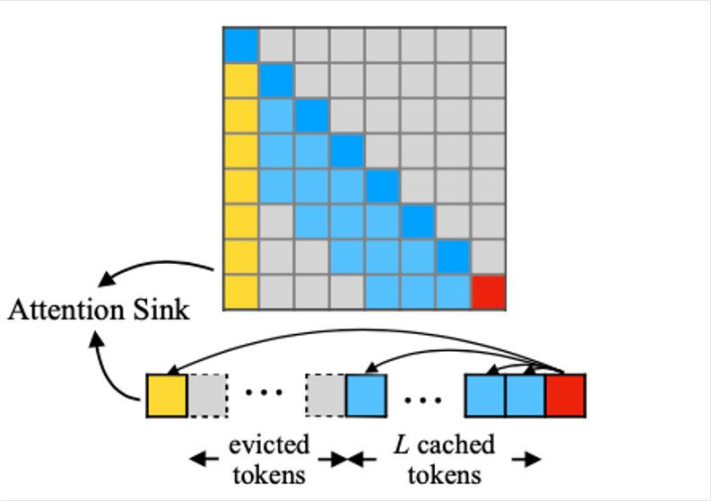


Gu et al. When Attention Sink Emerges in Language Models. ICLR 2025

Post-hoc Applications of Attention Sink

- Long context understanding / generation

- Only computing attention on the first token and recent tokens

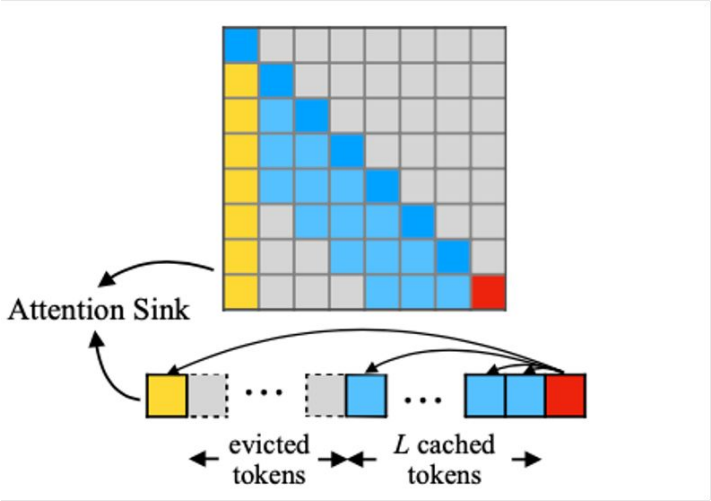


Xiao et al. Efficient Streaming Language Models with Attention Sinks. ICLR 2024

Post-hoc Applications of Attention Sink

- KV cache optimization

- Only retaining KV cache of sink tokens and recent tokens

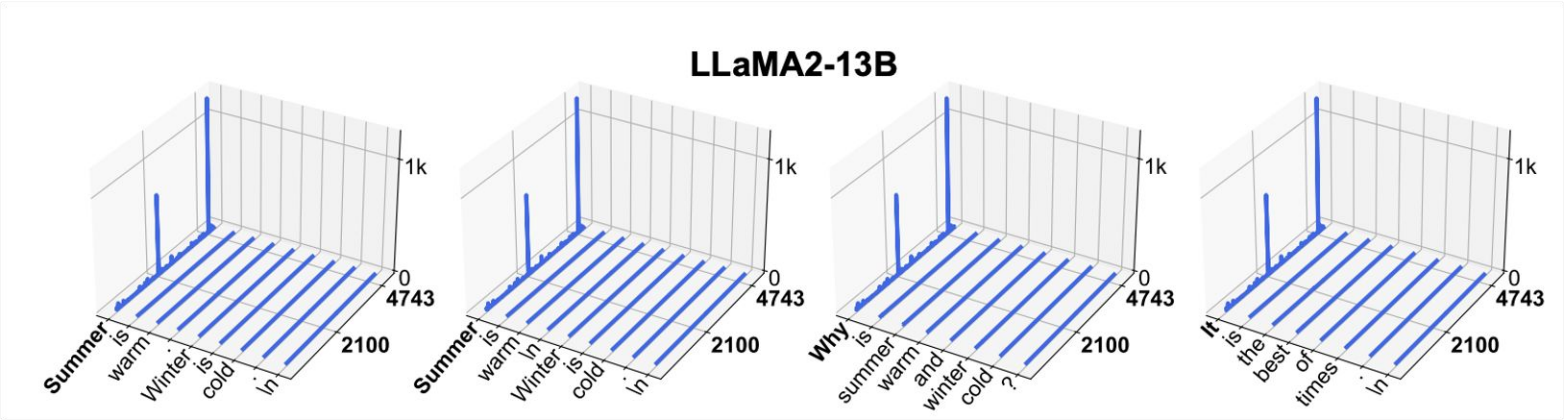


Ge et al. Model Tells You What to Discard: Adaptive KV Cache Compression for LLMs. ICLR 2024

Post-hoc Applications of Attention Sink

- Model quantization

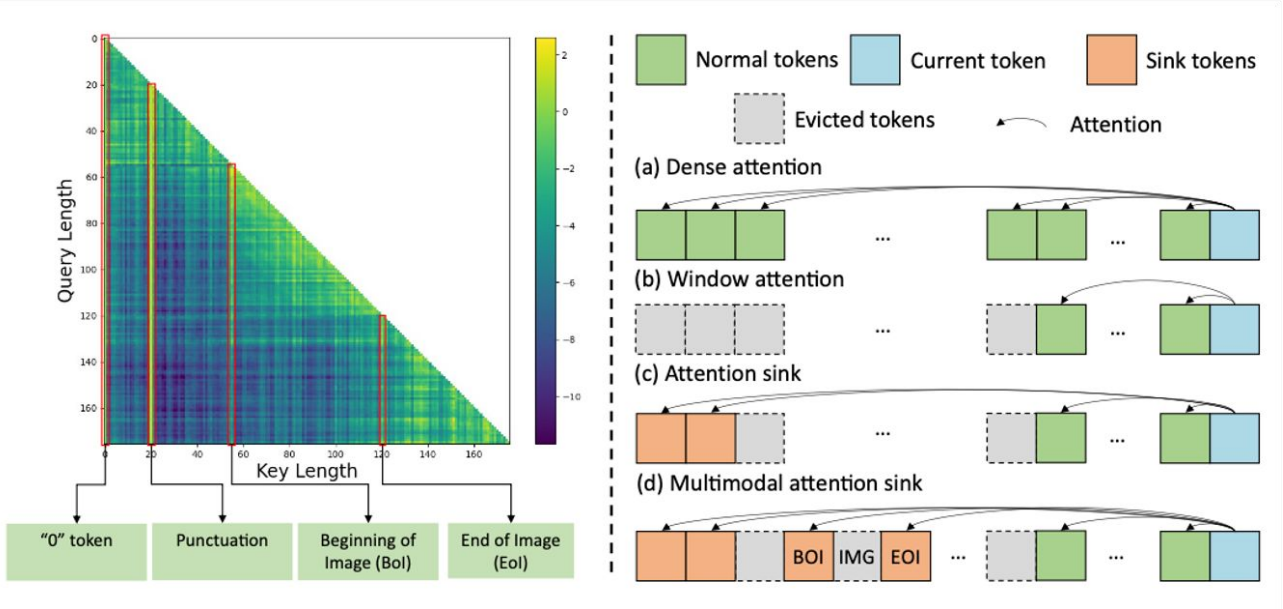
- Preserving the full precision of KV cache of sink token



Liu et al. IntactKV: Improving Large Language Model Quantization by Keeping Pivot Tokens Intact. ACL Findings 2024

Post-hoc Applications of Attention Sink

- Multimodal language modeling



Yang et al. SEED-Story: Multimodal Long Story Generation with Large Language Model. Arxiv 2024

I am attempting to answer …

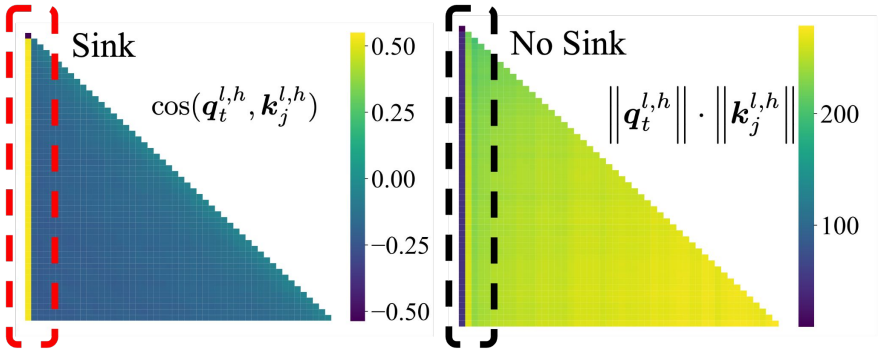
- Mechanism understanding of Attention Sink?
- When Attention Sink Emerges in LLMs?
- Why LLMs need Attention Sink?
- Why GPT-OSS and Qwen3-Next consider Attention Sink in the Model Design?

