UNCOMP: UNCERTAINTY-AWARE LONG-CONTEXT COMPRESSOR FOR EFFICIENT LARGE LANGUAGE MODEL INFERENCE

Anonymous authors

Paper under double-blind review

Abstract

Deploying large language models (LLMs) is challenging due to their high memory and computational demands, especially during long-context inference. While keyvalue (KV) caching accelerates inference by reusing previously computed keys and values, it also introduces significant memory overhead. Existing KV cache compression methods-such as eviction and merging-typically compress the KV cache after it is generated and overlook the hidden states, failing to improve the speed of the prefilling stage. Additionally, applying a uniform compression rate across different attention heads can harm crucial retrieval heads in needle-in-ahaystack tasks due to excessive compression. In this paper, we propose UNComp, an uncertainty-aware compression scheme that leverages matrix entropy to estimate model uncertainty across layers and heads at the token sequence level. By grouping layers and heads based on their uncertainty, UNComp adaptively compresses both the hidden states and the KV cache. Our method achieves a $1.6 \times$ speedup in the prefilling stage and reduces the KV cache to 4.74% of its original size, resulting in a $6.4 \times$ increase in throughput and a $1.4 \times$ speedup in inference with only a 1.41% performance loss. Remarkably, in needle-in-a-haystack tasks, UNComp outperforms the full-size KV cache even when compressed to 9.38% of its original size. Our approach offers an efficient, training-free Grouped-Query Attention paradigm that can be seamlessly integrated into existing KV cache schemes.

031 032 033

034

006

008 009 010

011

013

014

015

016

017

018

019

021

023

024

025

026

027

028

029

1 INTRODUCTION

The proliferation of large language models (LLMs) has led to unprecedented advancements in natural language processing (Achiam et al., 2023; Kaplan et al., 2020), enabling capabilities ranging from simple text generation to complex reasoning and dialogue. However, deploying and scaling LLMs are significantly hindered by extensive memory requirements and computational costs (Shazeer et al., 2017), especially during long-context inference. Processing long contexts leads to significant computational time during the prefilling stage, and the "attention sink" phenomenon (Xiao et al., 2023) during decoding impedes efficient long-text generation.

To mitigate these issues, *KV caching* (Pope et al., 2023; Liu et al., 2024b) stores and reuses keys and values to avoid redundant computations, improving inference speed. However, the memory overhead of maintaining the KV cache remains prohibitive for long contexts (Liu et al., 2024b), prompting the development of methods to reduce KV cache size while preserving performance.

Existing optimization methods include: *i*) Eviction Strategies (Ge et al., 2023; Zhang et al., 2024d; Li et al., 2024; Zhang et al., 2024c); *ii*) Merging Strategies (Liu et al., 2024b; Wan et al., 2024; Wang et al., 2024; Zhang et al.); *iii*) Quantization (Hooper et al., 2024; Zhang et al., 2024a; Liu et al., 2024e); *iv*) Compressing KV Cache Heads (Ainslie et al., 2023; Shazeer, 2019; Liu et al., 2024a; Yu et al., 2024). However, these methods often compress the KV cache after generation and neglect hidden states, failing to speed up the prefilling stage. Moreover, uniform compression across attention heads can degrade important retrieval heads due to over-compression.

Multi-Query Attention (MQA) (Ainslie et al., 2023; Yu et al., 2024; Brandon et al., 2024) reduces attention heads during inference by grouping heads and using a single head per group, significantly

reducing memory and improving speed while maintaining performance comparable to Multi-Head
 Attention (MHA). However, these methods typically require fine-tuning or training from scratch,
 which can be costly. A training-free approach to group heads during inference is more practical.

Inspired by these insights, we propose estimating the internal *uncertainty* across layers and heads
 within the KV cache and hidden states. Previous metrics based on cumulative attention distributions
 focus on token-level importance but overlook sequence-level sampling strategies such as estimating
 heads and layers. By measuring the effective information via *matrix entropy*, we quantify uncertainty
 across heads and layers, enabling adaptive compression of the KV cache and pruning of hidden states
 for faster inference. Our key contributions are:

- 1. We propose a novel method based on matrix entropy to explore the uncertainty within the hidden states and KV cache, analyzing their information compression patterns. This approach enables grouped compression of heads and layers. By compressing the hidden states, we achieve a $1.6 \times$ speedup in the prefilling stage in a single batch.
 - 2. We employ a training-free approach to adaptively determine the compression ratios for heads and layers across different groups. Compared to the full-size KV cache, our method achieves a compression rate of 4.74%, with a throughput increase of $6.4 \times$ and a $1.4 \times$ inference speedup in a single batch, incurring only a 1.41% performance loss.
- 3. Our method maintains performance even under extreme compression rates where some heads are removed. In the needle-in-a-haystack task, with a 9.38% compression rate (viz. compressed size over original size), our method even surpasses the performance of the full-size KV cache version.
- 077

063 064

065

066

067

068

069

070

071

073

075

076

- 2 RELATED WORK
- 079 080 081

082

2.1 ATTENTION-BASED TOKEN EVICTION POLICIES

083 Early works identify interesting attention patterns in long-context settings, such as the attention 084 sink phenomenon (Liu et al., 2024c; Xiao et al., 2023), where models aggregate information using tokens at the beginning and end. Additionally, certain parameters in LLMs remain in an active 085 state (Sun et al., 2024), inspiring researchers to explore the eviction of input prompts and generated 086 tokens. Recent methods employ cumulative attention scores for token eviction strategies (Zhang 087 et al., 2024c; Li et al., 2023; Jiang et al., 2024; Zhang et al., 2024d; Ge et al., 2023; Sheng et al., 088 2023; Liu et al., 2024d; Li et al., 2024). These methods aim to optimize memory usage while 089 preserving performance. However, they overlook compressing hidden states during the prefilling 090 stage, which is often the most time-consuming aspect. Further exploration is needed to leverage the 091 sparsity of hidden states to optimize compression rates and eviction strategies at this stage.

092

094 095

2.2 COMPRESSION OF THE KV CACHE HEADS

Recent studies show that Multi-Head Attention (MHA) varies across heads; some are highly effec-096 tive at retrieval tasks (Wu et al., 2024), while others specialize in preserving different token types, 097 reflecting inherent patterns of the model (Ge et al., 2023; Jiang et al., 2024). Leveraging the sparsity 098 across these head dimensions allows for designing different KV cache eviction strategies for each head, thereby improving inference speed. Methods like Multi-Query Attention (MQA) (Shazeer, 100 2019) share keys and values across heads to reduce the KV cache but at the cost of degraded per-101 formance. Grouped-Query Attention (GQA) (Ainslie et al., 2023) merges heads and fine-tunes the 102 model, while Multi-Head Latent Attention (MLA) (Liu et al., 2024a) compresses keys and values 103 into a low-rank subspace, reusing the KV cache during inference. However, these methods often 104 require retraining. Yu et al. (2024) use LoRA (Hu et al., 2021) to fine-tune compressed models, 105 minimizing errors in MHA-to-GQA transitions. CHAI (Agarwal et al., 2024) clusters tokens in the prefilling stage but adds significant computational overhead. Efficiently setting compression rates 106 for different heads without training remains an open challenge, requiring further exploration of the 107 sparsity patterns in the heads.

108 2.3 THE COMPRESSION BEHAVIOR OF LARGE LANGUAGE MODELS

110 Sections 2.1 and 2.2 discuss compressing the KV cache by utilizing sparsity patterns of the layer and head dimensions. However, this sparsity pattern is closely related to the model's internal matrix rank 111 and can alter the model's compression behavior (Feng et al., 2022). Recent work (Delétang et al., 112 2023) reveals that models exhibit spontaneous compression behavior during training, demonstrating 113 that LLMs are powerful general compressors and showcasing the scaling laws of model compression 114 capability. Similar phenomena are observed in (Tao et al., 2024; Huang et al., 2024). Moreover, 115 certain aggregation patterns within prompts in in-context learning are also noted (Wang et al., 2023). 116 These observations inspire us to further explore the internal compression patterns of the model, 117 particularly between different heads and across different layers. We introduce matrix entropy (Zhang 118 et al., 2023), which can be considered a measure of the rank of the KV cache; higher entropy 119 indicates more uncertainty and information aggregated by the tokens. 120

121 122

123

124

125

126 127

128

139 140

141 142

148

152

3 Method

Inspired by Giraldo et al. (2014), we derive the definition of matrix entropy and introduce our concept of truncated matrix entropy in this section. Additionally, we explore the relationship between matrix entropy and effective rank.

