



DHA: Learning Decoupled-Head Attention from Transformer Checkpoints via Adaptive Heads Fusion

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11/11/2024



Paper Link

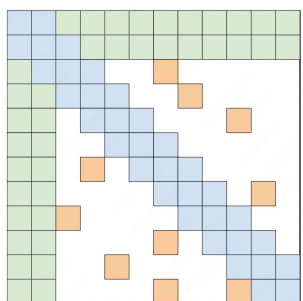
- **Background**
- **Motivation**
- **Method**
- **Experiments**
- **Summary**

- **Challenge: Large KV Cache with Long Context**
- **KV Cache:** During decoding phase, the key and value hidden states of all previous tokens in Attention block need to be stored to avoid re-computation.

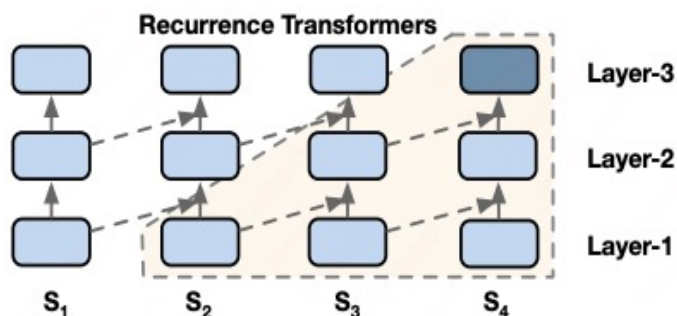
$$\text{Length} * \text{Batch-Size} * \text{Num-Layers} * \text{Num-Heads} * \text{Head-Dim} * 2 * 2\text{bytes}$$

KV Cache Memory Consumption (bf16)

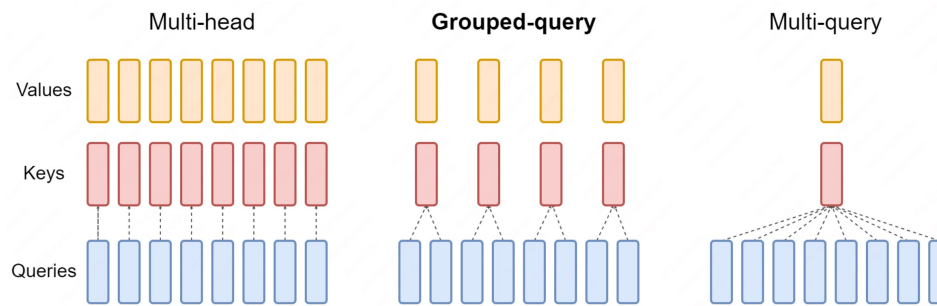
- **Difficulties in Efficient Transformer Re-training**
- Sparse Attention /Recurrence /Head Sharing



BigBird¹



ERNIE-Doc²



GQA³ & MQA

¹Big Bird: Transformers for Longer Sequences

²ERNIE-DOC: A Retrospective Long-Document Modeling Transformer ³GQA: Training Generalized Multi-Query Transformer Models from Multi-Head Checkpoints

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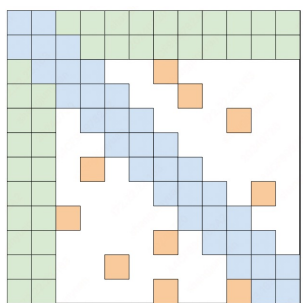
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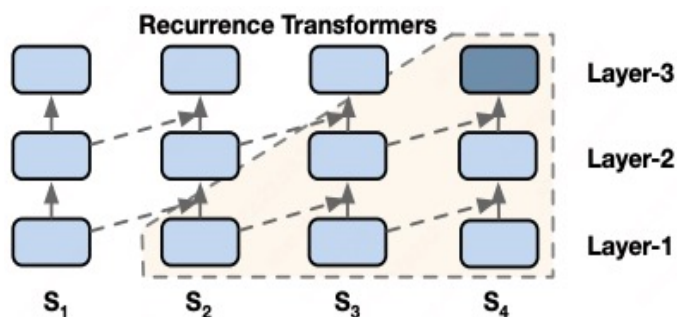
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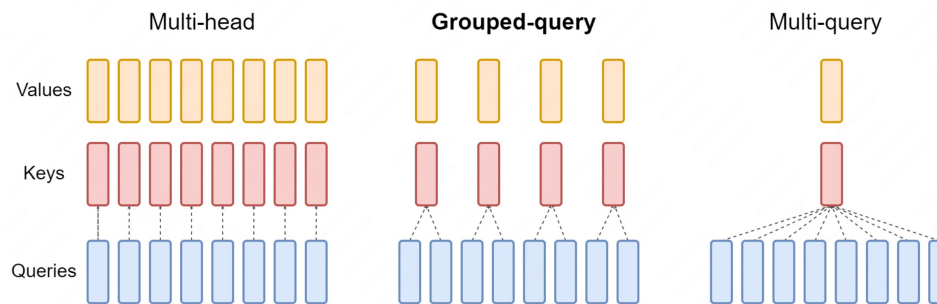
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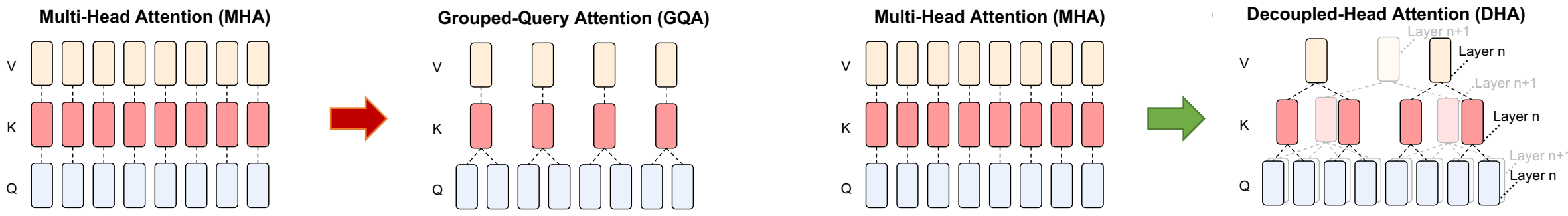
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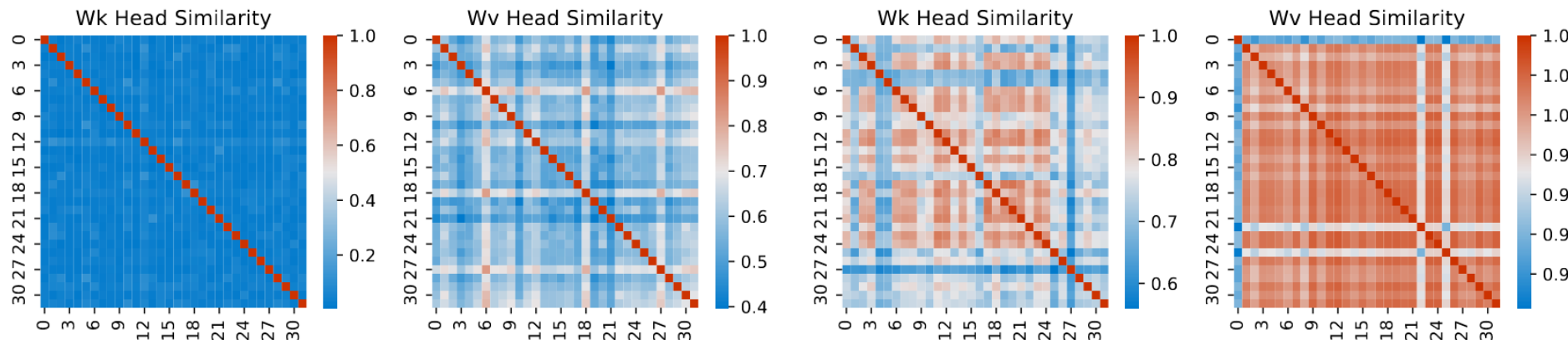
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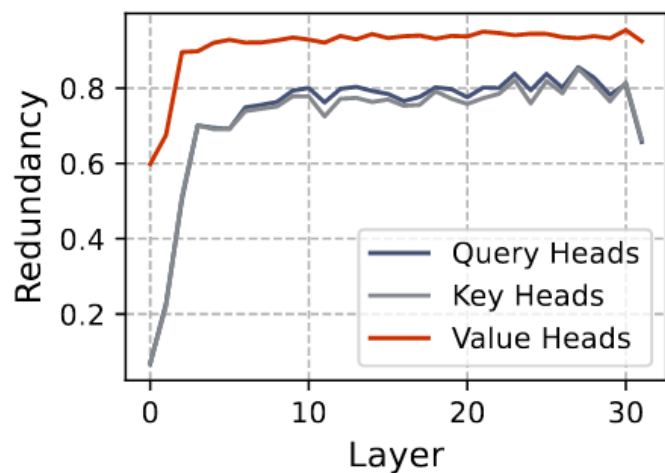
😄 **Resource-Efficient Re-training**
 😄 **Performance Maintenance**