Mechanism Understanding of Attention Sink

Attention sink is due to the key ***key*** bias of the sink token

$$\boldsymbol{q}_t^{l,h}\boldsymbol{k}_1^{l,h\top} \gg \boldsymbol{q}_t^{l,h}\boldsymbol{k}_{j\neq 1}^{l,h\top}$$

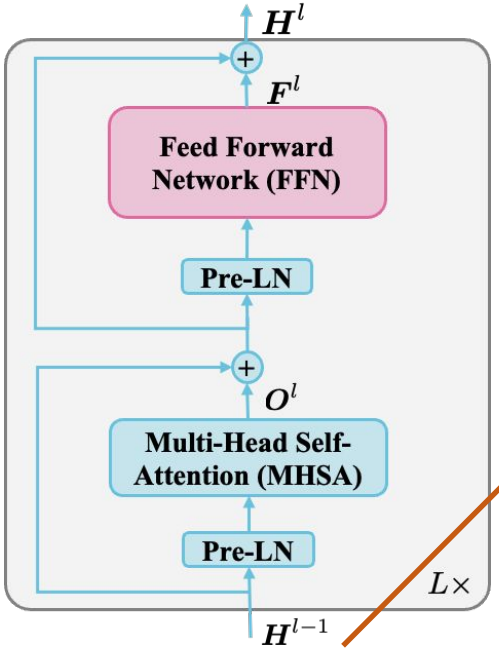
$$\cos(\boldsymbol{q}_t^{l,h}, \boldsymbol{k}_1^{l,h}) \gg \cos(\boldsymbol{q}_t^{l,h}, \boldsymbol{k}_{j\neq 1}^{l,h})$$

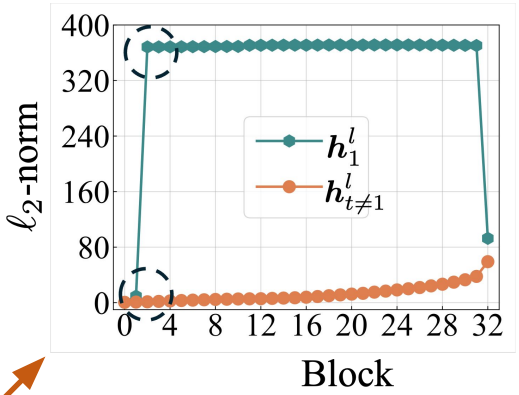


key of the sink token is located in the different manifold, it has small angles with any queries

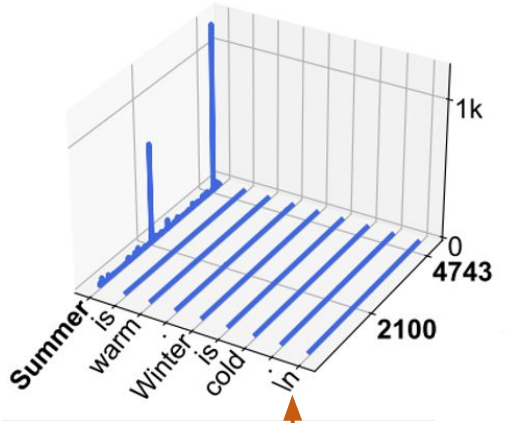
Mechanism Understanding of Attention Sink

- Massive Activations





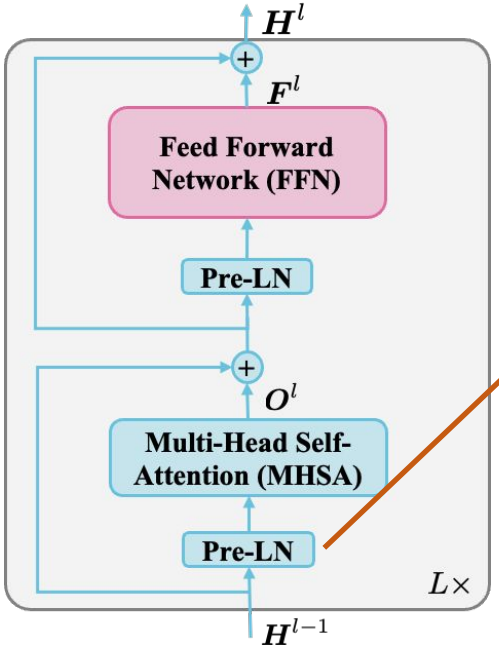
Activations extremely large



Few dimensions have spikes/outliers

Mechanism Understanding of Attention Sink

- Existence of massive activations is to support attention sink



$$\mathrm{LN}(\boldsymbol{h}) = \frac{\boldsymbol{h}}{\sqrt{\frac{1}{d}\sum_{i=1}^{d} \boldsymbol{h}_i^2}} \odot \boldsymbol{g}$$

Layer Norm only retain the spike dimensions (dominate the norm)

$$\boldsymbol{k}_t^{l,h} = \mathrm{LN}(\boldsymbol{h}_t^{l-1})\boldsymbol{W}_K^{l,h}\boldsymbol{R}_{\Theta,-t}$$

Linear transformations of spikes

Similar mechanism for small values

Mechanism Understanding of Attention Sink

Why all these phenomenon tend to happen in the first token (not necessary to be BOS)?

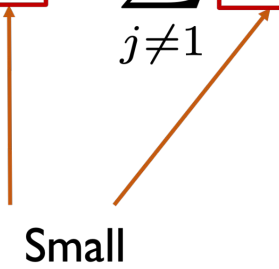
- Uniqueness of the first token: self-attention involves no other tokens, all hidden states in the forward path are equivalent to MLP transformations of input embeddings

- LLMs learn to map the input embeddings to massive activations after certain layers, leading to key bias, and then attention sink

Mechanism Understanding of Attention Sink

- Attention sink approximates “no-op”

$$\boldsymbol{v}_i^{\dagger} = \sum_{j=1}^{i} \boldsymbol{\alpha}_{ij}\boldsymbol{v}_j = \boldsymbol{\alpha}_{i1}\boldsymbol{v}_1 + \sum_{j\neq 1}^{i} \boldsymbol{\alpha}_{ij}\boldsymbol{v}_j$$



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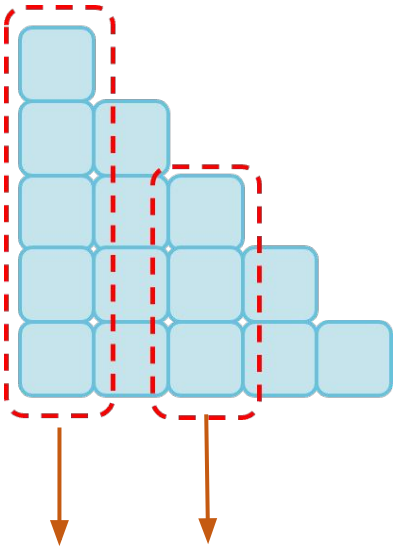
A metric to measure Attention Sink

- Motivations: attention scores of the first token dominates



Average

Importance score

$\alpha_k^{l,h}$

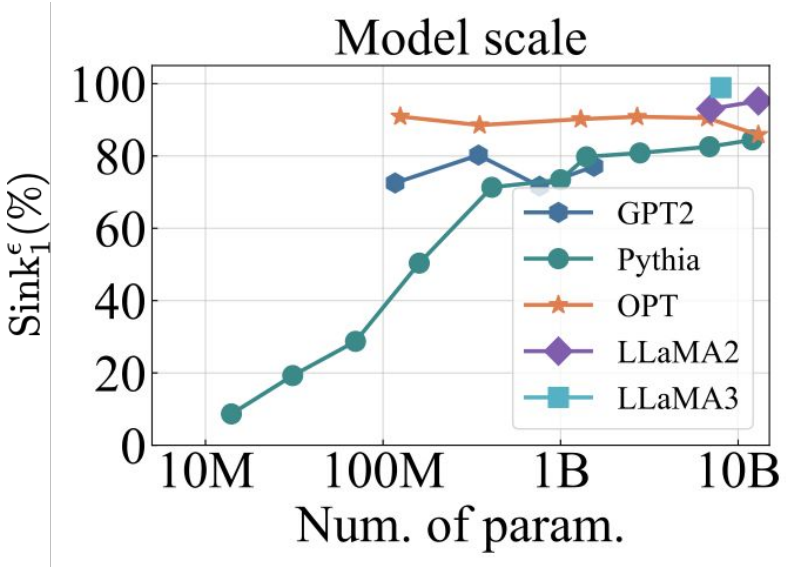
$$\text{Sink}_k^{\epsilon} = \frac{1}{L}\sum_{l=1}^{L}\frac{1}{H}\sum_{h=1}^{H}\mathbb{I}(\alpha_k^{l,h} > \epsilon)$$

Attention sink metric of the whole LM

Within a head, a threshold to decide sink, e.g., 0.3 for 64 tokens

Attention Sink w.r.t. Model Scale / Training Stage

- Attention sink emerges in small LMs, even with 14M params.



- Attention sink already emerges in LM pre-training.

LLM	$\text{Sink}_1^{\epsilon}(\%)$ Base	Chat
Mistral-7B	97.49	88.34
LLaMA2-7B	92.47	92.88
LLaMA2-13B	91.69	90.94
LLaMA3-8B	99.02	98.85

Attention Sink w.r.t. Different Inputs

- Attention sink emerges with / without BOS (for most LLMs), even with random tokens as input
- Under all the repeated tokens?