3.1 MATRIX ENTROPY

To derive the definition of matrix entropy, we first define the covariance matrix of the model's parameter matrix. In this context, it typically refers to the various heads of the KV cache and the different layers of the hidden state. The covariance matrix, $\Sigma_{\mathbf{X}}$, is derived from the token sequence matrix $\mathbf{X} = [\mathbf{x}_1, \mathbf{x}_2, \dots, \mathbf{x}_N]$, where $\mathbf{x}_i \in \mathbb{R}^D$ represents the *i*-th token vector in the sequence, and N denotes the sequence length. The covariance matrix $\Sigma_{\mathbf{X}} \in \mathbb{R}^{D \times D}$ is then computed as the average outer product of the centered token vectors:

$$\boldsymbol{\Sigma}_{\mathbf{X}} = \frac{1}{N} \sum_{i=1}^{N} \left(\frac{\mathbf{x}_{i} - \bar{\mathbf{x}}}{\|\mathbf{x}_{i} - \bar{\mathbf{x}}\|} \right) \left(\frac{\mathbf{x}_{i} - \bar{\mathbf{x}}}{\|\mathbf{x}_{i} - \bar{\mathbf{x}}\|} \right)^{T},$$
(1)

where $\bar{\mathbf{x}}$ is the mean vector of the sequence:

$$\bar{\mathbf{x}} = \frac{1}{N} \sum_{i=1}^{N} \mathbf{x}_i.$$
(2)

143 It can be shown that $Tr(\Sigma_X) = 1$, where $Tr(\cdot)$ represents the trace operator.

Based on the above definition of the covariance matrix, we derive the definition of matrix entropy. Specifically, following Giraldo et al. (2014), the matrix entropy of order $\alpha > 0$ based on $\Sigma_{\mathbf{X}}$ is defined as:

$$S_{\alpha}(\boldsymbol{\Sigma}_{\mathbf{X}}) = \frac{1}{1-\alpha} \log \left[\operatorname{Tr}\left(\left(\boldsymbol{\Sigma}_{\mathbf{X}} \right)^{\alpha} \right) \right].$$
(3)

Lemma 1. As $\alpha \to 1$, we obtain the definition of the von Neumann (matrix) entropy (Von Neumann, 2013):

$$H(\mathbf{\Sigma}_{\mathbf{X}}) = -Tr\left(\mathbf{\Sigma}_{\mathbf{X}}\log\left(\mathbf{\Sigma}_{\mathbf{X}}\right)\right).$$
(4)

153 154 **Lemma 2.** Let $\Sigma_{\mathbf{X}}$ be a symmetric positive definite matrix with eigenvalues $\sigma = (\sigma_1, \sigma_2, \dots, \sigma_D)^T$. 155 The matrix entropy of $\Sigma_{\mathbf{X}}$ can be expressed as:

$$H(\mathbf{\Sigma}_{\mathbf{X}}) = -\sum_{i=1}^{D} \sigma_i \log \sigma_i,$$
(5)

where D is the dimension of the covariance matrix of the model's hidden state layer or head. We
 define matrix entropy on the token sequence and provide the proof in Appendix C. To give an intu itive explanation of its role in the parameter matrix, we introduce effective rank, which links matrix

entropy to dimensionality, such as sequence length and number of heads, leading to meaningful conclusions.

Recent works (Zhang et al., 2023; Zhuo et al., 2023) explore the relationship between matrix entropy 165 and effective rank (Roy & Vetterli, 2007). Zhuo et al. (2023) discuss dimensional collapse and use 166 effective rank to explain asymmetric contrastive learning. Inspired by this, we use effective rank, i.e., 167 matrix entropy, to measure uncertainty across heads and layers, associating higher matrix entropy 168 with more information per token. We remark here that contrary to the conventional perception 169 that a higher rank represents more information and is less ready for truncation, we observe 170 that to the opposite, as the layer depth increases, since each token becomes more informative 171 by itself, we can thereby directly discard more tokens without hurting the overall information 172 content. This novel observation is justified by i): Previous efforts (Wang et al., 2023) find that higher-layer tokens gather more information, and a small number of tokens can represent the entire 173 sequence. *ii*): We observe the same phenomenon in Figure 1: the higher the layer, the higher the 174 matrix entropy of the entire sequence, which means that each token is more informative. *iii*): For 175 heads on the same layer, those with a higher effective rank should evict fewer tokens because 176 this head is more informative. iv): Tokens of the same head in different layers gradually share 177 information as the layers deepen, while tokens of different heads do not share information as the 178 layers deepen. Based on effective rank, we set different compression rates for different heads and 179 layers. The effective rank of $\Sigma_{\mathbf{X}}$, denoted erank($\Sigma_{\mathbf{X}}$), is defined as: 180

$$\operatorname{erank}(\mathbf{\Sigma}_{\mathbf{X}}) = \exp(H(\mathbf{\Sigma}_{\mathbf{X}})). \tag{6}$$

Lemma 3. The rank of the covariance matrix $\Sigma_{\mathbf{X}}$ is upper bounded by the rank of the input matrix \mathbf{X} :

$$rank(\Sigma_{\mathbf{X}}) \le rank(\mathbf{X}).$$
 (7)

Lemma 4. Eq. 6 can be interpreted as the dimension of the affine subspace spanned, i.e., the effective dimensionality of the parameter matrix in the head and layer dimensions. The bounds are:

$$1 \le erank(\mathbf{\Sigma}_{\mathbf{X}}) \le rank(\mathbf{\Sigma}_{\mathbf{X}}) \le D.$$
(8)



Figure 1: Effective ranks for the Q_m , K_m , and V_m across three different datasets in LongBench (Bai et al., 2023) and various layers.

We consider $\operatorname{erank}(\Sigma_{\mathbf{X}})$ as a measure of the model's uncertainty. In this work, we extend this concept to quantify the model's uncertainty in token sequence representations and derive an uncertainty measure for both the KV cache and the hidden states.

3.2 TRUNCATED MATRIX ENTROPY

181 182

183

185

186

187 188 189

190

191 192

193

194

196

197

199

200 201

202

203 204

205

206

207 208

209

To identify compression patterns in the hidden states and KV cache, we use matrix entropy. A key question is which matrix—key (K_m) , query (Q_m) , or value (V_m) —best captures the compression patterns in the token sequences mapped from the hidden states. To investigate this, we plot the matrix entropy trends for Q_m , K_m , and V_m across different layers and datasets (Figure 1). In our analysis, entropy fluctuations indicate ongoing compression and aggregation within the model layers. Figure 1 reveals: *i*) Q_m and K_m show a stronger compression trend than V_m . *ii*) Q_m and K_m have similar effective rank variation, making them equivalent in measuring the KV cache's





Figure 2: The eigenvalue distribution across three datasets in LongBench and various heads.