• **Heterogeneity of Head Similarity in Attention**



(a) Head Weight Similarity in 0th Layer

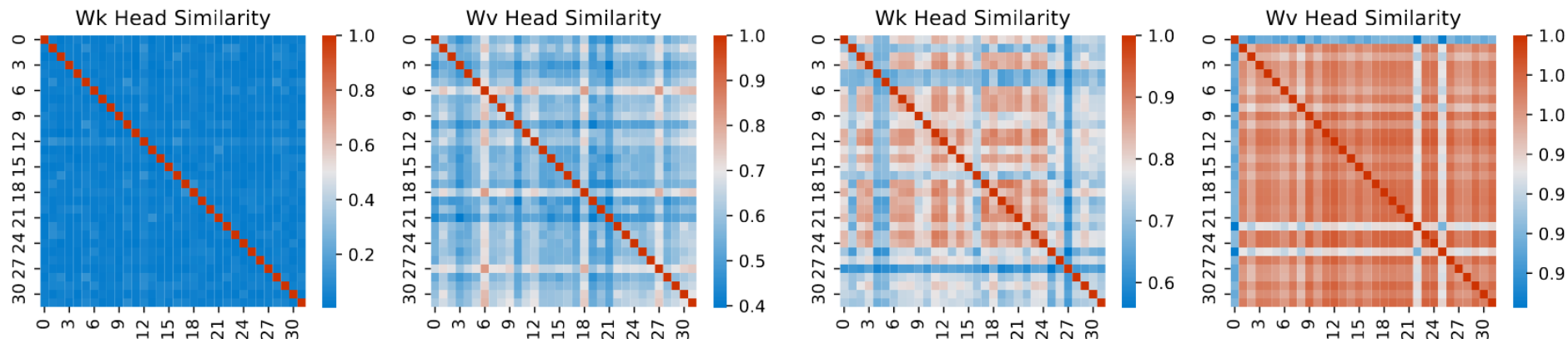
(b) Head Weight Similarity in 21st Layer



• **Head Similarity Observation Experiments**

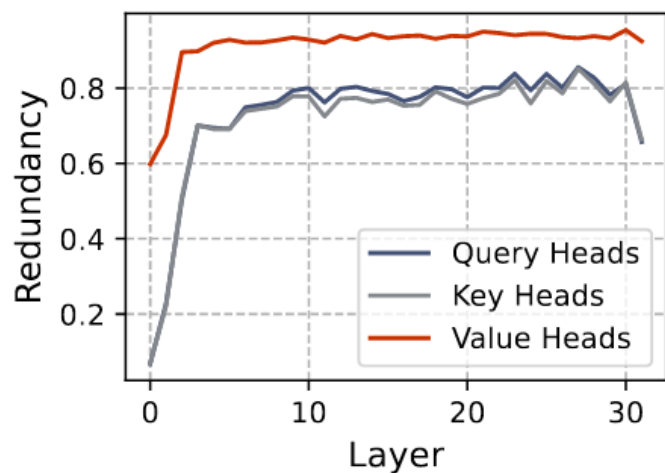
- The distribution of head **similarity varies significantly** across layers: the **initial** layers are relatively **sparse**, while the **later** layers are **more redundant**.
- The redundancy of **Values is higher than that of Keys**.

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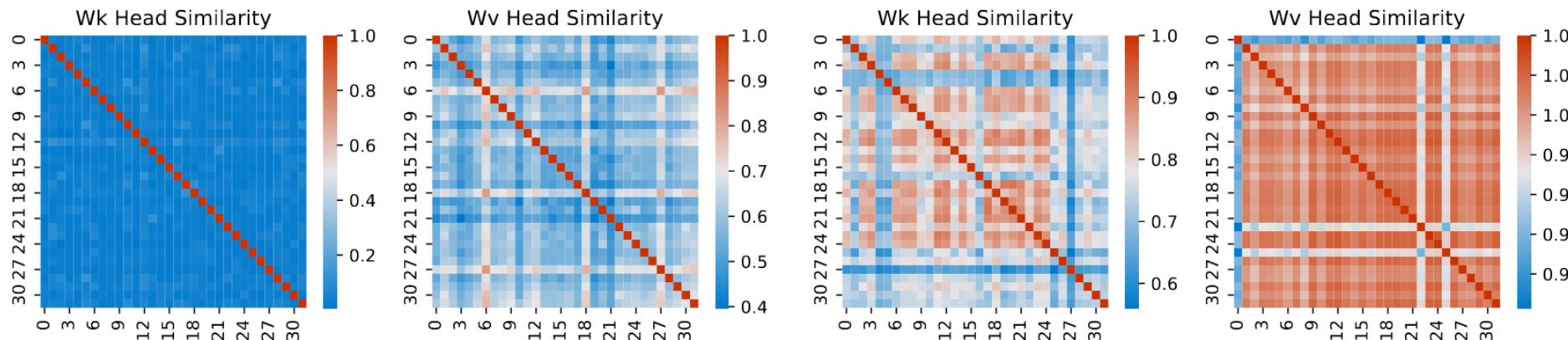
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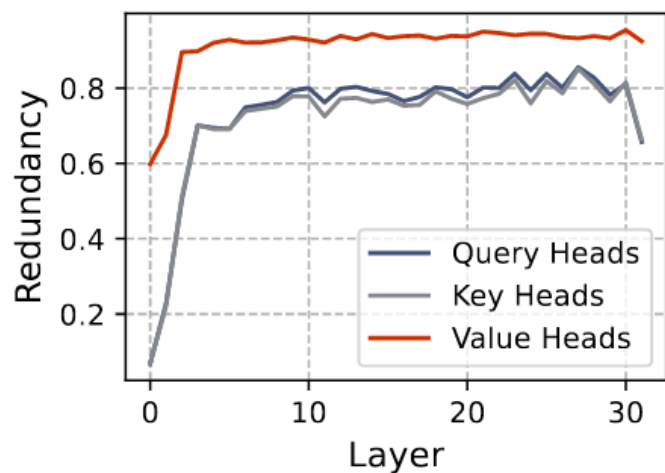
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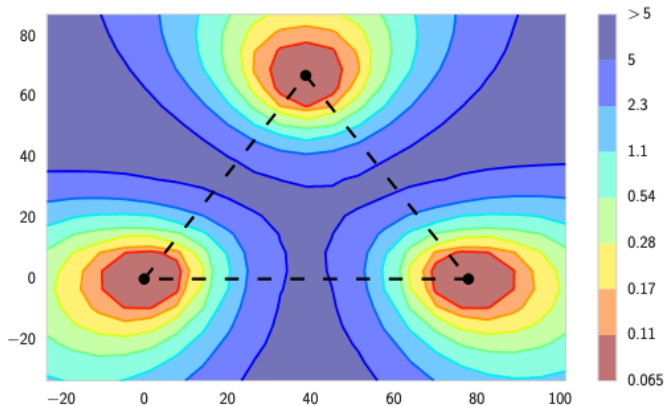
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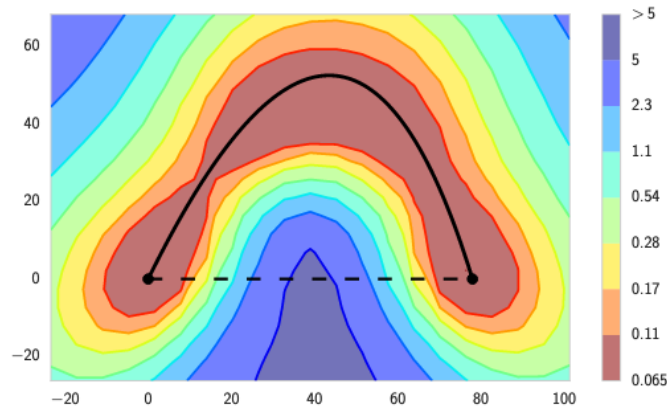


- **Motivation 1**
- By gradually **decoupling and reallocating the Head Budget across layers**, more heads can be assigned to **layers with lower redundancy** and specialized functions, while **compressing layers with higher redundancy**. This approach not only reduces model parameters but also enhances its performance.