LLM	$\text{Sink}_1^{\epsilon}(\%)$ natural	random	repeat
GPT2-XL	77.00	70.29	62.28
Mistral-7B	97.49	75.21	0.00
LLaMA2-7B Base	92.47	90.13	0.00
LLaMA3-8B Base	99.02	91.23	0.00

Related to positional embeddings

Attention Sink with Repeated Tokens as Inputs

- For LLMs with NOPE / Relative PE / ALiBi / Rotary

$$\boldsymbol{P} = \mathbf{0}$$

Residual streams before Transformer blocks

$$\boldsymbol{h}_t^0 = \boldsymbol{x}\boldsymbol{W}_E + \boldsymbol{P}$$

Then

$$\boldsymbol{h}_1^0 = \boldsymbol{h}_2^0 = \cdots = \boldsymbol{h}_T^0$$

Using induction, we can prove (all have massive activations, distribute the sink)

$$\boldsymbol{h}_1^l = \boldsymbol{h}_2^l = \cdots = \boldsymbol{h}_T^l, \ \ \forall \ 0 \le l \le L$$

Attention Sink with Repeated Tokens as Inputs

- We can even derive the closed form / upper bound attention distributions for NOPE / Relative PE / ALiBi / Rotary (see the paper).

- However, absolute / learnable PE (e.g., GPT2) have no such properties

LLM	$\text{Sink}_1^{\epsilon}(\%)$ natural	random	repeat
GPT2-XL	77.00	70.29	62.28
Mistral-7B	97.49	75.21	0.00
LLaMA2-7B Base	92.47	90.13	0.00
LLaMA3-8B Base	99.02	91.23	0.00

When Attention Sink Emerges in LLMs?

- Attention sink appears during LLM pre-training

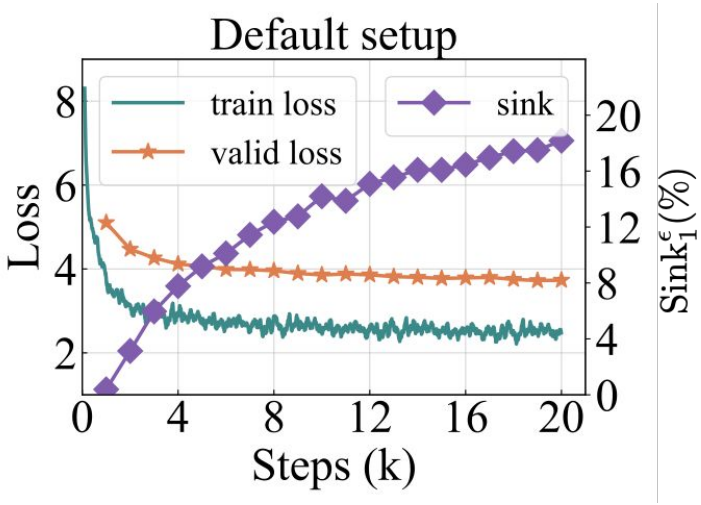
- Attributing attention sink phenomenon to LLM pre-training

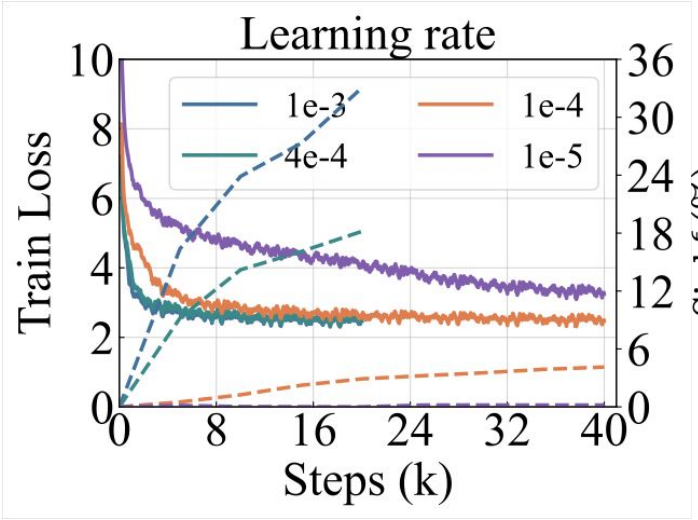
$$\min_{\theta} \mathbb{E}_{\boldsymbol{X} \sim p_{\text{data}}} \left[\mathcal{L} \left(p_{\theta}(\boldsymbol{X}) \right) \right]$$

Optimization Data distribution Loss function Model architecture

Effects of Optimization

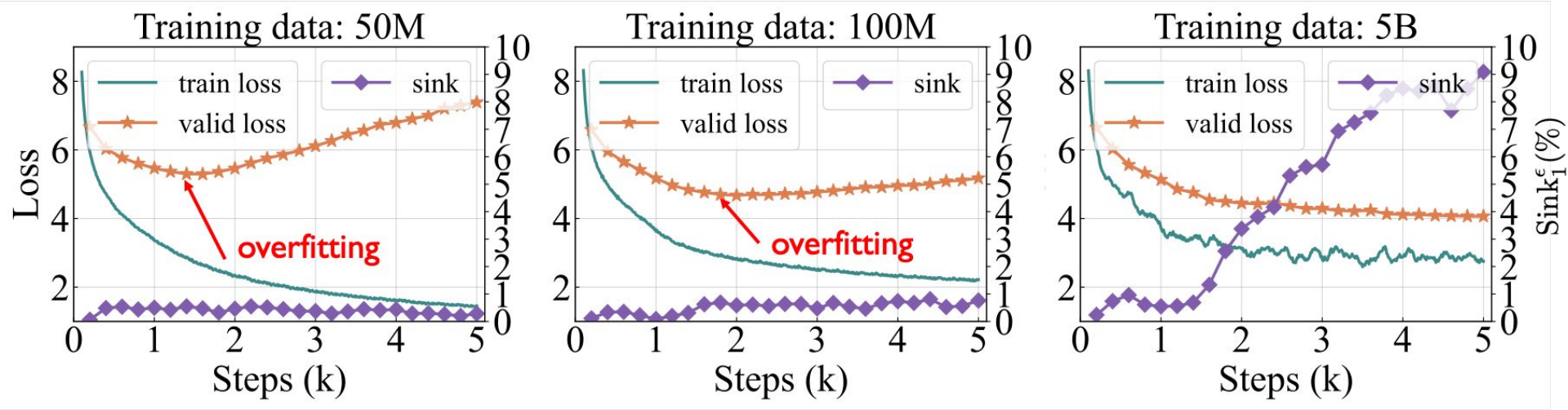
- Attention sink appears during LLM pre-training process (not initialization)
- Large LR encourages attention sink (even under the same LR*steps)





Effects of Data Distribution

- Attention sink emerges when we have enough unique training data amount



Effects of Loss function

- Weight decay encourages attention sink

L2 regularization

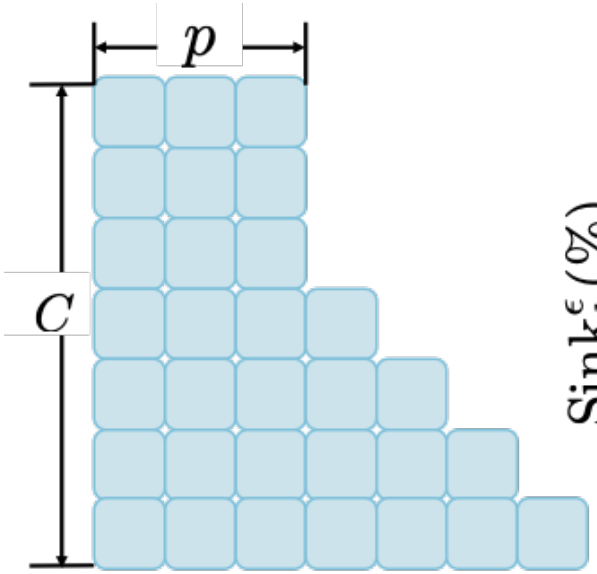
$$\mathcal{L} = \sum_{t=2}^{C} \log p_\theta(\boldsymbol{x}_t | \boldsymbol{x}_{<t}) + \gamma \|\theta\|_2^2$$

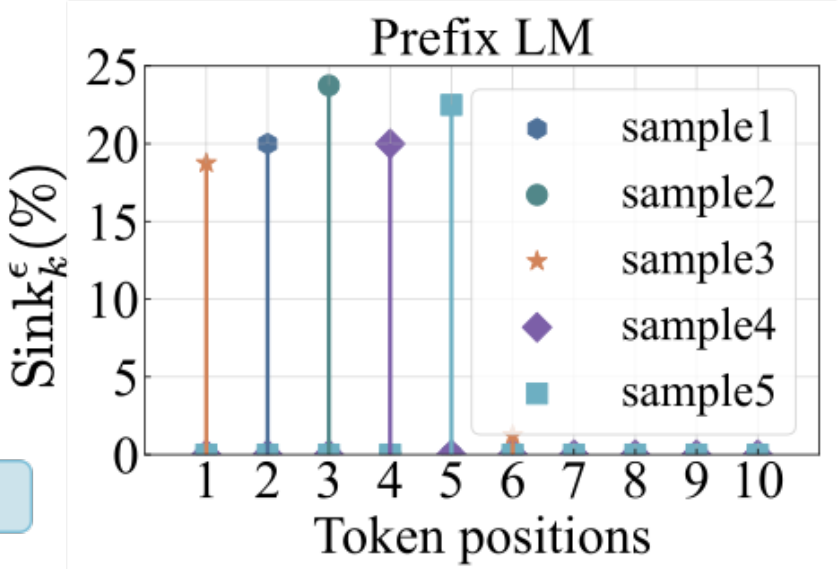
γ	0.0	0.001	0.01	0.1	0.5	1.0	2.0	5.0
$\text{Sink}_1^\epsilon(\%)$	15.20	15.39	15.23	18.18	41.08	37.71	6.13	0.01
valid loss	3.72	3.72	3.72	3.73	3.80	3.90	4.23	5.24