We visualize the eigenvalue distribution of Q_m across different heads in the model's final layer. As 233 the distributions show minimal differences across layers, we focus on the last layer over 128 hidden 234 dimensions. Figure 2 reveals: i) The initial part of the eigenvalue distribution varies significantly. 235 ii) Eigenvalue distributions across heads differ significantly in the leading part of the distribution. 236 iii) Different datasets exhibit a similar long-tailed distribution. These findings suggest some heads 237 operate in limited dimensions, suffering from representation collapse, motivating the use of varying 238 compression rates during inference. 239

According to Lemma 2, we require Σ_{Q_m} to be a positive definite matrix, though it is typi-240 cally positive semi-definite. To address this, we compute the effective rank using a subma-241 trix because it is positive definite. Intuitively, to exclude collapsed dimensions when calculating 242 matrix entropy, we adopt a PCA-like method, selecting the top-k eigenvalues before the elbow 243 point (Thorndike, 1953) to determine the effective rank, which represents the entropy of the low-244 rank matrix. Thus, we introduce the concept of truncated matrix entropy, obtaining the effective 245 rank of a positive definite submatrix to quantify uncertainty. From Eq. 9 and Eq. 6, the truncated 246 effective rank of matrix Q_m is defined by its top k eigenvalues:

 $H_k(\mathbf{\Sigma}_{Q_m}) = -\sum_{i=1}^k \sigma_i \log \sigma_i,$

 $\operatorname{erank}_{k}(\Sigma_{Q_{m}}) = \exp\left(H_{k}\left(\Sigma_{Q_{m}}\right)\right),$

where $H_k(\Sigma_{Q_m})$ denotes the entropy calculated using the top-k eigenvalue vector σ of the matrix Σ_{Q_m} . With the definition of erank $_k(\Sigma_{Q_m})$ established, we apply it to the different heads of Q_m

(9)

(10)

247 248

221

222

223

224

225

226

227

228 229

230 231

232

249

250

251

252 253 254

255

256

across various layers.

3.3 UNCERTAINTY-AWARE COMPRESSION STRATEGY

257 With the aforementioned conclusions, we begin to apply them to compress the heads of the KV 258 cache and each layer of the hidden state. Given that the hidden state and KV cache exhibit similar 259 matrix entropy behavior, we similarly use matrix entropy to adaptively estimate their compression 260 rates. We consider erank_k($\Sigma_{\mathbf{X}}$) as a measure of uncertainty for these matrices. The higher the 261 value, the greater the uncertainty, which implies more information in the token sequence matrix and 262 a lower compression rate for layer and a higher compression rate for head. We present the workflow 263 of our method in Figure 3. 264

265 Inter-layer Compression Regarding inter-layer compression, we focus on compressing hidden 266 states H_m , used to generate Q_m , K_m , and V_m . This involves measuring model uncertainty of 267 hidden states during the prefilling stage to obtain sparse attention. Unlike previous work (Xu et al., 2023; Li et al., 2023), which prunes the input prompt with a retrieval method before the prefilling 268 stage, we don't require an additional retrieval model, and pruning is conducted internally. Previous 269 work computes all hidden states during the prefilling stage and generates the complete KV cache



Figure 3: Overview of UNComp method. During the preparation stage, before inference on all datasets, we use a small amount of data in Wikitext2 (Merity, 2016) to group the model's layers 291 and heads. Layer grouping is based on Inter-layer Compression, while attention head grouping is 292 determined by Inter-head Compression. At the token level, we determine the cumulative attention 293 score by comparing matrix entropy trends before and after K_m compression (Paragraph 4.2). In the inference stage, compression is guided by the groupings from the preparation phase, and the KV 295 cache size is dynamically managed. The darker the color, the higher the effective rank of the Q_m 296 of the head, and thereby fewer tokens can be evicted. The Q_{mi} refers to the query matrix at layer i 297 before compression. The H/R^{j} (Paragraph 4.2) refers to the ratio of the number of historical tokens 298 (H) to the number of recent tokens (R), where j represents the j-th ratio in different H/R ratio 299 combination. The K_{mi}^{j} means the key matrix sampled at layer i with H/R^{j} . Correlation coefficient 300 refers to the Pearson correlation coefficient (Cohen et al., 2009). 301

302 before evicting them. Our method differs: we perform eviction on hidden states before generating 303 the KV cache, and the compressed H_m are used to generate the KV cache.

304 We divide the hidden states of tokens from all layers into C groups, where the token length in each 305 group is consistent across layers. As the group number increases, erank_k(X) increases, and more 306 tokens are pruned. By observing Figure 1(a), we can identify some patterns. We determine whether 307 to perform compression at two layers where erank $k(\mathbf{X})$ decreases beyond a threshold ϵ . This results 308 in the total number of compression stages, C:

$$C = \sum_{i=1}^{n-1} \mathbf{1} \left(\operatorname{erank}_{k}(\boldsymbol{\Sigma}_{H_{m}}^{(i)}) - \operatorname{erank}_{k}(\boldsymbol{\Sigma}_{H_{m}}^{(i+1)}) > \epsilon \wedge \operatorname{erank}_{k}(\boldsymbol{\Sigma}_{H_{m}}^{(i)}) > \operatorname{erank}_{k}(\boldsymbol{\Sigma}_{H_{m}}^{(i+1)}) \right), \quad (11)$$

where 1 is the indicator function that evaluates to 1 if the decrease in effective rank between layer i and i + 1 exceeds the threshold ϵ , and 0 otherwise, and n represents the total number of layers in 314 the model. Eq. 11 is a partition function that determines the division of the model's layers into C315 groups. The context size at each subsequent group is calculated as follows: 316

$$S_{i+1} = S_i + \Delta s, \quad i = 1, 2, \dots, C - 1,$$
(12)

310 311 312

313

317 318

- $\Delta s = \frac{S_{\max} S_{\min}}{C 1},$ (13)
- 320 where $S_{\text{max}} = S_1, S_{\text{min}} = S_C. \Delta s$ represents the incremental increase in context size between 321 consecutive groups. 322
- After obtaining the specific compression rate for each layer group, we start to evict tokens from 323 group 2. The hidden states of the tokens in group 1 are usually full-size because in the initial layer,

347 348 349

350

351

352

353

355

356

357

359

364 365 366

324 the matrix entropy is typically small, and we want to retain as much information as possible. From 325 group 2 to group C, for all layers, we choose the attention distribution of the final tokens from the 326 previous layer in the prefilling stage and evict the hidden states of the tokens with lower attention 327 scores. In other words, we use the attention scores of the current layer to predict the tokens to be 328 evicted in the next layer.

After generating all the hidden states for the prefilling stage at each layer, we map H_m onto the three 330 matrices Q_m, K_m , and V_m , and during the decoding phase, we maintain a fixed cumulative attention 331 score window, denoted as w_h . The window size is $S_{i,h}$, which we will introduce in the next part. 332 Each time a new token is generated, the token with the smallest cumulative attention score in w_h is 333 discarded.



Figure 4: The heatmap of erank $_k(\Sigma_{Q_m})$ across different layers and heads.

Inter-head Compression Similar to previous works like MQA, GQA, and MLA, we estimate the compression rate in the head dimension. However, unlike their approaches, our method focuses solely on the training-free setting, and we apply different compression rates to different head groups.

We sample 500 data points for observation, typically not included in the current test set, and find that the head patterns across different layers are consistent across datasets, as shown by the effective 354 rank distribution in Figure 4 (More details presented in Appendix A.4). Therefore, we conclude that the effective rank of the heads is not data-dependent, as it is an intrinsic characterization of the model's uncertainty measures. We rank the heads within each layer based on their effective rank and divide them into m groups. The groups are then arranged according to the ranking of the truncated 358 effective rank of each group. Typically, the larger the effective rank, the more information the head contains, the greater the compression ratio, and the fewer tokens are evicted.

360 After determining the context window S_i from Eq. 12 for each layer, we set different compression 361 rates for head groups based on their truncated effective rank. Specifically, we set the step size Δs_h , 362 decreasing the context size from $S_{i,1}$, which has the largest effective rank, down to $S_{i,m}$ as follows: 363

$$S_{i,h} = S_{i,h-1} - (h-1) \cdot \Delta s_h, \quad h = 1, 2, \dots, m,$$
(14)

367 where $S_{i,b}$ represents the context size for the *h*-th head group at layer *i*, and Δs_{b} is the fixed step 368 size applied between consecutive groups. During decoding, each head maintains its context window 369 according to the compression rate of the group it belongs to. For different heads, we maintain a window of size $S_{i,h}$ using the cumulative attention scores of the last l tokens. 370

371 Additionally, we investigate scenarios with extreme compression rates where certain groups with 372 low effective rank are completely removed, excluding them from the forward process. In such cases, 373 the dimensions of the modified attention output are dictated by the altered key and value, leading to 374 a dimensional mismatch with the original attention output. To resolve this, we compute the cosine 375 distance between the attention distributions of the removed and retained heads. These distributions are based on the cumulative attention over the last l tokens. We then fill the attention output ma-376 trix with the attention distribution from the head most similar to the removed head's distribution, 377 ensuring alignment with the dimension of the original attention output.