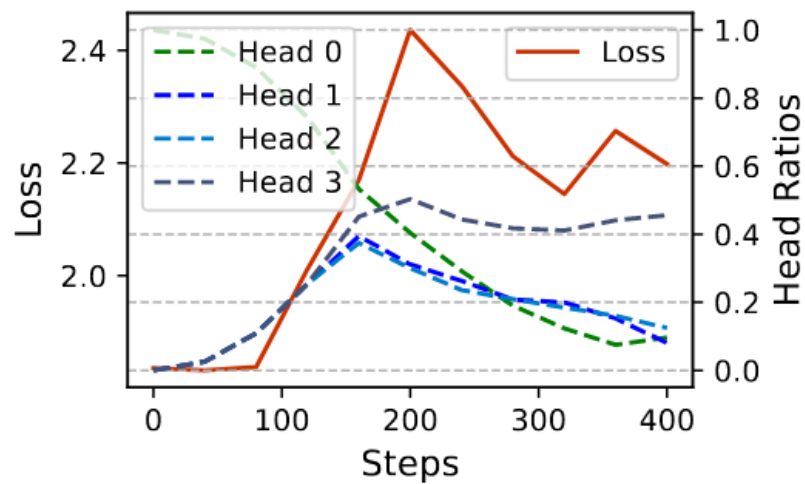
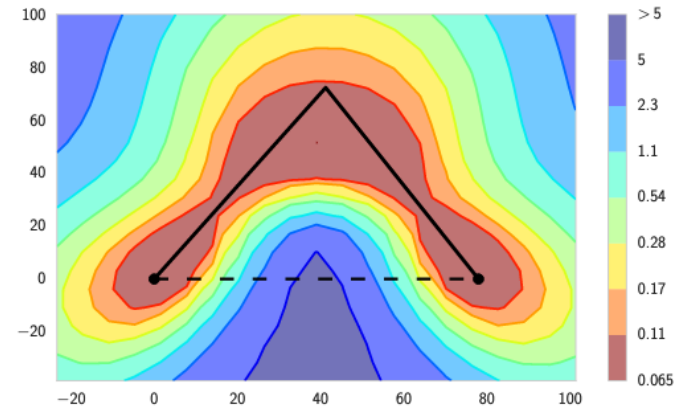
• **Connectivity of head parameters**



Independent DNNs



Connectable path between optimal points in loss landscape¹²

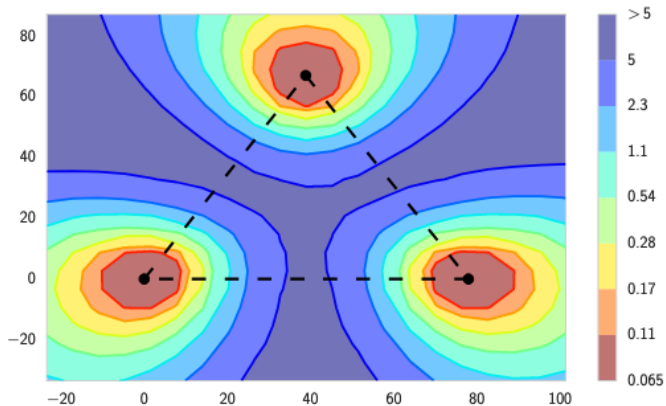


• **Head Fusion Observation Experiments**

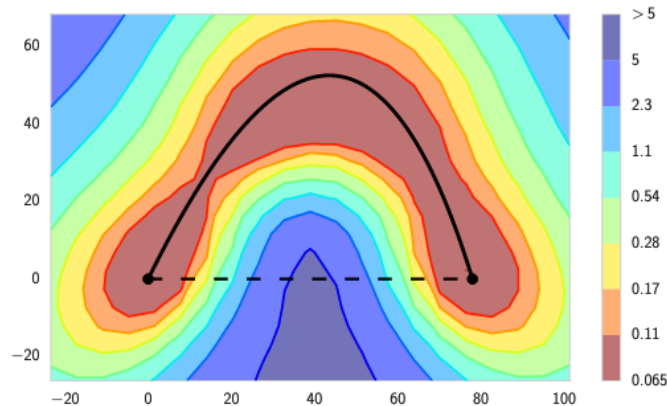
$$W_{k/v}^{d^{K/V}(h,l)} = \sum_{j=1}^{g^{K/V}} \omega_{hj} W_{k/v}^j$$

1. Loss Surfaces, Mode Connectivity, and Fast Ensembling of DNNs.
 2. Exploring Mode Connectivity for Pre-trained Language Models

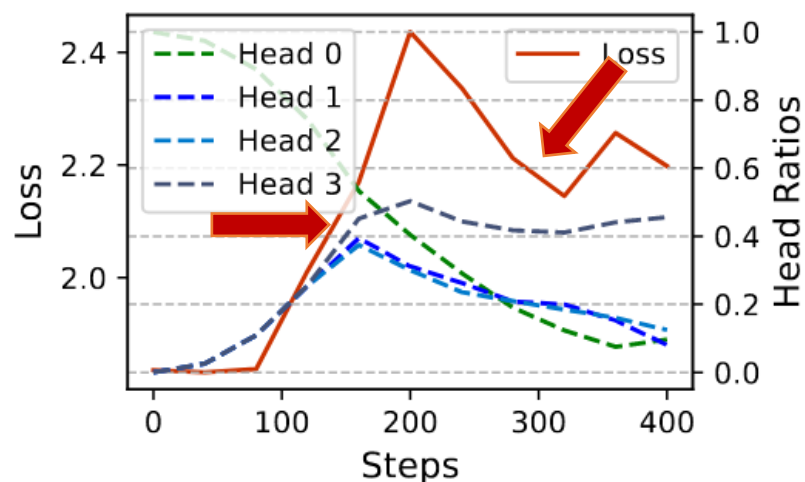
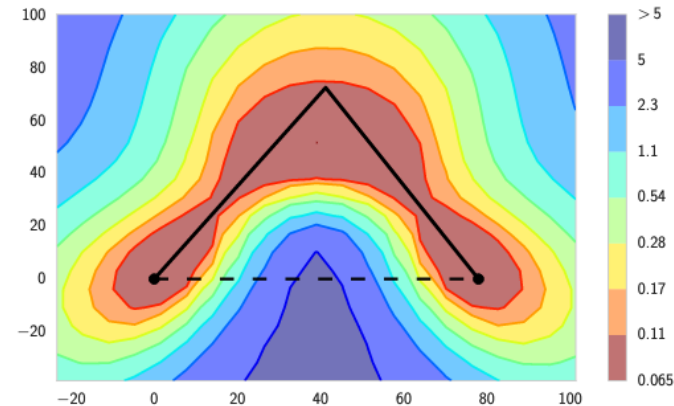
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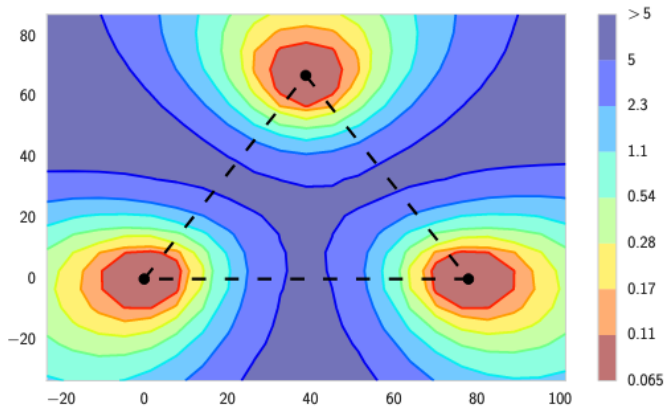


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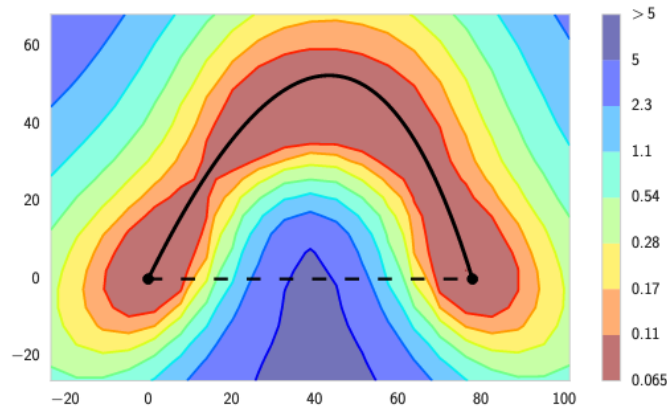
$$W_{k/v}^{d^{K/V}(h,l)} = \sum_{j=1}^{g^{K/V}} \omega_{hj} W_{k/v}^j$$

The loss **increases** when the head parameter **ratio approaches 0.5** but **decreases and stabilizes** toward the end.