Effects of Loss function

- Prefix language modeling: sink token shifts from the first token to other positions within the prefix

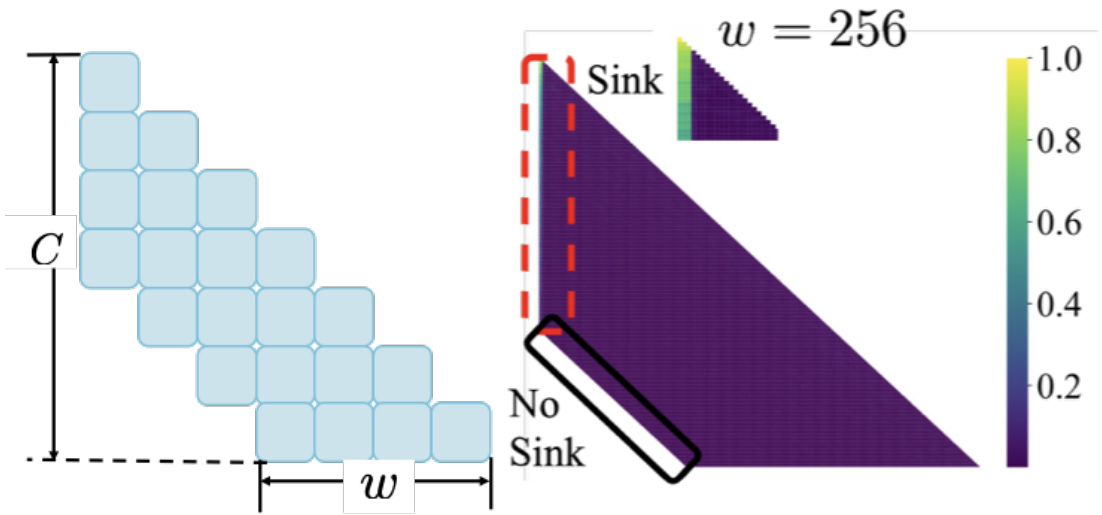
$$\mathcal{L} = \sum_{t=p+1}^{C} \log p_\theta(\boldsymbol{x}_t | \boldsymbol{x}_{p+1:t-1}, \boldsymbol{x}_{1:p})$$





Effects of Loss function

- Shift window attention: attention sink appears on the absolute, not the relative first token
- Small window size mitigates attention sink



Validating sink token has key bias

$$\mathcal{L} = \sum_{t=2}^{C} \log p_\theta(\boldsymbol{x}_t | \boldsymbol{x}_{t-w:t-1})$$

Effects of Model Architecture

The following designs do not affect the emergence of attention sink

- Positional embeddings

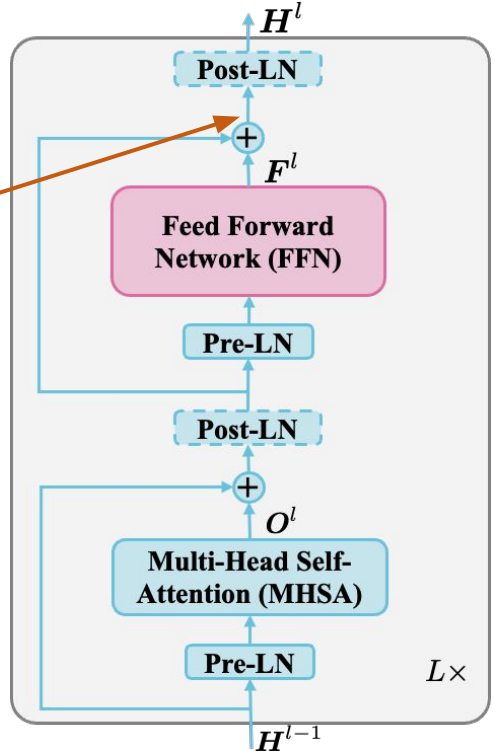
NOPE, learnable PE, absolute PE, relative PE, Rotary, ALIBI

Effects of Model Architecture

The following designs do not affect the emergence of attention sink

- Positional embeddings
- Pre-norm or post-norm

Massive activations happen before LN



Effects of Model Architecture

The following designs do not affect the emergence of attention sink

- Positional embeddings
- Pre-norm or post-norm
- FFNs with different activation functions
- Number of attention heads, how to combine multiple heads
- ...

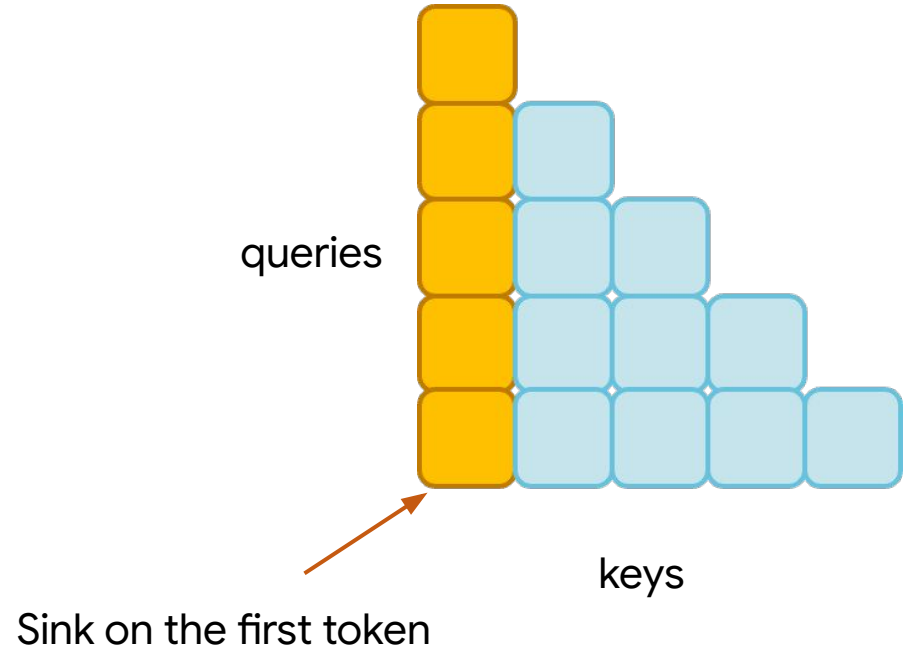
Effects of Model Attention Design

- Standard softmax attention

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}$$

queries keys values

Casual mask



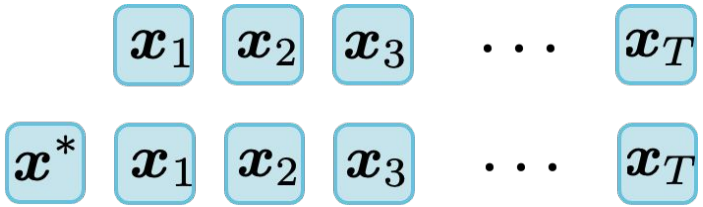
Effects of Model Attention Design

- Softmax attention with a learnable sink token

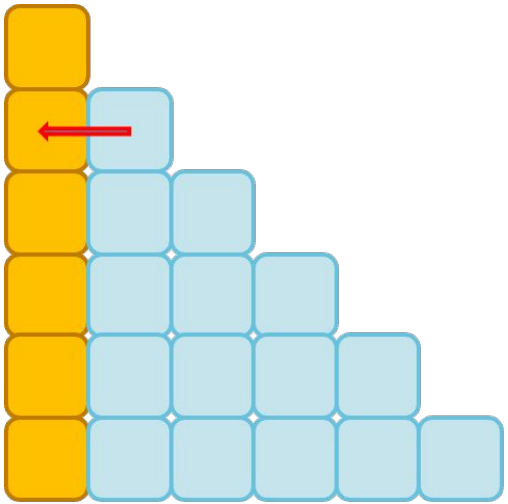
$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\begin{bmatrix}\boldsymbol{q}^{*l,h}\\ \boldsymbol{Q}^{l,h}\end{bmatrix}\begin{bmatrix}\boldsymbol{k}^{*l,h\top} & \boldsymbol{K}^{l,h\top}\end{bmatrix}+\boldsymbol{M}\right)\begin{bmatrix}\boldsymbol{v}^{*l,h}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

QKV for sink token

queries



Learnable sink token



keys

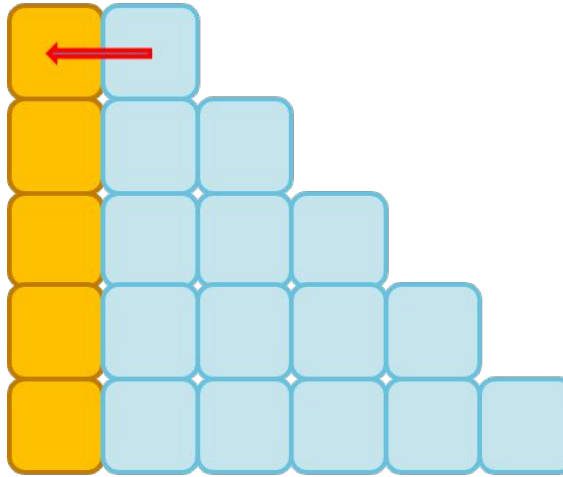
Sink on the learnable sink token

Effects of Model Attention Design

- Softmax attention with learnable KV biases

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\left[\boldsymbol{k}^{*l,h\top} \quad \boldsymbol{K}^{l,h\top}\right] + \boldsymbol{M}\right)\begin{bmatrix}\boldsymbol{v}^{*l,h}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