EXPERIMENT

4.1 EXPERIMENTAL SETTINGS

Models, Baselines, and Tasks We evaluate three models: Llama2-7B/13B-chat-hf (Touvron et al., 2023), Llama-3-8B-Inst (AI, 2024), and Mistral-7B-Instruct-v0.1 (Jiang et al., 2023). Llama2 and Llama3 are optimized for dialogue and question-answering, while Mistral is instruction-tuned for similar tasks. We compare our method with existing KV cache eviction methods H2O (Zhang et al., 2024d), PyramidKV (Zhang et al., 2024c), SnapKV (Li et al., 2024), and the head pruning method CHAI (Agarwal et al., 2024) under the same compression rate. Details are in Appendix A. UNComp is tested on 16 LongBench (Bai et al., 2023) benchmarks, including 2WikiMQA, GovReport, Nar-rativeQA, HotpotQA, Musique, Qasper, QMSum, MultiNews, MultifieldQA, TriviaQA, SAMSum, TREC, PCount, PRe, Lcc, and RB-P. We also compare our model's accuracy, inference speed, and throughput under extreme compression and evaluate it on the 'Needle in a Haystack' task (Liu et al., 2024c).

392		Single	-Docume	nt QA	Mult	i-Docume	nt QA	Su	mmarizat	ion	Few	shot Lea	ming	Synt	hetic	Co	ode		
393	Methods	NITY OA	oasper	MFen	HotpotQA	WikiMQ	Musique	CovRepor	oMSum	MultiNews	TREC	TriviaQA	SAMSum	pCount	pRe	Lee	RB.P	Avg. (s	Time / sample)
394		<u>,</u>	u	<i>y</i> .	v	<i>v</i> .	<i>A</i> .					•	5,	`					
395		10.01	10.01	25.10	20.55	20.42	10.05	Llama2-	7B-chat-h	f, KV Size	= FULI	-		# 00	40.00	<i>c</i> 1.10			0.07
396	FullKV	19.34	18.61	35.19	30.66	28.42	10.05	25.19	20.18	25.73	63.00	83.62	41.60	5.00	10.00	61.40	55.45	35.34	0.86
007		11.05	11.00	17.10	Jama-2-/1	B-chat-hi	KV Size	= 384 , Co	mpressio	anty 15 9.38	% (Exc		method)		5.00		50.04		
397	H2O SnapKV	14.96 16.27	14.60 17.34	30.37	26.72 33.04	27.97	6.11 9.92	17.83	20.33	20.17 22.63	47.00 59.50	83.50	39.39 38.45	4.50 5.50	5.00 12.50	57.08 59.18	50.31 55.28	27.84 31.94	0.94 0.82
398	Pyramidkv	16.86	18.26	31.01	31.59	27.93	8.69	19.88	20.15	22.43	62.00 57.00	83.86	38.98	5.50	10.00	58.94	52.80	31.81	0.84
399	Ours-group-stage	17.61	20.39	33.56	30.52	26.75	9.91	20.42	20.55	23.54	63.00	82.51	38.16	4.50	8.00	59.76	52.55	31.98	0.61
400	Ours-group	17.33	19.34	34.16	31.54	28.23	10.04	20.38	20.51	23.33	63.00	84.11	39.35	5.50	9.50	59.93	54.87	32.57	0.81
400							Llama	a2-13B-ch	at-hf, KV	Size = FUI	L								
401	FullKV	18.20	26.07	37.06	36.20	32.44	14.19	25.82	20.20	26.00	66.50	87.49	35.93	3.12	11.50	53.29	52.73	34.17	2.01
402				L	lama-2-13	B-chat-hf	, KV Size	e = 384 , C	ompressit	ility is 9.38	8% (Exc	ept CHAI	method)						
102	H2O SpepKV	14.11	18.36	22.78	33.03	27.58	12.94	18.97	18.69	20.37	53.50	85.75	34.15	3.55	6.00	50.97	47.56	29.27	2.57
403	PyramidKV	16.33	22.81	34.37	30.75 37.54	30.25	13.82	19.70	20.00 20.11	22.91	64.50	86.45	36.62	4.05	12.00	51.76 52.06	50.58	32.70	3.50
101	CHAI	17.06	23.51	31.01	33.70	27.78	11.73	23.03	19.59	24.66	65.00	86.18	15.93	4.00	8.50	45.57	48.74	30.37	2.50
404	Ours-group-stage	15.20	23.03	35.44	36.66	30.21	12.67	20.70	19.53	24.05	63.50	85.10	35.71	3.65	9.50	49.76	46.78	31.97	1.74
405	Ours-group	18.16	23.90	36.56	36.29	30.48	14.36	21.22	19.93	24.06	67.00	88.11	36.02	4.00	11.50	51.59	51.53	33.42	1.85
100							Llam	a3-8B-Ins	ruct, KV	Size = FUI	L								
406	FullKV	23.31	31.18	38.09	43.67	35.26	21.43	28.42	22.9	26.64	73.5	89.76	42.2	4.78	67.88	60.12	56.76	41.62	2.88
407				L	lama-3-8F	B-Instruct	, KV Size	= 384 , C	ompressib	ility is 4.74	% (Exc	ept CHAI	method)						
408	H2O	18.80	13.76	21.20	38.90	31.38	14.81	20.38	20.70	22.03	61.00	82.07	39.49	5.12	66.92	58.59	54.98	35.63	3.98
-100	SnapKV	21.47	19.77	33.97	43.10	32.79	21.48	21.69	22.01	22.92	63.00	89.69	39.78	5.06	67.83	60.19	56.82	38.85	2.68
409	CHAI	22.08	19.45	32.99	42.51	32.01	19.62	21.75	22.24	22.74	/1.00	89.59	40.51	4.23	67.75	58.92	36.12	38.88	2.78
100	Ours-group-stage	21.08	23.44	33.87	44 07	33.72	20.42	24.40	21.74	23.78	71 00	91 11	40.07	4.92	60.50	62.10	57.36	39.52	2.65
410	Ours-group	22.85	24.27	35.32	44.30	34.42	20.46	22.25	22.25	23.74	71.00	89.64	40.43	4.56	68.00	61.71	58.13	40.21	2.45
/111							Mistr	al-7B-Inst	ruct, KV	Size = FUL	L								
410	FullKV	20.53	27.28	47.67	38.57	26.75	15.46	30.88	22.00	26.99	70.50	86.28	43.23	1.30	29.42	56.60	52.18	37.22	2.74
412				N	listral-7B	-Instruct,	KV Size	= 384 , Co	mpressib	ility is 9.38	% (Exce	ept CHAI	method)						
413	H2O	14.68	14.92	28.43	30.04	20.92	11.21	20.03	19.37	21.05	58.00	81.48	41.08	2.42	11.04	54.76	48.78	29.89	3.13
	SnapKV	19.09	23.06	46.73	35.76	25.41	15.37	23.23	21.61	23.78	64.00	85.34	41.79	1.09	28.92	55.46	51.52	35.14	2.55
414	Pyramidkv	17.59	22.82	46.34	36.01	25.07	14.47	22.64	21.83	22.83	69.00	85.85	42.42	1.67	27.98	53.32	49.03	34.93	2.57
445	CHAI	15.01	17.23	39.41	23.53	21.12	9.00	24.83	20.59	23.17	49.50	84.08	33.28	1.07	19.25	46.85	44.62	29.53	3.55
415	Ours-group-stage Ours-group	19.65 18.98	21.93 23.30	44.08 48.77	35.30 36.80	23.21 24.83	12.84 15.22	24.61 24.87	22.08 21.65	24.36 23.78	67.00 69.50	84.31 85.93	41.81 43.17	1.48 0.94	28.81 27.38	54.84 55.28	52.10 50.91	34.90 35.71	2.27 2.79
416																			

Table 1: Performance Comparison across Different Tasks: Ours-group-stage compresses both hid-den states and KV cache, while Ours-group compresses only the KV cache. For 150 data points, Ours-group-stage is 1.4x faster than Ours-group, with only a 0.59% performance loss. All methods, except CHAI, compress key and value caches at the same compression ratio. In contrast, CHAI pri-marily compresses the key cache, leaving the value cache uncompressed and performing selection at the attention head level, achieving a 77.54% compression ratio. The last column represents the average time per sample.