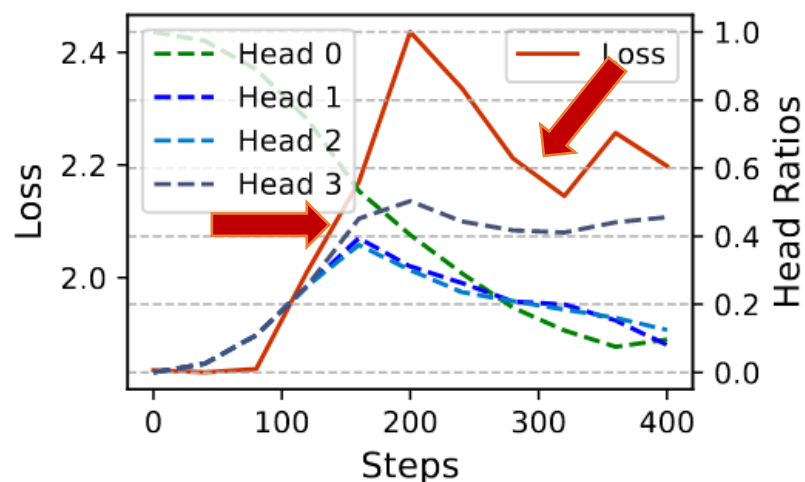
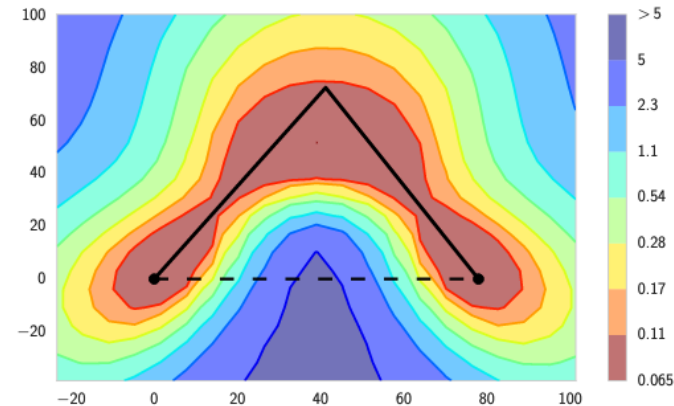
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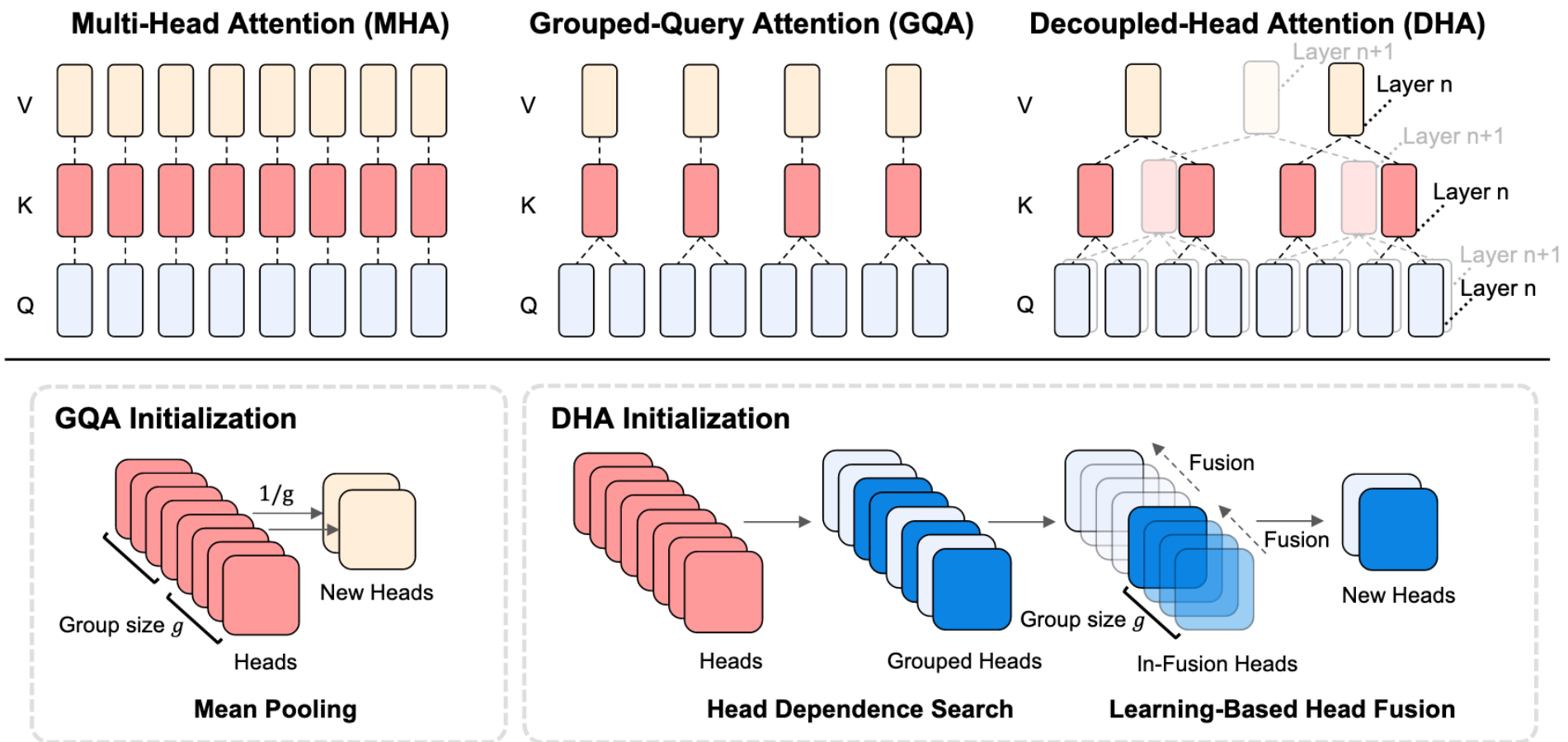


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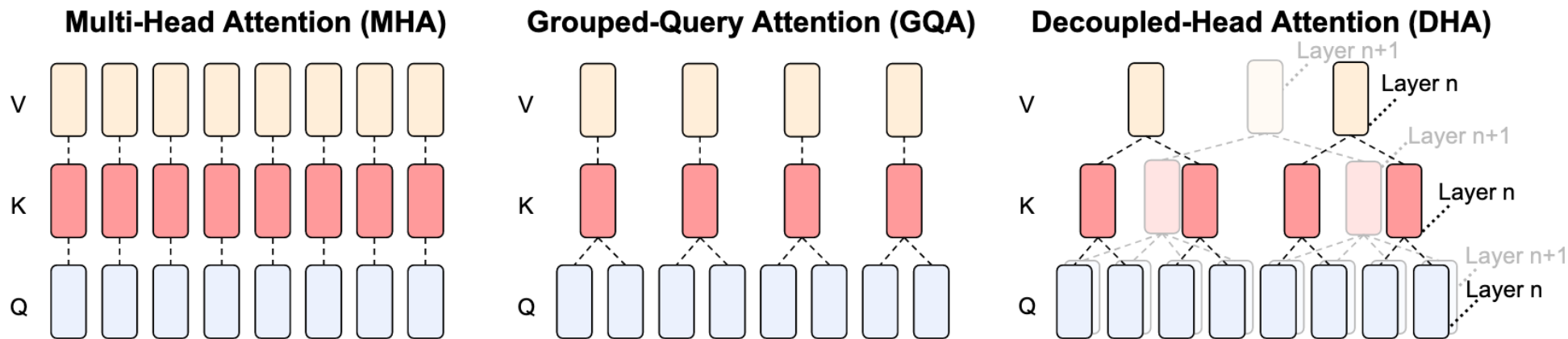
• **Motivation 2**

Parameter fusion can **reconstruct the functionality** of the original parameters while **reducing the number of heads**



How can we construct a more efficient model while keeping costs as low as possible?