Learnable KV biases



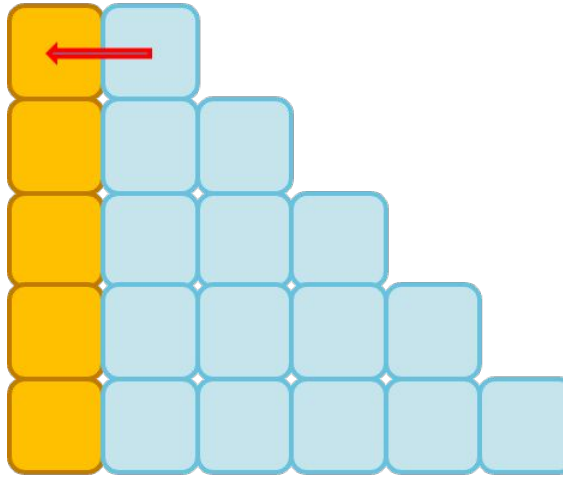
Sink on the learnable K biases

Effects of Model Attention Design

- Softmax attention with learnable K biases

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\left[\boldsymbol{k}^{*l,h\top} \quad \boldsymbol{K}^{l,h\top}\right] + \boldsymbol{M}\right)\begin{bmatrix}\boldsymbol{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

Learnable K biases,
zero V biases



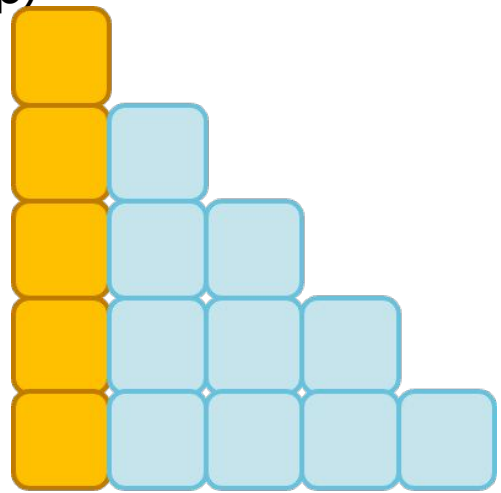
Sink on the learnable
key biases

Effects of Model Attention Design

- Softmax attention with learnable K biases (control group)

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}+\boldsymbol{v}^{*l,h}$$

Learnable V biases



Sink on the first token,
no effects

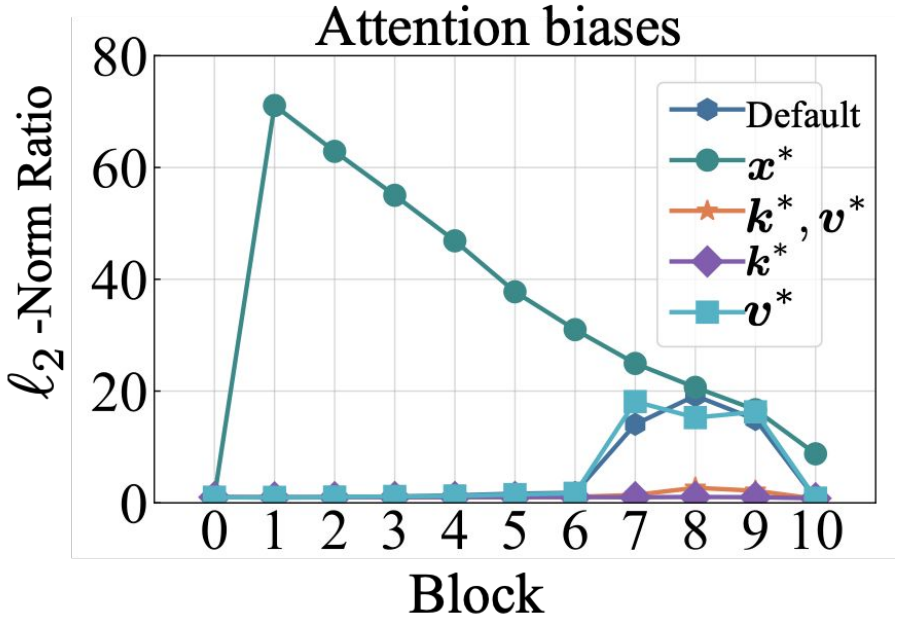
Effects of Attention Biases

- Attention biases can absorb attention sink from the actual first token

Attention in each head	$\text{Sink}_*^\epsilon(\%)$	$\text{Sink}_1^\epsilon(\%)$	valid loss
$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}$	-	18.18	3.73
$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\begin{bmatrix}\boldsymbol{q}^{*l,h}\\ \boldsymbol{Q}^{l,h}\end{bmatrix}\begin{bmatrix}\boldsymbol{k}^{*l,h\top} & \boldsymbol{K}^{l,h\top}\end{bmatrix}+\boldsymbol{M}\right)\begin{bmatrix}\boldsymbol{v}^{*l,h}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$	74.12	0.00	3.72
$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\begin{bmatrix}\boldsymbol{k}^{*l,h\top} & \boldsymbol{K}^{l,h\top}\end{bmatrix}+\boldsymbol{M}\right)\begin{bmatrix}\boldsymbol{v}^{*l,h}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$	72.76	0.04	3.72
$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\begin{bmatrix}\boldsymbol{k}^{*l,h\top} & \boldsymbol{K}^{l,h\top}\end{bmatrix}+\boldsymbol{M}\right)\begin{bmatrix}\boldsymbol{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$	73.34	0.00	3.72
$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}+\boldsymbol{v}^{*l,h}$	-	17.53	3.73

Effects of Attention Biases

- Key biases can significantly mitigates massive activations, as no need to develop new biases



Effects of Attention Biases

- Value bias needs to be close to zero

$\boldsymbol{v}^{*l,h}$	$\mathbf{0}$	$\boldsymbol{v}'$	$5\boldsymbol{v}'$	$20\boldsymbol{v}'$	$\boldsymbol{v}''$	$5\boldsymbol{v}''$	$20\boldsymbol{v}''$
$\text{Sink}_*^\epsilon(\%)$	73.34	70.03	44.43	1.51	69.74	27.99	0.00
$\text{Sink}_1^\epsilon(\%)$	0.00	0.06	3.71	25.88	2.15	5.93	11.21
valid loss	3.72	3.72	3.72	3.71	3.72	3.72	3.73

$$\boldsymbol{v}' = [1, 0, 0, .., 0] \qquad \boldsymbol{v}'' = [1, 1, 1, .., 1]/\sqrt{d_h}$$

Effects of Attention Biases

- Key bias is low-rank

d_a	1	2	4	8	16	32	64
$\text{Sink}_*^\epsilon(\%)$	32.18	30.88	30.94	31.39	23.30	51.23	69.19
$\text{Sink}_1^\epsilon(\%)$	4.74	4.96	4.39	4.54	2.19	1.94	0.04
valid loss	3.73	3.72	3.72	3.73	3.73	3.73	3.72

Comparing different Attention Biases

- Learnable key biases, zero value biases

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\left[\boldsymbol{k}^{*l,h\top} \quad \boldsymbol{K}^{l,h\top}\right] + \boldsymbol{M}\right)\begin{bmatrix}\mathbf{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

- Softmax off-by-one

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\left[\mathbf{0}^{*l,h\top} \quad \boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}\right] + \boldsymbol{M}\right)\begin{bmatrix}\mathbf{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

- Learnable attention score biases (single number for each head, layer)

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\left[\boldsymbol{b}^{*l,h\top} \quad \boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}\right] + \boldsymbol{M}\right)\begin{bmatrix}\mathbf{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

$$\boldsymbol{b}^{*l,h} = b^{*l,h}[1, 1, 1, .., 1]$$

Comparing different Attention Biases

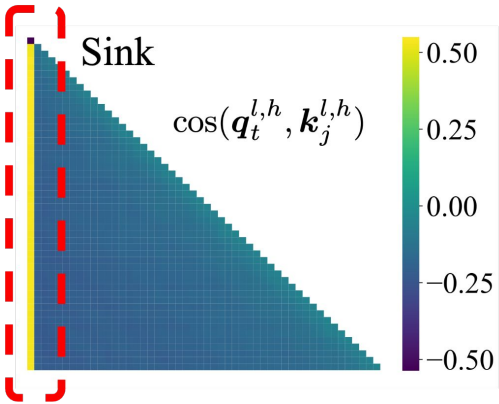
- Softmax off-by-one: with any query, the cosine similarity is zero

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\left[\mathbf{0}^{*l,h\top} \quad \boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}\right] + \boldsymbol{M}\right)\begin{bmatrix}\mathbf{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

- Original format:

$$(\text{softmax}_1(x))_i = \frac{\exp(x_i)}{1+\sum_j \exp(x_j)}$$

- Zero may already be enough



Effects of Attention Biases

The learnable key bias and **zero** value bias experiments show that:

- Large attention score does not mean important in semantic
- Sink token save extra attention, adjusts the dependence among tokens

But why LLMs need such a mechanism?