4.2 EXPERIMENTAL COMPARISON IN MEMORY-CONSTRAINED SETTING

Main Results Our main experimental results are shown in Table 1, where we present the per-formance of current mainstream LLMs tested on LongBench. We perform the comparison under a unified setting with a KV cache size of 384. The heads in the main table are divided into two groups, with KV cache sizes set to 512 and 256, respectively, in descending order of effective rank. To ensure a fair comparison with others, we set the KV cache size of the other models to 384.

From Table 1, we draw the following conclusions: i) Our method achieves the best performance on LLaMA3, delivering a speedup of up to 1.4 times on a single batch instance with a compression

100			Llama2.7	B-chat-hf KV	Size = 64				
432			2.1.111122-7			DG /			
433	Methods	Qasper	Musique	GovReport	TREC	PCount	Lcc	Average score	
434	FullKV	18.61	10.05	25.19	63.00	5.00	61.40	30.54	
435	H2O	13.84	1.33	8.57	18.00	0.50	28.86	11.85	
	PyramidKV	16.10	6.58	12.07	46.00	5.50	46.09	22.06	
436	SnapKV	15.70	6.15	11.16	40.50	5.00	43.77	20.38	
437	Ours-group-stage	17.57	6.58	15.25	59.00	4.50	49.75	25.44	
-101	Ours-group	15.40	6.96	14.88	55.50	5.00	50.00	24.62	
438	T 1		Le VV C'	-f.O	W241. E-4				
439	Liama2-/B-chat-in, KV Size of One Group with Extreme Compression								
140	Methods	Qasper	Musique	GovReport	TREC	PCount	Lcc	Average score	
440	FullKV	18.61	10.05	25.19	63.00	5.00	61.40	30.54	
441	Ours-remain-tokens-256	19.67	9.80	20.19	63.00	5.50	60.28	29.74	
442	Ours-remain-tokens-128	18.67	9.75	20.02	63.00	5.50	59.60	29.42	
//3	Ours-remain-tokens-64	18.13	9.79	19.84	63.00	5.50	58.09	29.06	
	Ours-remain-tokens-32	18.04	9.24	19.31	63.00	5.50	57.04	28.69	
444	Ours-remain-tokens-16	18.48	8.08	18.21	63.00	5.00	47.29	26.68	
445	Ours-remain-tokens-12	17.31	8.78	18.16	62.00	5.00	45.23	26.08	
	Ours-delete-2-heads	18.30	8.58	18.98	63.00	5.50	59.38	28.96	
446	Ours-delete-4-heads	13.29	7.96	19.12	62.50	5.50	53.94	27.05	
447	Ours-delete-8-heads	12.64	6.60	9.87	63.50	3.21	37.87	22.28	

Table 2: Extreme Compression Conditions.

rate of 4.68%, confirmed by averaging multiple repeated experiments. *ii*) Our method exhibits nearlossless performance in certain models, especially compared to the full-size KV cache setting in
Llama2-7B/13B-chat-hf, with only a 0.77% performance loss while achieving a 9.38% compression
rate. *iii*) In comparison with the training-free head-pruning method CHAI, our *UNComp* outperforms in both single-batch inference speed and overall performance. With a KV cache compression
rate lower than CHAI's 68.55%, our method achieved 5.4 times faster inference speed.

The Result of Extreme Compression We compare performance under extreme compression settings to highlight our method's advantages. For this investigation, we use Llama-2-7B-chat-hf as the baseline model, categorizing the layer into five groups and attention heads into two groups. As shown in Table 2, we evaluate the effectiveness of our approach across increasingly extreme compression ratios. Importantly, when the compression rate of the KV cache is set to 1.56%, our method shows a substantial enhancement over existing alternatives.

462 We further explore the minimum achievable compression rate for the group with the lower effective 463 rank, as detailed in Table 2 where *Ours-remain-tokens-N* indicates the retention of N tokens per attention head within the group of lower effective rank, while the other group maintains a KV cache 464 size of 512. Furthermore, Ours-delete-K-head denotes the complete pruning of K heads per layer, 465 contingent on the effective rank order. The results underscore that our methodology can sustain 466 a high level of accuracy relative to the full KV cache size when only 12 tokens are preserved 467 or even certain heads are pruned. This finding further corroborates the validity of employing 468 differentiated compression ratios for various heads, aligned with their respective effective ranks. 469

Methods		NVIDIA A	100 80GB G	PU	AMD Instinct MI210 64G GPU					
	Attention Time (s)	Prefill Time (s)	Decoding Time (s)	Max Memory Usage (MB)	Attention Time (s)	Prefill Time (s)	Decoding Time (s)	Max Memory Usage (MB)		
FullKV	129.13	77.34	51.79	25900	189.92	116.64	73.27	23195		
H2O	140.92	90.56	50.37	22908	241.42	173.08	68.34	20247		
PyramidKV	126.03	78.98	47.05	22936	185.85	119.17	66.68	20295		
SnapKV	123.71	78.71	45.00	22920	184.59	120.26	64.33	20276		
Ours-group-stage	91.56	48.78	42.78	22964	155.60	100.17	55.43	20300		
Ours-group	121.85	79.60	42.25	22978	184.76	121.04	63.72	20335		

⁴⁷⁷ 478

448

449

479 480

481

Table 3: Single Batch Time Consumption and Memory Usage Analysis on Different GPUs. Analysis based on MultifieldQA dataset with 150 samples, and KV size is 384 per layer. The compression ratio of Ours-group-stage to hidden states in the prefill stage is 63.09%.

Analysis of Inference Time Latency and Performance We analyze the inference time latency
 and the specific time costs of each component. To achieve reliable time analysis, we synchronize
 the CPU and GPU clock frequencies to facilitate our measurements. We use the Llama2-7B-chat-hf
 model to measure 150 data points from the MultifieldQA collection in a single batch on an NVIDIA
 A100 80G GPU and an AMD INSTINCT MI210 64G GPU. We focus on the duration of the prefill-



Figure 5: Comparison of Inter-Layer Matrix Entropy Trends Across Different H/R.

ing stage, the decoding duration, and the total duration of the attention mechanism. We also record the maximum memory usage during runtime.

In Table 3, we compare our experimental results and present the following observations: *i*) For longcontext generation tasks, the prefilling stage takes up more time throughout the inference process. *ii*) Our method is optimized in the prefilling stage, greatly speeding up inference and outperforming other methods, with up to $1.58 \times$ acceleration over the full-size KV cache in a single batch. For throughput analysis, experiments with prompt and generation lengths set to 2048 + 8096 show that FullKV supports a maximum batch size of 6 with a token generation time of 15.67 ms. In contrast, our method supports a batch size of 32 with a token generation time of 2.45 ms, achieving 6.4 times the throughput of FullKV. More details are provided in Appendix E.

Needle in a Haystack Task The 'Needle in a Haystack' 511 task (Liu et al., 2024c) involves embedding key informa-512 tion randomly in long contexts to assess the model's abil-513 ity to handle complex, extended text. Table 4 compares 514 Llama2-4k and Llama3-8k, both with a KV size of 384. 515 The results show that our method outperforms FullKV at 516 a 9.38% compression rate, demonstrating its superiority. 517 This indicates that our uncertainty measurement method 518 based on effective rank can identify the heads crucial for 519 the retrieval task and effectively compress noisy heads.

Methods	Llama2-4k	Llama3-8k
FullKV	98.70	84.99
H2O	61.14	51.56
PyramidKV	93.24	79.08
SnapKV	94.50	81.27
CHAI	97.80	64.69
Ours-group	98.42	84.13
Ours-group-stage	e 98.80	83.73

Table 4: Needle-in-a-haystack results.