• Definition



• Multi-Head Attention (MHA)

$$\text{MHA} = \text{Concat}(\text{head}_1, \dots, \text{head}_H) W_O, \text{ where } \text{head}_h = \sigma \left(\mathbf{X}W_q^h (\mathbf{X}W_k^h)^T \cdot \frac{1}{\sqrt{d_k}} \right) \mathbf{X}W_v^h \quad (1)$$

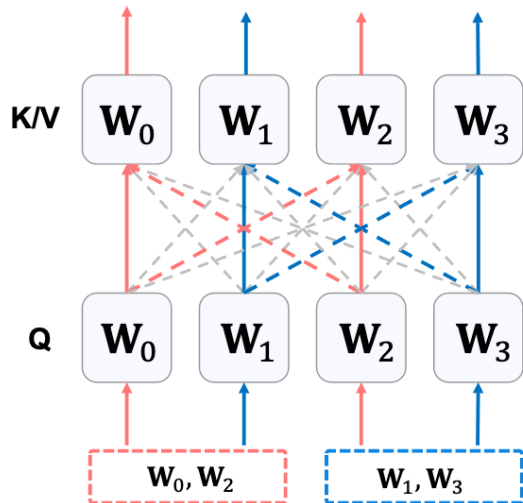
• Decoupled-Head Attention (DHA)

$$\text{head}_{h,l} = \sigma \left(\mathbf{X}W_q^h (\mathbf{X}W_k^{d^k(h,l)})^T \cdot \frac{1}{\sqrt{d_k}} \right) \mathbf{X}W_v^{d^v(h,l)} \quad (3)$$

DHA shares key and value heads in multi-query attention based **on independently mapped functions** across different layers.

DHA consists of $H = H^Q + \sum_{l=1}^L H_l^K + \sum_{l=1}^L H_l^V$ heads in total.

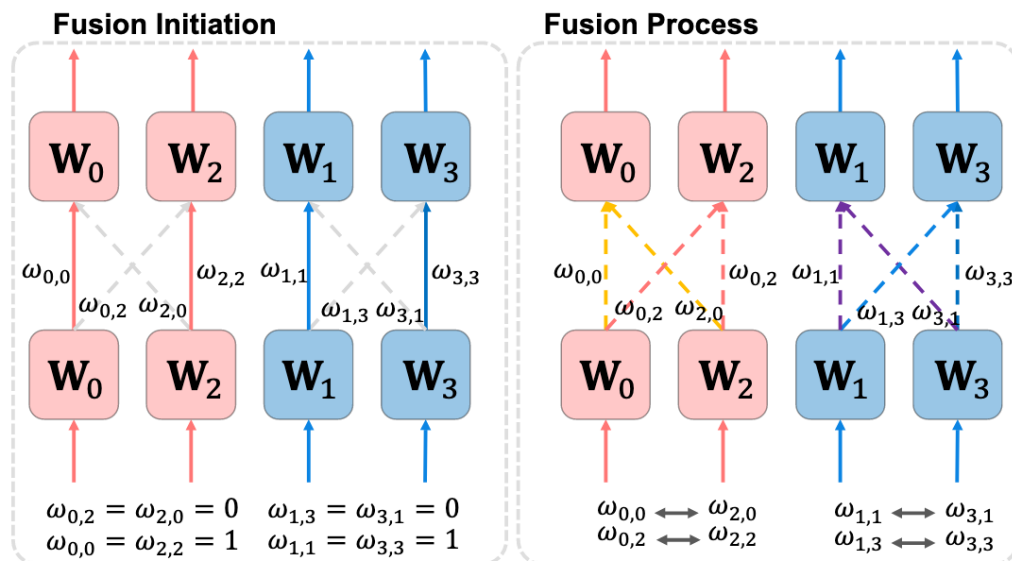
Dependence Search



$$\mathcal{L}_{\text{fusion}} = \frac{1}{64} \sum_{h=1}^4 \sum_{h'=h+1}^4 \sum_{j=1}^4 (\omega_{hj} - \omega_{h'j})^2$$

$$\mathcal{L} = \min_{\Theta, \mathcal{M}} [\mathcal{L}_{\text{lm}}(\mathcal{M}(\Theta^{\text{MHA}})) + \lambda \mathcal{L}_{\text{fusion}}]$$

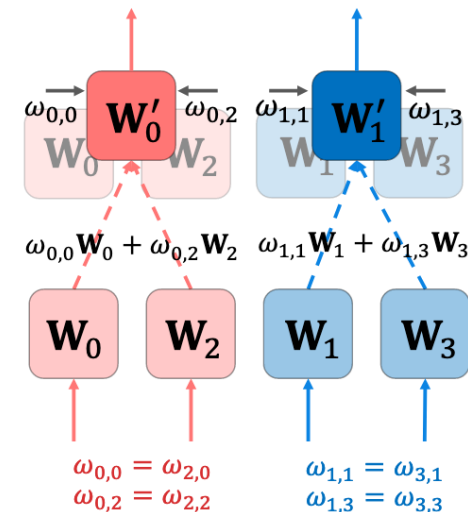
In-Group Head Fusion



$$\mathcal{L}_{\text{fusion}} = \text{Group_num} \times \frac{1}{8} \sum_{h=1}^2 \sum_{h'=h+1}^2 \sum_{j=1}^2 (\omega_{hj} - \omega_{h'j})^2$$

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Continued Pretraining



$$\Theta_{\text{K/V}}^{\text{DHA}} = [\mathbf{W}'_1, \dots, \mathbf{W}'_H]$$

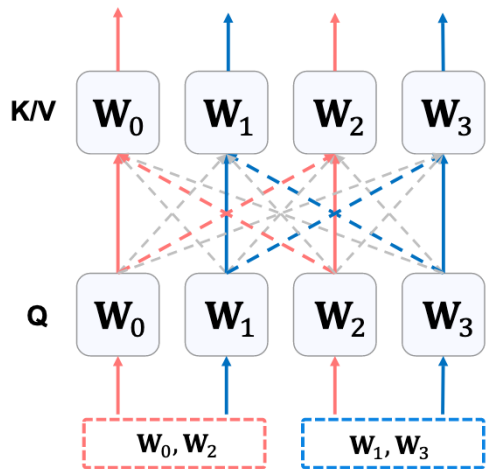
$$\mathcal{L} = \min_{\Theta} \mathcal{L}_{\text{lm}}(\Theta^{\text{DHA}})$$

• **Goal**

$$\arg \min_{\Theta, \mathcal{M}} \mathbb{E}_{\mathbf{x} \sim \mathcal{D}} \left[\mathcal{L}_{\text{lm}}(\mathbf{x}; \mathcal{M}(\Theta^{\text{MHA}})) + \lambda \mathcal{L}_{\text{fusion}}(\mathbf{x}; \mathcal{M}(\Theta^{\text{MHA}}), \Theta^{\text{DHA}}) \right] \quad (4)$$

By progressively merging head parameters, we reduce the number of heads while retaining the knowledge of the original model, thus decreasing training costs and enhancing performance.

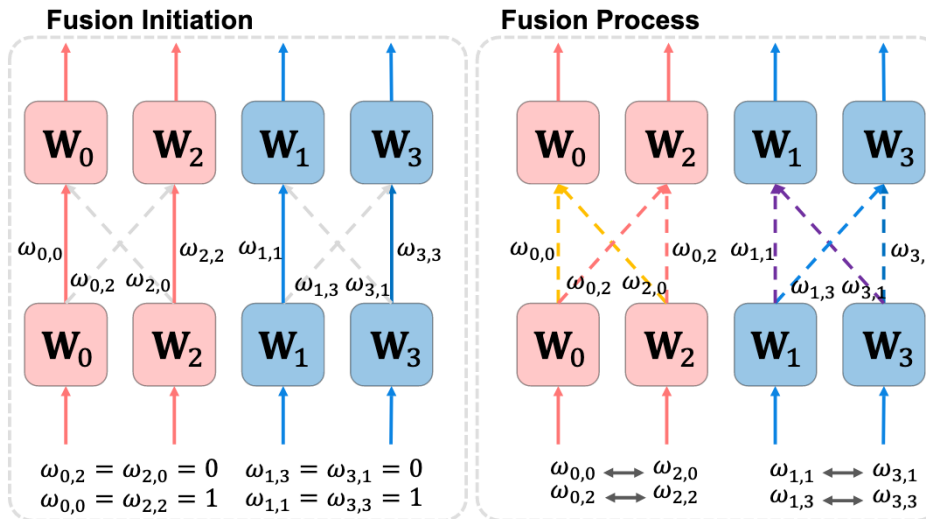
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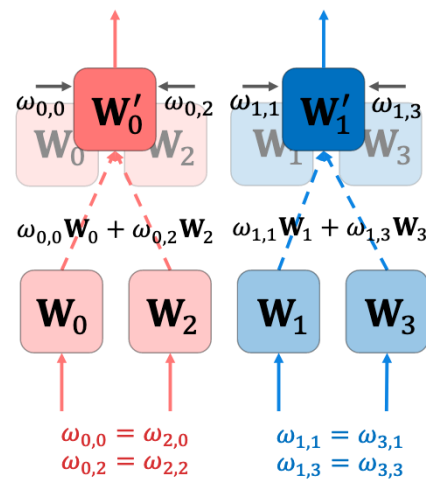
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Continued Pretraining



$$\theta_{\text{K/V}}^{\text{DHA}} = [W'_1, \dots, W'_H]$$

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Fusion Operator

$$\text{head}_{h,l} = \sigma \left(\mathbf{X} \mathbf{W}_q^h (\mathbf{X} \mathbf{W}_k^{d^{\text{K}}(h,l)})^T \cdot \frac{1}{\sqrt{d_k}} \right) \mathbf{X} \mathbf{W}_v^{d^{\text{V}}(h,l)}, \text{ where } \mathbf{W}_{k/v}^{d^{\text{K/V}}(h,l)} = \sum_{j=1}^{g^{\text{K/V}}} \omega_{h,j} \mathbf{W}_{k/v}^j \quad (5)$$