Effects of Normalization in Softmax Attention

Whether this is due to the normalization in Softmax attention?

$$\boldsymbol{v}_i^{\dagger} = \sum_{j=1}^{i} \frac{\alpha \mathrm{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_j))}{\sum_{j'=1}^{i} \mathrm{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_{j'}))} \boldsymbol{v}_j = \sum_{j=1}^{i} \frac{\mathrm{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_j))}{\sum_{j'=1}^{i} \mathrm{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_{j'}))} \boldsymbol{h}_j(\alpha \boldsymbol{W}_V),$$

$$\boldsymbol{o}_i' = \mathrm{Concat}_{h=1}^{H}(\boldsymbol{v}_i'^{h}) \boldsymbol{W}_O.$$

Scaling the normalization $\boldsymbol{Z}_i \to \boldsymbol{Z}_i/\alpha$, equivalent to scaling weight matrices, and then scaling the LR, mitigates attention sink

$$\begin{aligned} \boldsymbol{W}_O^{s+1} &= \boldsymbol{W}_O^s - \eta \nabla_{\boldsymbol{W}_O^s} \mathcal{L}(\alpha \boldsymbol{W}_O^s) \\ &= \boldsymbol{W}_O^s - \alpha\eta \nabla_{\boldsymbol{W}} \mathcal{L}(\boldsymbol{W})|_{\boldsymbol{W}=\alpha \boldsymbol{W}_O^s}, \end{aligned}$$

$$\begin{aligned} \hat{\boldsymbol{W}}_O^{s+1} &= \hat{\boldsymbol{W}}_O^s - \eta' \nabla_{\hat{\boldsymbol{W}}_O^s} \mathcal{L}(\hat{\boldsymbol{W}}_O^s) \\ &= \alpha \boldsymbol{W}_O^s - \eta' \nabla_{\boldsymbol{W}} \mathcal{L}(\boldsymbol{W})|_{\boldsymbol{W}=\alpha \boldsymbol{W}_O^s}, \end{aligned}$$

Effects of Normalization in Softmax Attention

Power of sum to one: may mitigate attention sink but does not prevent, sensitive to LR, large LR may incentivize attention sink

$$\boldsymbol{v}_i^\dagger = \frac{\sum_{j=1}^{i} \mathrm{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_j))\boldsymbol{v}_j}{\left(\sum_{j'=1}^{i} \mathrm{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_{j'}))^p\right)^{\frac{1}{p}}} \qquad \boldsymbol{v}_i^\dagger = \sum_{j=1}^{i} \left(\frac{\exp(\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h/p}})}{\sum_{j'=1}^{i} \exp(\frac{\boldsymbol{q}_i \boldsymbol{k}_{j'}^\top}{\sqrt{d_h/p}})} \right)^{\frac{1}{p}} \boldsymbol{v}_j$$

Effects of Normalization in Softmax Attention

- Removing the normalization in Softmax attention

Using sigmoid attention (exponential kernel in Softmax tends to explode)

$$\text{Sigmoid}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}$$

Or ELU plus one attention

No normalization -> No attention sink; add back - > attention sink

Effects of Normalization in Softmax Attention

Other attention variants

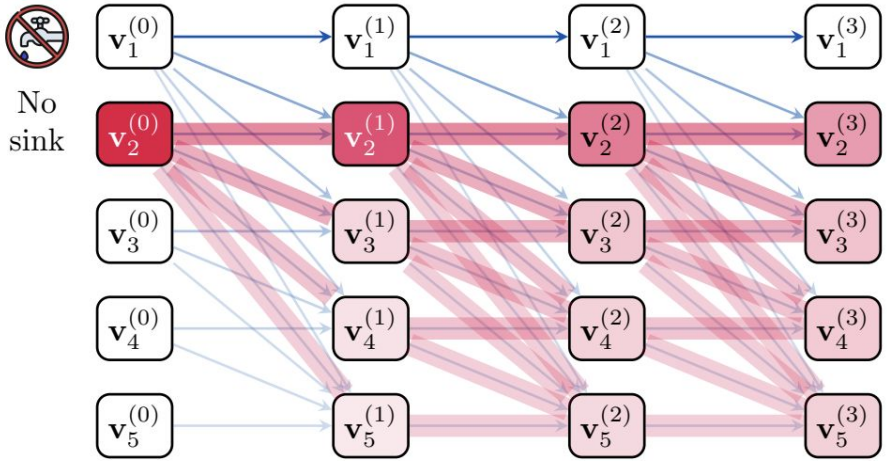
$\text{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_j))$	$\boldsymbol{Z}_i$	$\text{Sink}_1^{\epsilon}(\%)$	valid loss
$\exp(\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}})$	$\sum_{j'=1}^{i} \exp(\frac{\boldsymbol{q}_i \boldsymbol{k}_{j'}^\top}{\sqrt{d_h}})$	18.18	3.73
$\text{sigmoid}(\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}})$	1	0.44*	3.70
$\text{sigmoid}(\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}})$	$\sum_{j'=1}^{i} \text{sigmoid}(\frac{\boldsymbol{q}_i \boldsymbol{k}_{j'}^\top}{\sqrt{d_h}})$	30.24	3.74
$\text{elu}(\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}}) + 1$	1	0.80*	3.69
$\text{elu}(\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}}) + 1$	$\sum_{j'=1}^{i} \text{elu}(\frac{\boldsymbol{q}_i \boldsymbol{k}_{j'}^\top}{\sqrt{d_h}}) + 1$	-	-
$\frac{(\text{elu}(\boldsymbol{q}_i)+1)(\text{elu}(\boldsymbol{k}_j)+1)^\top}{\sqrt{d_h}}$	$\sum_{j'=1}^{i} \frac{(\text{elu}(\boldsymbol{q}_i)+1)(\text{elu}(\boldsymbol{k}_{j'})+1)^\top}{\sqrt{d_h}}$	53.65*	4.19
$\frac{(\text{elu}(\boldsymbol{q}_i)+1)(\text{elu}(\boldsymbol{k}_j)+1)^\top}{\sqrt{d_h}}$	1	-	-
$\boldsymbol{q}_i \boldsymbol{k}_j^\top$	$\max\left(\left\lvert \sum_{j'=1}^{i} \boldsymbol{q}_i \boldsymbol{k}_{j'}^\top \right\rvert, 1\right)$		

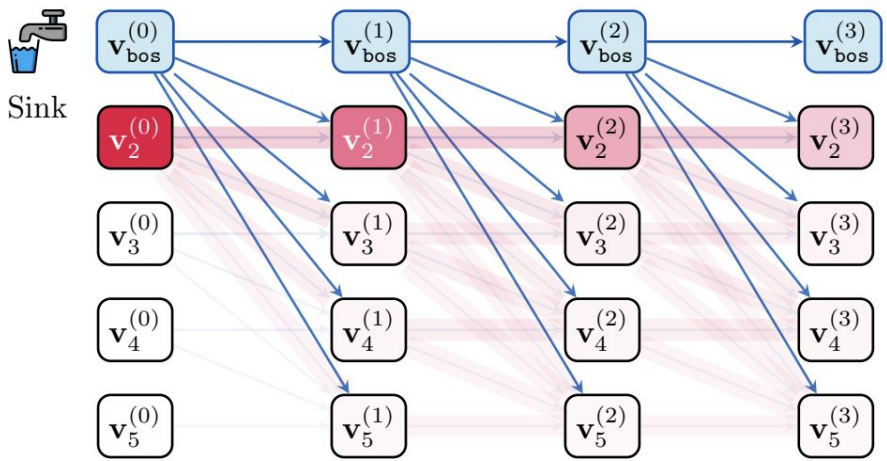
I am attempting to answer …

- Mechanism understanding of Attention Sink?
- When Attention Sink Emerges in LLMs?
- Why LLMs need Attention Sink?
- Why GPT-OSS and Qwen3-Next consider Attention Sink in the Model Design?

LLMs need attention sink to prevent over-mixing

- Attention blocks try to mix representations
- Attention sink serves as a mechanism to prevent over-mixing (see the paper for theory, longer context needs stronger mechanism)