520 The Ratio of Recent Tokens to Historical Window Tokens This part examines the ratio H/R, 521 comparing the number of historical tokens (H) to the most recent l tokens (R). Our experiment 522 reveals that matrix entropy trends across layers at various H/R ratios align with those of the full-523 size KV cache. As shown in Figure 5(a), different proportions of historical and recent tokens produce distinct trends. Notably, a compressed key matrix trend more similar to the full KV cache indicates 524 better performance, given the same KV cache compression ratio. We confirm this through multiple 525 experiments. To measure this similarity, we use the Pearson correlation coefficient. As depicted in 526 Figure 5(b), higher similarity in matrix entropy trends corresponds to improved model performance. 527

528 529 5 CONCLUSION

500

530 We introduced UNComp, an uncertainty-aware approach for compressing the KV cache and hid-531 den states in LLMs. By employing matrix entropy to measure model uncertainty across layers and heads, UNComp adaptively determines compression rates, achieving a balance between memory ef-532 ficiency and model performance. Our experiments demonstrate that UNComp can reduce memory 533 usage significantly, achieving up to a $1.6 \times$ speedup during the prefilling stage, a $6.4 \times$ throughput 534 improvement, and compressing the KV cache to 4.74% of its original size. Despite this high com-535 pression, UNComp maintains a minimal performance loss of only 1.41%, and even surpasses the 536 performance of the full-size KV cache in specific needle-in-a-haystack tasks. This indicates that our 537 method provides an effective solution for optimizing long-context LLM inference without requiring 538 additional training. Moving forward, our approach can serve as a foundation for further exploration into adaptive compression techniques in large-scale model deployment.

540 REFERENCES

548

554

- Josh Achiam, Steven Adler, Sandhini Agarwal, Lama Ahmad, Ilge Akkaya, Florencia Leoni Aleman, Diogo Almeida, Janko Altenschmidt, Sam Altman, Shyamal Anadkat, et al. Gpt-4 technical
 report. *arXiv preprint arXiv:2303.08774*, 2023.
- Saurabh Agarwal, Bilge Acun, Basil Homer, Mostafa Elhoushi, Yejin Lee, Shivaram Venkataraman,
 Dimitris Papailiopoulos, and Carole-Jean Wu. Chai: Clustered head attention for efficient llm
 inference. *arXiv preprint arXiv:2403.08058*, 2024.
- 549 Meta AI. Llama 3: A family of large language models. https://llama.meta.com, 2024.
 550 URL https://llama.meta.com. Instruction-tuned version.
- Joshua Ainslie, James Lee-Thorp, Michiel de Jong, Yury Zemlyanskiy, Federico Lebrón, and Sumit
 Sanghai. Gqa: Training generalized multi-query transformer models from multi-head check *arXiv preprint arXiv:2305.13245*, 2023.
- Yushi Bai, Xin Lv, Jiajie Zhang, Hongchang Lyu, Jiankai Tang, Zhidian Huang, Zhengxiao Du, Xiao Liu, Aohan Zeng, Lei Hou, et al. Longbench: A bilingual, multitask benchmark for long context understanding. *arXiv preprint arXiv:2308.14508*, 2023.
- William Brandon, Mayank Mishra, Aniruddha Nrusimha, Rameswar Panda, and Jonathan Ragan
 Kelly. Reducing transformer key-value cache size with cross-layer attention. *arXiv preprint arXiv:2405.12981*, 2024.
- Israel Cohen, Yiteng Huang, Jingdong Chen, Jacob Benesty, Jacob Benesty, Jingdong Chen, Yiteng Huang, and Israel Cohen. Pearson correlation coefficient. *Noise reduction in speech processing*, pp. 1–4, 2009.
- Grégoire Delétang, Anian Ruoss, Paul-Ambroise Duquenne, Elliot Catt, Tim Genewein, Christo pher Mattern, Jordi Grau-Moya, Li Kevin Wenliang, Matthew Aitchison, Laurent Orseau, et al.
 Language modeling is compression. *arXiv preprint arXiv:2309.10668*, 2023.
- Ruili Feng, Kecheng Zheng, Yukun Huang, Deli Zhao, Michael Jordan, and Zheng-Jun Zha. Rank diminishing in deep neural networks. *Advances in Neural Information Processing Systems*, 35: 33054–33065, 2022.
- Suyu Ge, Yunan Zhang, Liyuan Liu, Minjia Zhang, Jiawei Han, and Jianfeng Gao. Model tells
 you what to discard: Adaptive kv cache compression for llms. *arXiv preprint arXiv:2310.01801*, 2023.
- Luis Gonzalo Sanchez Giraldo, Murali Rao, and Jose C Principe. Measures of entropy from data using infinitely divisible kernels. *IEEE Transactions on Information Theory*, 61(1):535–548, 2014.
- Coleman Hooper, Sehoon Kim, Hiva Mohammadzadeh, Michael W Mahoney, Yakun Sophia Shao,
 Kurt Keutzer, and Amir Gholami. Kvquant: Towards 10 million context length llm inference with
 kv cache quantization. *arXiv preprint arXiv:2401.18079*, 2024.
- 582
 583
 584
 584
 585
 585
 586
 587
 588
 588
 588
 589
 589
 580
 580
 580
 581
 581
 582
 582
 583
 584
 585
 584
 585
 584
 585
 585
 585
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
 586
- Edward J Hu, Yelong Shen, Phillip Wallis, Zeyuan Allen-Zhu, Yuanzhi Li, Shean Wang, Lu Wang,
 and Weizhu Chen. Lora: Low-rank adaptation of large language models. *arXiv preprint arXiv:2106.09685*, 2021.
- Yuzhen Huang, Jinghan Zhang, Zifei Shan, and Junxian He. Compression represents intelligence linearly. *arXiv preprint arXiv:2404.09937*, 2024.
- Albert Q Jiang, Alexandre Sablayrolles, Arthur Mensch, Chris Bamford, Devendra Singh Chaplot,
 Diego de las Casas, Florian Bressand, Gianna Lengyel, Guillaume Lample, Lucile Saulnier, et al.
 Mistral 7b. arXiv preprint arXiv:2310.06825, 2023.