During DHA initialization, the fusion operator constructs new heads based on a **linear combination of original key and value heads** within each group. The initial forward of DHA are **fully equivalent** to those of MHA.

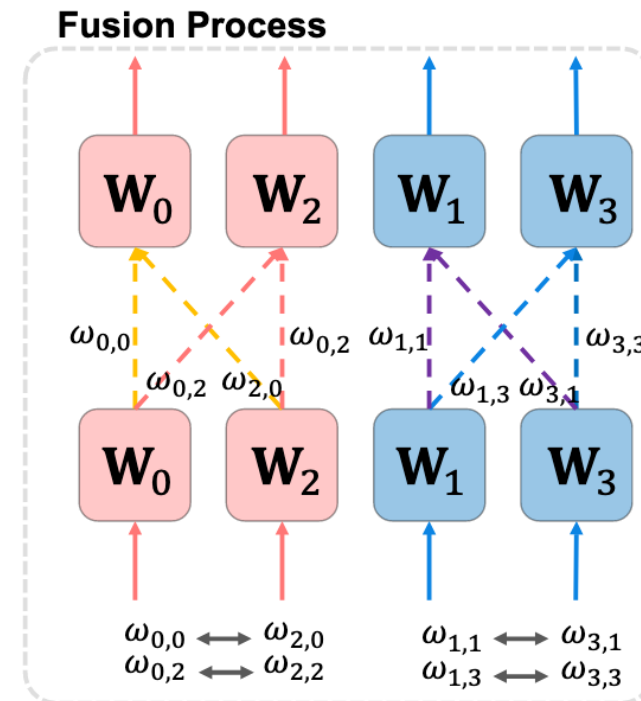
• **Optimization**

The goal is to enable **a single fused key or value head to be shared across multiple query heads** in DHA. We design a fusion loss to **optimize the initial mapping functions to a single unified mapping function**.

$$\mathcal{L}_{\text{head}_l^n}(h, h') = \frac{1}{g} \left\| \sum_{j=1}^g \omega_{hj} \mathbf{W}_{k/v}^j - \sum_{j=1}^g \omega_{h'j} \mathbf{W}_{k/v}^j \right\|^2 = \frac{1}{g} \left(\sum_{j=1}^g (\omega_{hj} - \omega_{h'j}) \mathbf{W}_{k/v,ij}^j \right)^2 \quad (6)$$

Since W can be considered a scalar, we **only need to optimize the fusion variable ω** .

$$\mathcal{L}_{\text{fusion}} = \sum_{l=1}^L \sum_{n=1}^N \sum_{h=1}^g \sum_{h'=h+1}^g \mathcal{L}_{\text{head}_l^n}(h, h'), \text{ subject to } \mathcal{L}_{\text{head}_l^n}(h, h') = \frac{1}{g} \sum_{h=1}^g \sum_{j=1}^g (\omega_{hj} - \omega_{h'j})^2 \quad (7)$$



Challenge: We must **optimize the fusion loss to a near-zero minimum**, enabling effective **sharing** of the new DHA key-value head parameters **across queries within the group**.

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• Augmented Lagrangian Approach

In the **early stages of training**, We encourage the model to **tolerate differences** among parameters to promote exploration. As training progresses, the **algorithm gradually enforces stricter reduction** of these differences, **improving parameter alignment** within each group.

$$\max_{\lambda} \min_{\Theta, \mathcal{M}} \mathbb{E}_{\mathbf{x} \sim \mathcal{D}} \left[\mathcal{L}_{\text{lm}}(\mathbf{x}; \mathcal{M}(\Theta^{\text{MHA}})) + \lambda \max(\mathcal{L}_{\text{fusion}} - t, 0) \right], \text{ where } t = \max\left(0, b^s \left(1 - \frac{s}{k}\right)\right) \quad (8)$$

t as the target loss, b as the base decay factor, s as the current global step, k as warm-up step

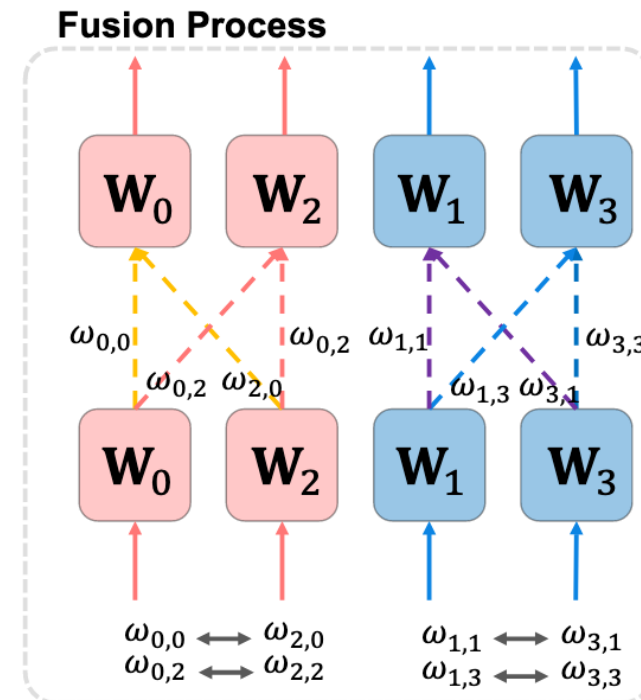
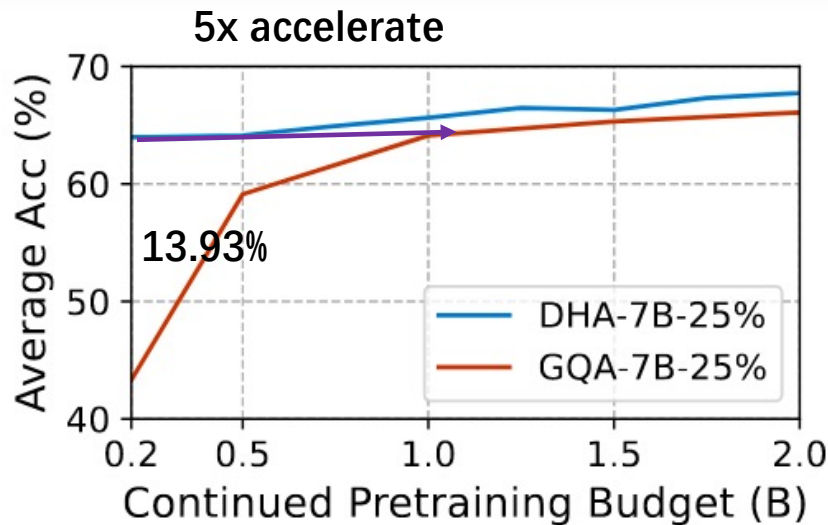
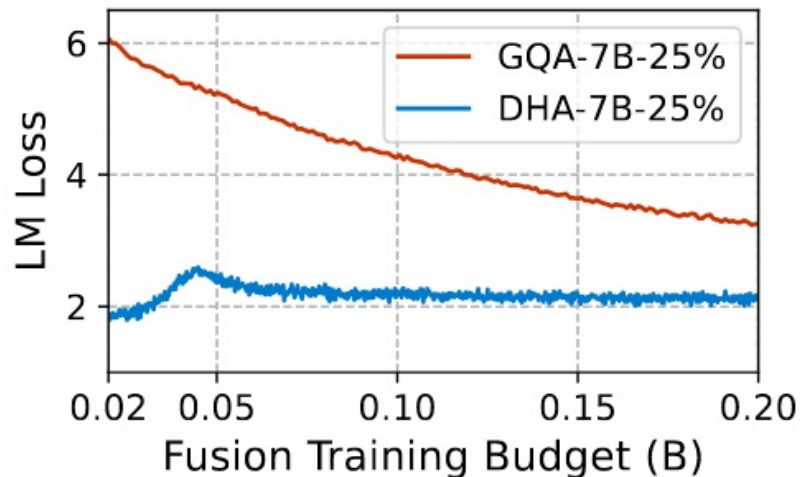


Table 1: Comprehensive assessment of model’s fundamental capabilities, in which DHA models demonstrate competitive performance while requiring significantly fewer training resources. Models with [†] use MHA.