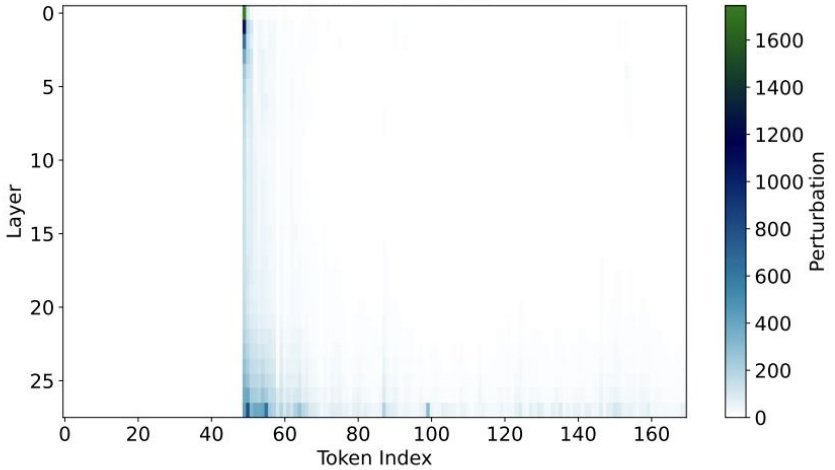




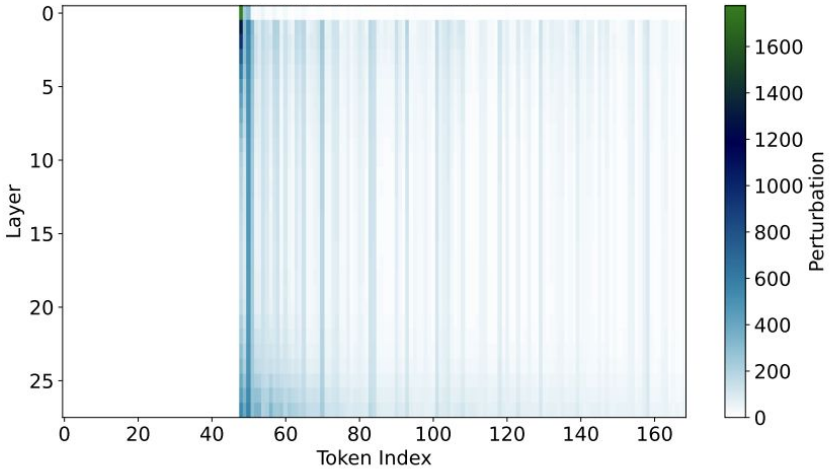
LLMs need attention sink to prevent over-mixing

With attention sink, perturbation on one token (“greatest”->”best”) won’t change token representations a lot

Sink



No sink

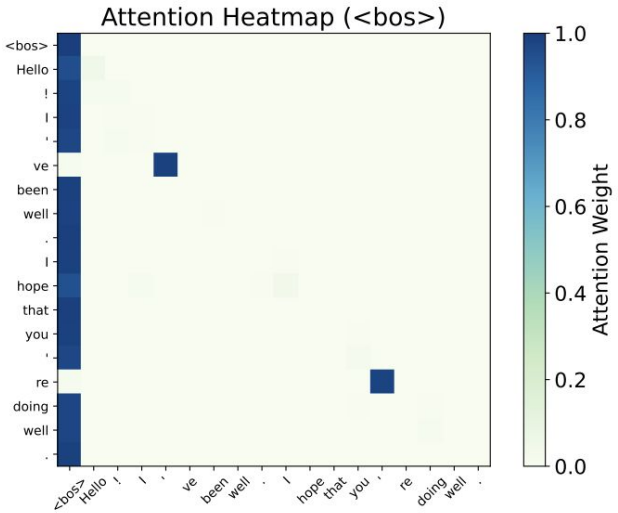


Attention sink implements “no-op”

- Attention sink approximates “no-op”: either sharply to attend one important token or attend to the first token
- From the representation mixing perspective, LLMs need “no-op” to prevent over-mixing

$$\boldsymbol{v}_i^{\dagger} = \sum_{j=1}^{i} \boldsymbol{\alpha}_{ij} \boldsymbol{v}_j = \boldsymbol{\alpha}_{i1} \boldsymbol{v}_1 + \sum_{j \neq 1}^{i} \boldsymbol{\alpha}_{ij} \boldsymbol{v}_j$$

Small

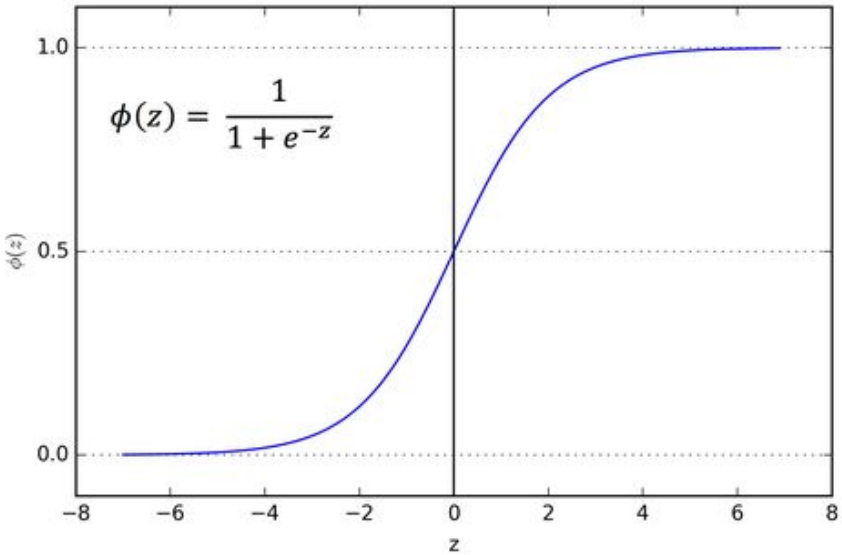


Interpreting attention variants using “no-op”

Sigmoid attention allows approximate

zero attention

$$\text{Sigmoid}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}+\boldsymbol{M}\right)\boldsymbol{V}^{l,h}$$



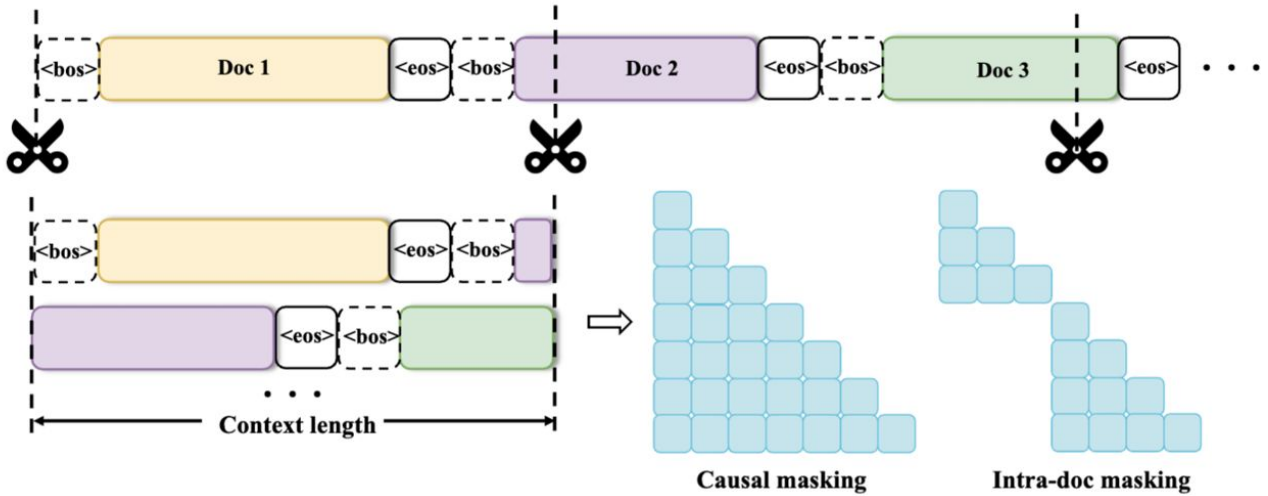
Interpreting attention variants using “no-op”

The following linear attention could have all zero attention scores

$\text{sim}(\varphi(\boldsymbol{q}_i), \varphi(\boldsymbol{k}_j))$	$\boldsymbol{Z}_i$	$\text{Sink}_1^{\epsilon}(\%)$	valid loss
$\exp(\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}})$	$\sum_{j'=1}^{i} \exp(\frac{\boldsymbol{q}_i \boldsymbol{k}_{j'}^\top}{\sqrt{d_h}})$	18.18	3.73
$\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}}$	$\max\left(\left\lvert\sum_{j'=1}^{i} \frac{\boldsymbol{q}_i \boldsymbol{k}_{j'}^\top}{\sqrt{d_h}}\right\rvert, 1\right)$	-	-
$\frac{\boldsymbol{q}_i \boldsymbol{k}_j^\top}{\sqrt{d_h}}$	1	0.00*	3.99
$\frac{\text{mlp}(\boldsymbol{q}_i)\text{mlp}(\boldsymbol{k}_j)^\top}{\sqrt{d_h}}$	$\max\left(\left\lvert\sum_{j'=1}^{i} \frac{\text{mlp}(\boldsymbol{q}_i)\text{mlp}(\boldsymbol{k}_{j'})^\top}{\sqrt{d_h}}\right\rvert, 1\right)$	0.19*	3.85
$\frac{\text{mlp}(\boldsymbol{q}_i)\text{mlp}(\boldsymbol{k}_j)^\top}{\sqrt{d_h}}$	1	0.74*	3.91

When Attention Sink Attaches to <BOS>

Data packing (fixed <BOS> in the first position will have similar behavior as Gemma)

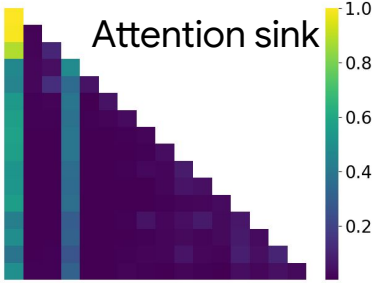


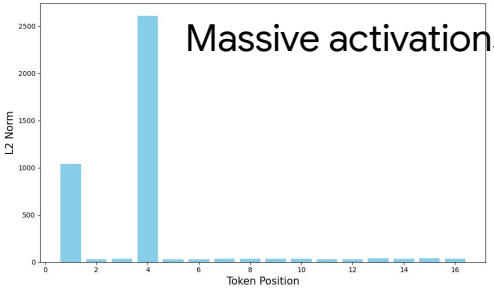
Attention sink / “No-op” widely exists in Transformer family