594 Huiqiang Jiang, Yucheng Li, Chengruidong Zhang, Qianhui Wu, Xufang Luo, Surin Ahn, Zhenhua 595 Han, Amir H Abdi, Dongsheng Li, Chin-Yew Lin, et al. Minference 1.0: Accelerating pre-filling 596 for long-context llms via dynamic sparse attention. arXiv preprint arXiv:2407.02490, 2024. 597 Jared Kaplan, Sam McCandlish, Tom Henighan, Tom B Brown, Benjamin Chess, Rewon Child, 598 Scott Gray, Alec Radford, Jeffrey Wu, and Dario Amodei. Scaling laws for neural language models. arXiv preprint arXiv:2001.08361, 2020. 600 601 Yucheng Li, Bo Dong, Chenghua Lin, and Frank Guerin. Compressing context to enhance inference 602 efficiency of large language models. arXiv preprint arXiv:2310.06201, 2023. 603 Yuhong Li, Yingbing Huang, Bowen Yang, Bharat Venkitesh, Acyr Locatelli, Hanchen Ye, Tianle 604 Cai, Patrick Lewis, and Deming Chen. Snapky: Llm knows what you are looking for before 605 generation. arXiv preprint arXiv:2404.14469, 2024. 606 607 Aixin Liu, Bei Feng, Bin Wang, Bingxuan Wang, Bo Liu, Chenggang Zhao, Chengqi Dengr, Chong 608 Ruan, Damai Dai, Daya Guo, et al. Deepseek-v2: A strong, economical, and efficient mixture-609 of-experts language model. arXiv preprint arXiv:2405.04434, 2024a. 610 Akide Liu, Jing Liu, Zizheng Pan, Yefei He, Gholamreza Haffari, and Bohan Zhuang. Mini-611 cache: Kv cache compression in depth dimension for large language models. arXiv preprint 612 arXiv:2405.14366, 2024b. 613 614 Nelson F Liu, Kevin Lin, John Hewitt, Ashwin Paranjape, Michele Bevilacqua, Fabio Petroni, and 615 Percy Liang. Lost in the middle: How language models use long contexts. Transactions of the Association for Computational Linguistics, 12:157–173, 2024c. 616 617 Zichang Liu, Aditya Desai, Fangshuo Liao, Weitao Wang, Victor Xie, Zhaozhuo Xu, Anastasios 618 Kyrillidis, and Anshumali Shrivastava. Scissorhands: Exploiting the persistence of importance 619 hypothesis for llm kv cache compression at test time. Advances in Neural Information Processing 620 Systems, 36, 2024d. 621 622 Zirui Liu, Jiayi Yuan, Hongye Jin, Shaochen Zhong, Zhaozhuo Xu, Vladimir Braverman, Beidi Chen, and Xia Hu. Kivi: A tuning-free asymmetric 2bit quantization for kv cache. arXiv preprint 623 arXiv:2402.02750, 2024e. 624 625 Stephen Merity. The wikitext long term dependency language modeling dataset. Salesforce Meta-626 mind, 9, 2016. 627 628 Alexander Peysakhovich and Adam Lerer. Attention sorting combats recency bias in long context language models. arXiv preprint arXiv:2310.01427, 2023. 629 630 Reiner Pope, Sholto Douglas, Aakanksha Chowdhery, Jacob Devlin, James Bradbury, Jonathan 631 Heek, Kefan Xiao, Shivani Agrawal, and Jeff Dean. Efficiently scaling transformer inference. 632 Proceedings of Machine Learning and Systems, 5:606–624, 2023. 633 Olivier Roy and Martin Vetterli. The effective rank: A measure of effective dimensionality. In 2007 634 15th European signal processing conference, pp. 606–610. IEEE, 2007. 635 636 Noam Shazeer. Fast transformer decoding: One write-head is all you need. arXiv preprint 637 arXiv:1911.02150, 2019. 638 639 Noam Shazeer, Azalia Mirhoseini, Krzysztof Maziarz, Andy Davis, Quoc Le, Geoffrey Hinton, and Jeff Dean. Outrageously large neural networks: The sparsely-gated mixture-of-experts layer. 640 arXiv preprint arXiv:1701.06538, 2017. 641 642 Ying Sheng, Lianmin Zheng, Binhang Yuan, Zhuohan Li, Max Ryabinin, Beidi Chen, Percy Liang, 643 Christopher Ré, Ion Stoica, and Ce Zhang. Flexgen: High-throughput generative inference of 644 large language models with a single gpu. In International Conference on Machine Learning, pp. 645 31094-31116. PMLR, 2023. 646 Mingjie Sun, Xinlei Chen, J Zico Kolter, and Zhuang Liu. Massive activations in large language 647

models. arXiv preprint arXiv:2402.17762, 2024.

- 648 Jiaming Tang, Yilong Zhao, Kan Zhu, Guangxuan Xiao, Baris Kasikci, and Song Han. Quest: 649 Query-aware sparsity for efficient long-context llm inference. arXiv preprint arXiv:2406.10774, 650 2024. 651 Chaofan Tao, Qian Liu, Longxu Dou, Niklas Muennighoff, Zhongwei Wan, Ping Luo, Min Lin, and 652 Ngai Wong. Scaling laws with vocabulary: Larger models deserve larger vocabularies. arXiv 653 preprint arXiv:2407.13623, 2024. 654 655 Robert L Thorndike. Who belongs in the family? *Psychometrika*, 18(4):267–276, 1953. 656 657 Hugo Touvron, Louis Martin, Kevin Stone, Peter Albert, Amjad Almahairi, Yasmine Babaei, Nikolay Bashlykov, Soumya Batra, Prajjwal Bhargava, Shruti Bhosale, et al. Llama 2: Open founda-658 tion and fine-tuned chat models. arXiv preprint arXiv:2307.09288, 2023. 659 660 John Von Neumann. Mathematische grundlagen der quantenmechanik, volume 38. Springer-Verlag, 661 2013. 662 663 Zhongwei Wan, Xinjian Wu, Yu Zhang, Yi Xin, Chaofan Tao, Zhihong Zhu, Xin Wang, Siqi Luo, 664 Jing Xiong, and Mi Zhang. D20: Dynamic discriminative operations for efficient generative 665 inference of large language models. arXiv preprint arXiv:2406.13035, 2024. 666 Lean Wang, Lei Li, Damai Dai, Deli Chen, Hao Zhou, Fandong Meng, Jie Zhou, and Xu Sun. Label 667 words are anchors: An information flow perspective for understanding in-context learning. arXiv 668 preprint arXiv:2305.14160, 2023. 669 670 Zheng Wang, Boxiao Jin, Zhongzhi Yu, and Minjia Zhang. Model tells you where to merge: Adap-671 tive kv cache merging for llms on long-context tasks. arXiv preprint arXiv:2407.08454, 2024. 672 Wenhao Wu, Yizhong Wang, Guangxuan Xiao, Hao Peng, and Yao Fu. Retrieval head mechanisti-673 cally explains long-context factuality. arXiv preprint arXiv:2404.15574, 2024. 674 675 Guangxuan Xiao, Yuandong Tian, Beidi Chen, Song Han, and Mike Lewis. Efficient streaming 676 language models with attention sinks. arXiv preprint arXiv:2309.17453, 2023. 677 678 Guangxuan Xiao, Jiaming Tang, Jingwei Zuo, Junxian Guo, Shang Yang, Haotian Tang, Yao Fu, and Song Han. Duoattention: Efficient long-context llm inference with retrieval and streaming 679 heads. arXiv preprint arXiv:2410.10819, 2024. 680 681 Fangyuan Xu, Weijia Shi, and Eunsol Choi. Recomp: Improving retrieval-augmented lms with 682 compression and selective augmentation. arXiv preprint arXiv:2310.04408, 2023. 683 684 Shuo Yang, Ying Sheng, Joseph E Gonzalez, Ion Stoica, and Lianmin Zheng. Post-training sparse 685 attention with double sparsity. arXiv preprint arXiv:2408.07092, 2024. 686 Hao Yu, Zelan Yang, Shen Li, Yong Li, and Jianxin Wu. Effectively compress ky heads for llm. 687
 - Tianyi Zhang, Jonah Yi, Zhaozhuo Xu, and Anshumali Shrivastava. Kv cache is 1 bit per channel: Efficient large language model inference with coupled quantization. *arXiv preprint arXiv:2405.03917*, 2024a.

arXiv preprint arXiv:2406.07056, 2024.

688 689

690

691

- Kinrong Zhang, Yingfa Chen, Shengding Hu, Zihang Xu, Junhao Chen, Moo Hao, Xu Han, Zhen
 Thai, Shuo Wang, Zhiyuan Liu, et al. ∞ bench: Extending long context evaluation beyond
 100k tokens. In *Proceedings of the 62nd Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, pp. 15262–15277, 2024b.
- Yichi Zhang, Bofei Gao, Tianyu Liu, Keming Lu, Wayne Xiong, Yue Dong, Baobao Chang, Junjie
 Hu, Wen Xiao, et al. Pyramidkv: Dynamic kv cache compression based on pyramidal information
 funneling. *arXiv preprint arXiv:2406.02069*, 2024c.
- 701 Yifan Zhang, Zhiquan Tan, Jingqin Yang, Weiran Huang, and Yang Yuan. Matrix information theory for self-supervised learning. *arXiv preprint arXiv:2305.17326*, 2023.

Yuxin Zhang, Yuxuan Du, Gen Luo, Yunshan Zhong, Zhenyu Zhang, Shiwei Liu, and Rongrong Ji. Cam: Cache merging for memory-efficient llms inference. In Forty-first International Conference on Machine Learning. Zhenyu Zhang, Ying Sheng, Tianyi Zhou, Tianlong Chen, Lianmin Zheng, Ruisi Cai, Zhao Song, Yuandong Tian, Christopher Ré, Clark Barrett, et al. H2o: Heavy-hitter oracle for efficient gen-erative inference of large language models. Advances in Neural Information Processing Systems, 36, 2024d. Zhijian Zhuo, Yifei Wang, Jinwen Ma, and Yisen Wang. Towards a unified theoretical understanding of non-contrastive learning via rank differential mechanism. arXiv preprint arXiv:2303.02387, 2023.