Model	Budget	Commonsense & Comprehension						Continued		LM	Average
		SciQ	PIQA	Wino.	ARC-E	ARC-C	HellaS.	LogiQA	BoolQ	LAMB.	
LLaMA2-7B [†]	2T	94.1	78.1	69.1	76.3	49.7	58.9	25.7	80.8	74.1	67.4
DHA-7B-50%	50B	93.4	78.5	69.1	73.8	45.9	58.6	22.5	79.1	71.1	65.8
DHA-7B-25%	50B	92.4	78.5	68.6	72.9	43.9	57.6	22.4	76.7	70.2	64.8
GQA-7B-50%	1B	90.7	76.8	66.5	71.3	41.9	53.6	22.4	70.5	67.0	62.3
DHA-7B-50%	1B	90.8	76.5	66.7	71.3	44.6	55.1	22.4	74.8	67.2	63.3
GQA-7B-25%	1B	86.5	74.3	59.1	67.6	37.5	49.2	24.1	65.8	58.3	58.0
DHA-7B-25%	1B	90.0	75.2	63.8	70.4	39.3	52.2	21.1	72.3	62.9	60.7
S.-LLaMA-2.7B [†]	2T	91.2	76.1	64.9	67.3	38.8	52.2	22.1	74.4	68.3	61.7
GQA-2.7B-50%	1B	86.7	74.8	59.0	64.0	34.2	48.2	23.8	64.9	60.3	57.3
DHA-2.7B-50%	1B	86.8	75.1	59.5	64.6	35.1	48.7	22.4	66.4	61.7	57.8
GQA-2.7B-25%	1B	82.0	72.8	54.9	58.4	31.0	42.9	21.7	58.5	49.6	52.4
DHA-2.7B-25%	1B	85.6	74.1	57.6	61.5	32.4	45.9	21.7	63.1	56.9	55.4
S.-LLaMA-1.3B [†]	2T	87.0	73.6	58.2	60.9	29.5	45.4	21.8	65.5	61.3	55.9
GQA-1.3B-50%	1B	84.3	72.3	55.8	57.5	28.2	41.8	20.7	62.9	52.9	52.9
DHA-1.3B-50%	1B	84.5	72.0	55.2	58.1	28.7	42.6	21.5	63.7	55.4	53.6
GQA-1.3B-25%	1B	76.6	70.0	52.9	51.9	23.5	37.6	21.0	59.9	41.0	48.3
DHA-1.3B-25%	1B	82.8	71.1	54.0	55.4	25.8	40.5	21.5	57.6	48.6	50.8

- Under the **same training budget**, DHA **surpasses** GQA.
- **Higher compression rates** lead to **greater relative performance gains** for DHA.
- Achieves 97.5% performance with **just 0.05% of the training budget**.



- DHA initial loss is only **slightly above** the original model loss.
- DHA retains original model knowledge, achieving **a higher performance.**
- **0.1B data is enough** to get a good DHA initial point.

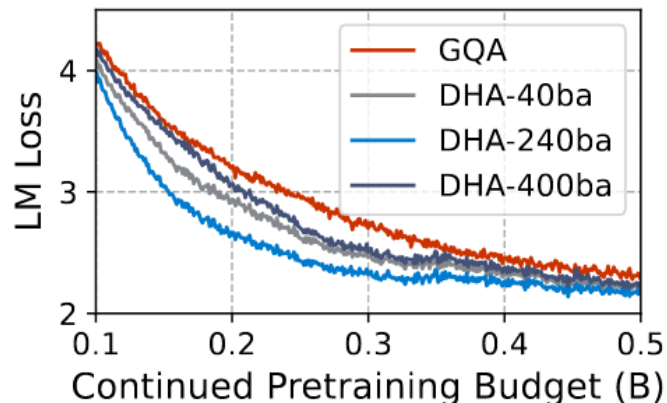
Table 2: Ablation Results of DHA *w.o.* Linear Heads Fusion and Adaptive Transformation. Experiments are conducted with LLaMA2-7B with 25% heads budget and 0.5B & 1B training budget on 0-shot Evaluation.

Models	SciQ	PiQA	Wino.	ARC-E.	ARC-C.	LogiQA	LAMB.	Average	Diff
DHA-7B-25% (0.5B)	88.6	75.9	61.3	68.2	36.1	23.8	63.2	59.6	—
<i>w.o.</i> Linear Heads Fusion	83.4	73.7	57.3	63.6	29.4	22.0	51.9	54.5	-5.1
<i>w.o.</i> Adaptive Transformation	87.9	74.1	60.1	69.4	34.7	19.5	62.1	58.3	-0.4
DHA-7B-25% (1B)	90.0	75.2	63.8	70.4	37.5	21.1	62.9	60.1	—
<i>w.o.</i> Linear Heads Fusion	87.5	74.5	60.7	67.3	32.8	21.7	58.3	57.5	-2.6
<i>w.o.</i> Adaptive Transformation	89.5	74.6	62.8	69.1	36.3	21.6	62.4	59.5	-0.6
DHA-7B-25% (5B)	91.7	76.8	64.4	70.9	42.8	21.8	68.4	62.4	—
GQA-7B-25% (5B)	91.5	76.6	63.9	70.5	42.3	22.1	67.8	62.1	-0.4

Table 3: Data budget allocation to fusion and continued pre-training(CT) and 0-shot Task Average Accuracy (%) in DHA-1.3B.

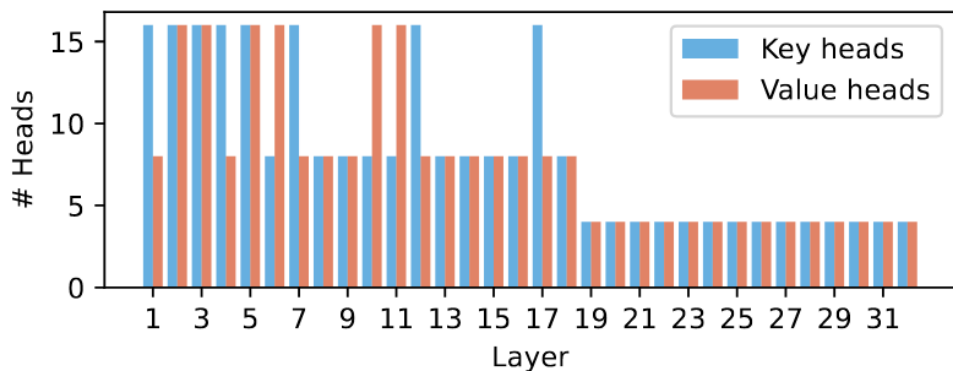
Fusion		CT	
Tokens	Avg.Acc	Tokens	Avg.Acc
0.05B	33.74	4.95B	59.08
0.10B	38.32	4.90B	59.53
0.15B	48.26	4.85B	59.46
0.20B	52.54	4.80B	59.16

• Is the DHA architecture truly efficient?



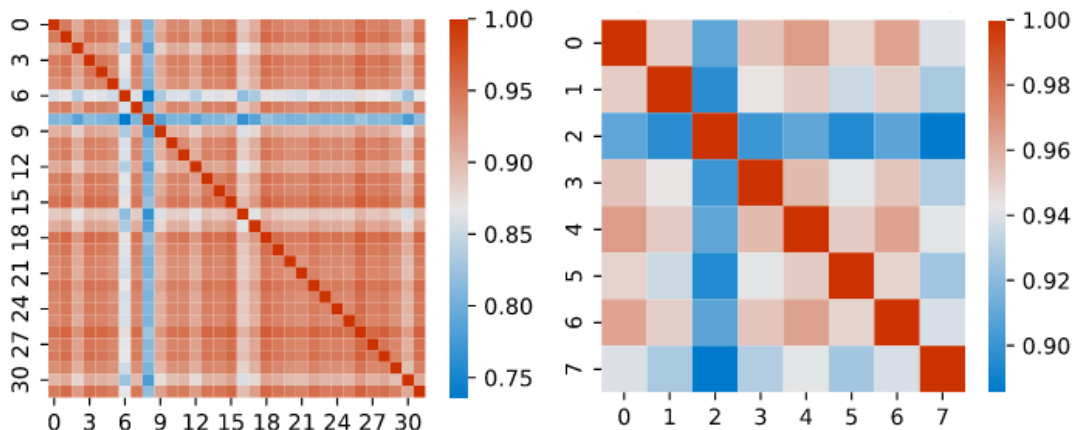
Training from scratch using the DHA-searched architecture achieves faster training speeds and better performance than GQA.