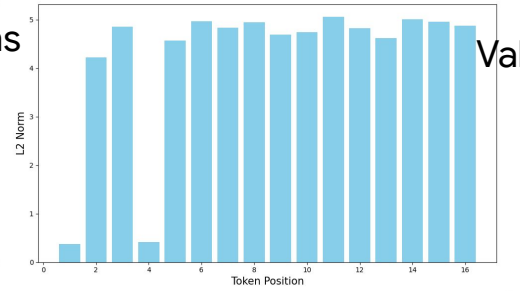
LLaMA

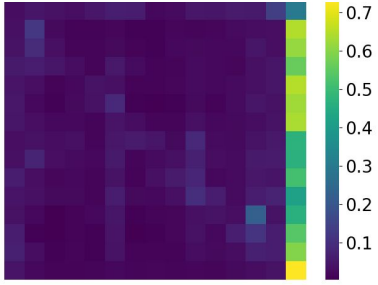
BERT

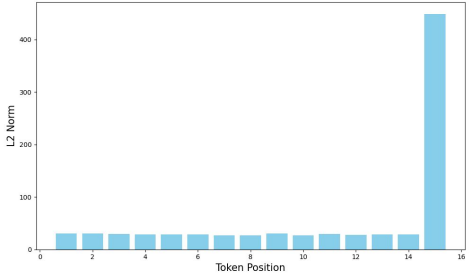
ViT

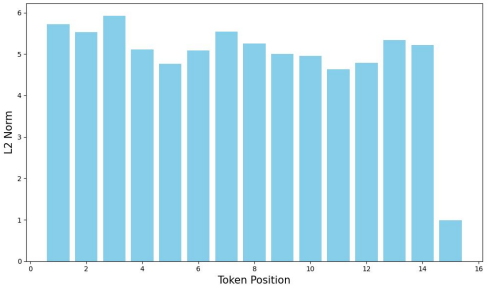


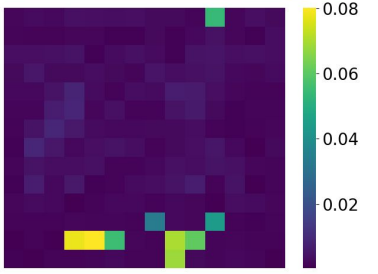


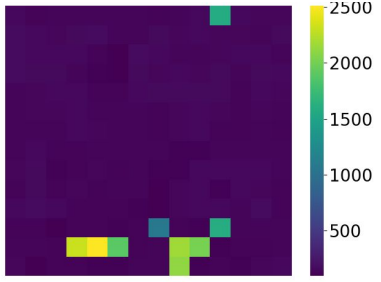


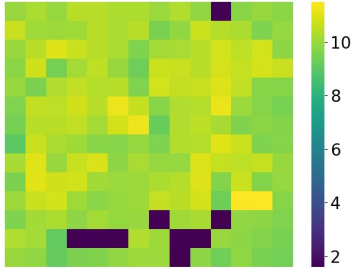












Also appear in diffusion transformers

I am attempting to answer …

- Mechanism understanding of Attention Sink?
- When Attention Sink Emerges in LLMs?
- Why LLMs need Attention Sink?
- Why GPT-OSS and Qwen3-Next consider Attention Sink in the Model Design?

GPT-OSS adopts Attention Biases

- Learnable key biases, zero value biases

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\begin{bmatrix}\boldsymbol{k}^{*l,h\top} & \boldsymbol{K}^{l,h\top}\end{bmatrix}+\boldsymbol{M}\right)\begin{bmatrix}\mathbf{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

- Softmax off-by-one

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\begin{bmatrix}\mathbf{0}^{*l,h\top} & \boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}\end{bmatrix}+\boldsymbol{M}\right)\begin{bmatrix}\mathbf{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

- Learnable attention score biases (single number for each head, layer)

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\begin{bmatrix}\boldsymbol{b}^{*l,h\top} & \boldsymbol{Q}^{l,h}\boldsymbol{K}^{l,h\top}\end{bmatrix}+\boldsymbol{M}\right)\begin{bmatrix}\mathbf{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

$$\boldsymbol{b}^{*l,h}=b^{*l,h}[1,1,1,..,1]$$

GPT-OSS adopts Attention Biases

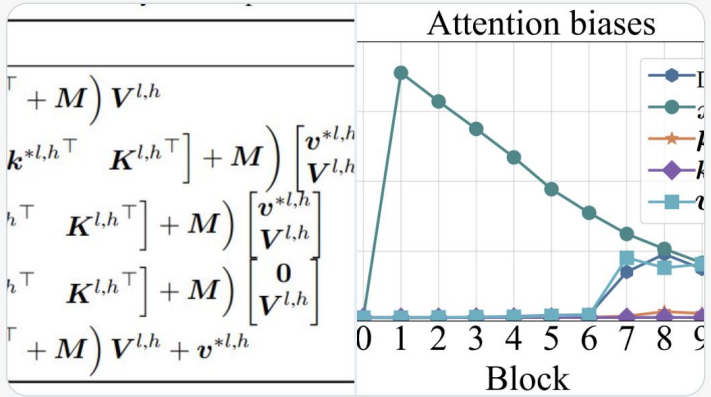
The first token does not to develop strong attention sink, thus mitigating massive activations/outliers

Benefits 1: facilitate quantization, pre-training stability

Pinned

Xiangming Gu @gu_xiangming · Aug 6

I noticed that @OpenAI added learnable bias to attention logits before softmax. After softmax, they deleted the bias. This is similar to what I have done in my ICLR2025 paper: openreview.net/forum?id=78Nn4....
I used learnable key bias and set corresponding value bias zero. In this way,
Show more



OpenAI @OpenAI · Aug 6

Our open models are here.
Both of them.

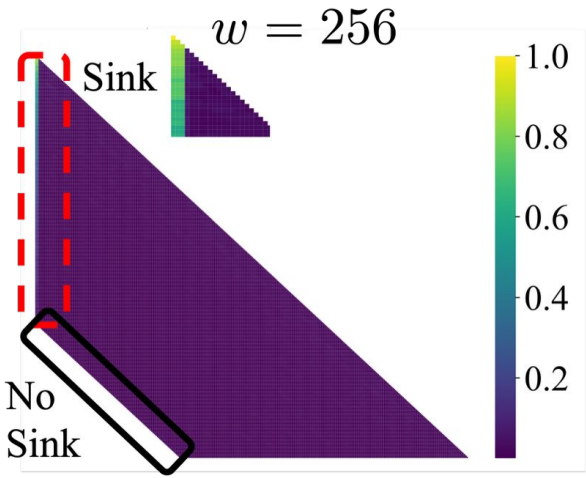
openai.com/open-models

22 185 1.7K 276K

GPT-OSS adopts Attention Biases

- Attention sink only happens in ***absolute*** first token,

not ***relative*** first token



- Tokens beyond window size have no sinks to attend,

possible over-mixing

$$\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}\left[\boldsymbol{k}^{*l,h\top} \quad \boldsymbol{K}^{l,h\top}\right] + \boldsymbol{M}\right)\begin{bmatrix}\boldsymbol{0}\\ \boldsymbol{V}^{l,h}\end{bmatrix}$$

- Facilitate long context, especially in LLMs with alternative shifted window / full attention

Xiaomi MiMo-V2-Flash adopts Attention Biases

Attention biases work both on language modeling and long context scenarios

General LLM benchmarks

Model	MMLU	BBH	TriviaQA	GSM8K	MATH	CMMLU	MBPP
All GA	57.3	54.7	53.2	34.2	9.5	50.3	54.7
Hybrid SWA(W = 128, w/o sink)	54.9	52.4	52.8	36.9	8.9	-	-
Hybrid SWA(W = 128, w/ sink)	**58.3**	**56.1**	53.7	36.9	**10.3**	**53.3**	**56.3**
Hybrid SWA(W = 512, w/ sink)	**58.3**	54.9	**54.9**	**37.9**	10.0	52.3	53.2

Long-context benchmarks

Model	GSM-Infinite	NoLiMa	RULER-32k	MRCR
All GA	12.3	49.7	**89.4**	32.5
Hybrid SWA(W = 128, w/ sink)	**17.3**	**51.2**	**89.4**	**34.4**
Hybrid SWA(W = 512, w/ sink)	17.2	38.5	84.7	19.6

Reasoning benchmarks

Model	AIME24/25	LiveCodebench	GPQA-Diamond	Average
All GA	45.5	40.0	41.7	42.4
Hybrid SWA(W = 128, w/ sink)	**47.1**	**43.9**	**48.1**	**46.3**

Qwen3-Next adopts Gated Attention

$$\text{Sigmoid}(\boldsymbol{G}^{l,h}) \odot \left[\text{Softmax}\left(\frac{1}{\sqrt{d_h}}\boldsymbol{Q}^{l,h}{\boldsymbol{K}^{l,h}}^{\top} + \boldsymbol{M}\right)\boldsymbol{V}^{l,h}\right]$$

Transformations of inputs

Sigmoid gate allows “no-op”, no need to only rely on attention sink for “no-op” → No attention sink, massive activations, better long context, pre-training stability

Zihan et al. Gated Attention for Large Language Models: Non-linearity, Sparsity, and Attention-Sink-Free. NeurIPS 2025 Best Paper Award

Thank you for listening!