• How does DHA allocate the head budget?



DHA allocates more parameters to critical layers. DHA generally preserves parameters in the early layers. DHA compresses parameters in the later layers.

• What is the head similarity distribution before and after DHA fusion?



- DHA merges multiple heads within **each cluster into a single head** while preserving **inter-cluster relationships**.
- Maintains the **same overall distribution** trend as MHA.
- Effectively **reduces head parameter redundancy**.

• Performance of the Instruction Tuned DHA model

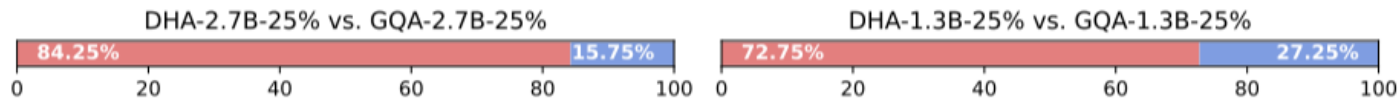


Figure 10: In model scale of 7B, 3B, and 1.3B, DHA significantly outperforms GQA and achieves comparable performance with MHA after instruction tuning .

Heterogeneous Attention Efficient Architecture

- Increases training speed
- Enhances the capability of key components
- Compresses parameters of redundant components

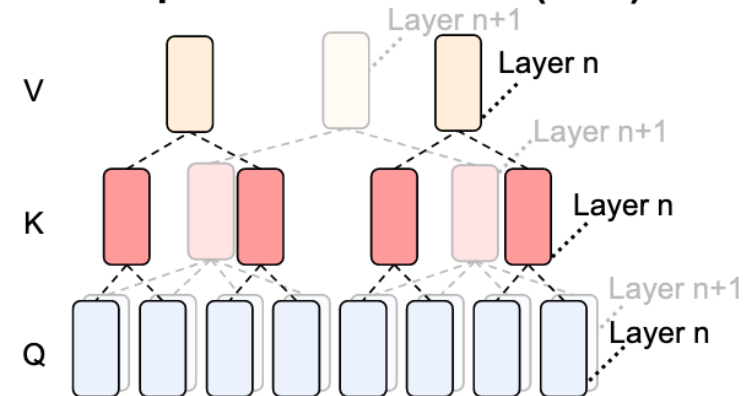
Progressive Head Parameter Fusion

- Significantly boosts training speed
- Achieves 5x training acceleration
- Reconstructs model functionality

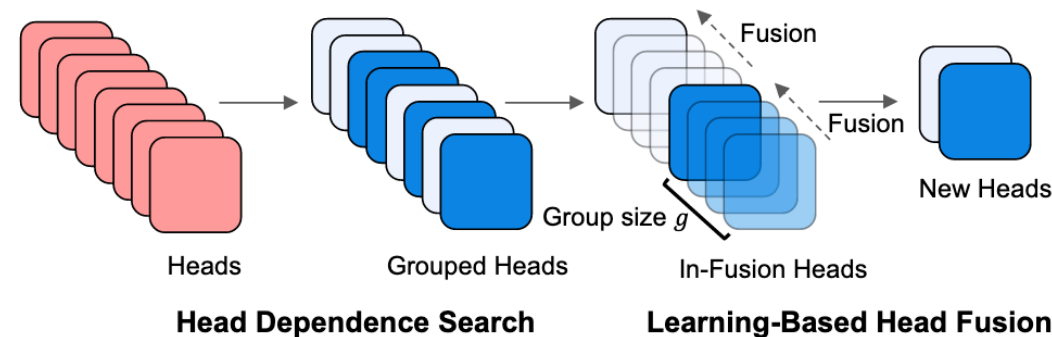
Stronger and More Efficient Model

- 13.93% improvement with 0.01% budget
- 4% improvement with 0.05% budget
- 75% KVCache compression

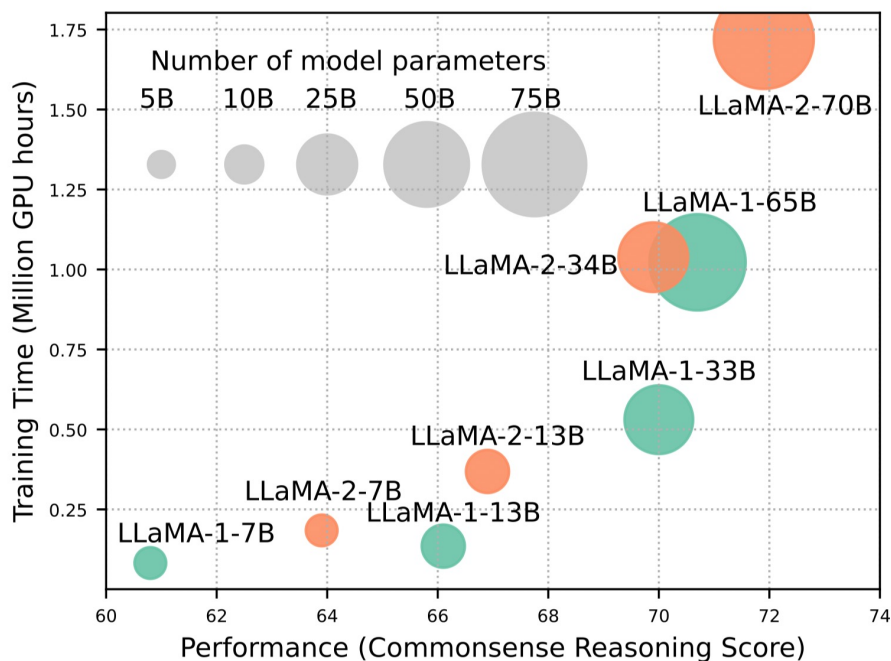
Decoupled-Head Attention (DHA)



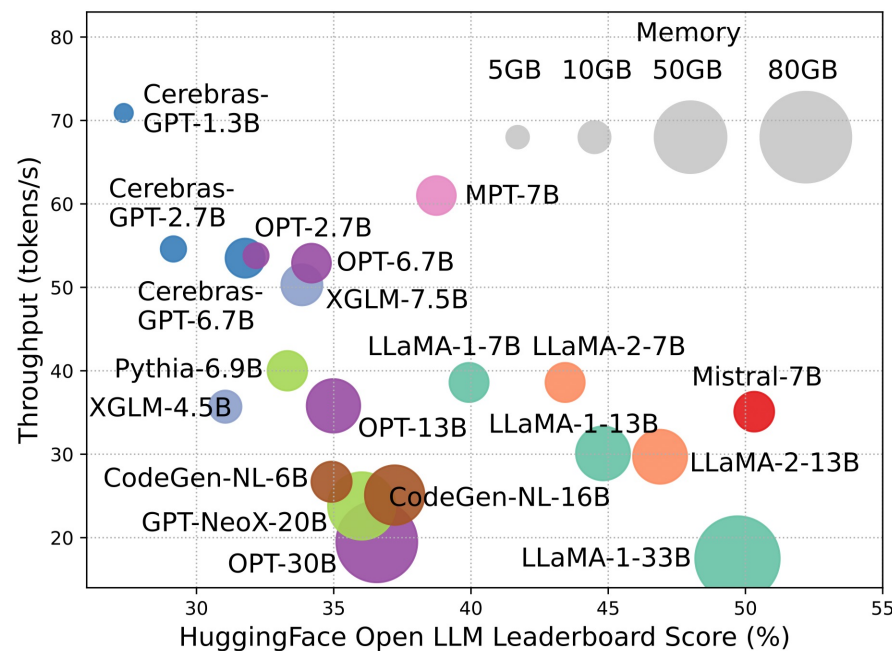
DHA Initialization



- Considering that the training and deployment of large-scale LMs require a large amount of computing resources, **Efficient-LMs are more cost-effective** in actual production environments.



Larger models are powerful but have **exponential training costs**¹



Larger models use **more memory** and are **slower at inference** [1]