A IMPLEMENTATION DETAILS

758 A.1 MACHINE ENVIRONMENT 759

Main of our experiments are conducted on eight AMD INSTINCT MI210 64G GPUs. For the time test analysis, we conducted the experiment on a single NVIDIA A100 80GB GPU and a single AMD INSTINCT MI210 64G GPU.

764 A.2 MODEL SELECTION

In all of our experiments, the model's weights are downloaded from huggingface. For all llama architectures, Llama2-7b model uses the 'meta-llama/Llama-2-7b-chat-hf' version, Llama2-13b model uses the 'meta-llama/Llama-2-13b-chat-hf' version, Llama3-8b model uses the 'meta-llama/Meta-Llama-3-8B-Instruct' version. For mistral architecture, 'mistralai/Mistral-7B-Instruct-v0.2' version is used.

770

771 A.3 Hyperparameter setting

We conduct the experiment in a scenario with an average KV size of 384 per layer. The experiment is governed by six main hyperparameters, the selection of last l token's cumulative attention score, the threshold ϵ , the setting of minimum context length S_{min} , the numbers of groups (called GN) and the selections of $S_{i,1}$ and Δs_h .

In our experiment, we select the cumulative attention scores of the last 8 tokens, and threshold ϵ is set to 1. S_{min} is set to 1536 and S_{max} is determined by the maximum context length of the model. We conduct the experiment under two groups, setting GN to 2. The groups with the higher truncated matrix entropy are assigned a higher compression rate, while the groups with the lower truncated matrix entropy are assigned a lower compression rate. The $S_{i,1}$ is set to 512, and the corresponding Δs_h is set to 256.

783 More specifically, we randomly sample several Wikitext2 datasets and calculate the matrix entropy 784 inter-layer trend of the query matrix in the prefill stage. Based on the method outlined in the paper, 785 we partition the 32 attention layers of Llama2-7B, Mistral-7B, and Llama3-8B into five distinct groups: layers 0–1, 2–14, 15–25, 26–30, and layer 31. The reserved capacities for these groups 786 are configured as 4096, 3456, 2816, 2176, and 1536, respectively, in Llama2-7B and Mistral-7B. 787 For Llama3-8B, the corresponding reserved sizes are set to 8096, 6456, 4816, 3176, and 1536. For 788 Llama2-13B, which consists of 40 attention layers, we categorize the layers into eight groups: layer 789 0, layers 1-2, 3-14, 15-22, 23-30, 31-34, 35-36, and 37-39, with the reserved sizes designated as 790 4096, 3731, 3366, 3001, 2636, 2271, 1906, and 1536, respectively. 791

- 792
- 793

A.4 ATTENTION HEAD TYPE SCREENING

In this study, we use the Wikitext2 dataset to categorize attention heads. Taking Llama2-7B-chat-hf
 as an example, we divide the attention heads into two groups for demonstration purposes.

Initially, we randomly select 500 data samples and input them into a large model for generation.
During the prefilling stage, we compute the truncated matrix entropy of the query matrix for each layer's 32 attention heads. Attention heads with higher truncated matrix entropy are assigned a value of 1, while those with lower entropy are assigned a value of 0, and the results are output to a file.
Once the data generation process is complete, we collect 500 files containing 32x32 matrices.

In the actual generative task, we load the previously generated file. For each layer, we count the number of 1s per attention head and group the 16 heads with the highest counts together, assigning them a higher compression rate. The remaining 16 attention heads are grouped separately and assigned a lower compression rate.

806 807

808

B DETAILS OF EVALUATION

Longbench is the first benchmark for assessing the long-context understanding capabilities of large language models in a bilingual and multitask framework. It evaluates multilingual capabilities in

both Chinese and English, consisting of six major categories and twenty-one tasks. Key application scenarios include single-document QA, multi-document QA, summarization, few-shot learning, synthetic tasks, and code completion. We use Longbench to evaluate the performance of our method on contextual input tasks. The details of metrics at Table 5.

Additionally, once the data sample is encoded into tokens, if its length exceeds the model's maximum allowable length, we truncate it by taking equal portions from the beginning and the end.

Dataset	Metric	Language	Data Length	Dataset	Metric	Language	Data Length
NarrativeQA	F1	English	200	MultiNews	range-l	English	200
Qasper	F1	English	200	trec	classification accuracy	English	200
MultifieldQA	F1	English	150	TriviaQA	English	F1	200
HotpotQA	F1	English	200	SAMSum	range-1	English	200
2WikiMQA	F1	English	200	PCount	exact match accuracy	English	200
Musique	F1	English	200	PRe	exact match accuracy	English	200
GovReport	range-1	English	200	Lcc	edit similarity	Python/C#/Java	500
QMSum	range-1	English	200	RB-P	edit similarity	Python/Java	500

Table 5: The details of statistics in LongBench

C APPENDIX FOR PROOFS

Proof Lemma 1

 Proof. To derive the von Neumann entropy from the Rényi entropy, we first need to clarify the relationship between the two. The von Neumann entropy can be seen as a special case of the Rényi entropy in the limit where the Rényi parameter $\alpha \rightarrow 1$. The Rényi entropy is defined as:

$$S_{\alpha}(\mathbf{\Sigma}_{\mathbf{X}}) = \frac{1}{1-\alpha} \log \left(\operatorname{Tr}((\mathbf{\Sigma}_{\mathbf{X}})^{\alpha}) \right), \tag{15}$$

where α is the order of the Rényi entropy, $\Sigma_{\mathbf{X}}$ is the density matrix, and $\operatorname{Tr}(\rho^{\alpha})$ is the trace of the density matrix raised to the power of α . To derive the von Neumann entropy, we need to examine the limit of the Rényi entropy as $\alpha \to 1$. Let's consider the form of the Rényi entropy:

$$S_{\alpha}(\mathbf{\Sigma}_{\mathbf{X}}) = \frac{1}{1-\alpha} \log\left(\sum_{i} \sigma_{i}^{\alpha}\right), \tag{16}$$

where σ_i are the eigenvalues of the density matrix Σ_X . As $\alpha \to 1$, we can apply L'Hôpital's rule to compute this limit:

$$S(\mathbf{\Sigma}_{\mathbf{X}}) = \lim_{\alpha \to 1} S_{\alpha}(\rho) = \lim_{\alpha \to 1} \frac{1}{1 - \alpha} \log\left(\sum_{i} \sigma_{i}^{\alpha}\right)$$
(17)

To proceed, consider the Taylor expansion of $\sum_i \sigma_i^{\alpha}$:

$$\sum_{i} \sigma_{i}^{\alpha} = \sum_{i} \sigma_{i} \cdot e^{(\alpha-1)\log\sigma_{i}} \approx \sum_{i} \sigma_{i} \left(1 + (\alpha-1)\log\sigma_{i}\right) = 1 + (\alpha-1)\sum_{i} \sigma_{i}\log\sigma_{i} \quad (18)$$

Thus,

$$S_{\alpha}(\mathbf{\Sigma}_{\mathbf{X}}) \approx \frac{1}{1-\alpha} \log \left(1 + (\alpha - 1) \sum_{i} \sigma_{i} \log \sigma_{i} \right)$$
 (19)

As $\alpha \to 1$, we can use the approximation $\log(1 + x) \approx x$ for small x. Therefore, we get:

$$S_{\alpha}(\mathbf{\Sigma}_{\mathbf{X}}) \approx -\sum_{i} \sigma_{i} \log \sigma_{i}$$
⁽²⁰⁾

which is exactly the expression for the von Neumann entropy:

$$H(\mathbf{\Sigma}_{\mathbf{X}}) = -\mathrm{Tr}(\mathbf{\Sigma}_{\mathbf{X}}\log(\mathbf{\Sigma}_{\mathbf{X}}))$$
(21)

Proof Lemma 2

Proof. In this section, we present a continuous proof of the transformation from the matrix entropy formula to the eigenvalue form.

$$H(\mathbf{\Sigma}_{\mathbf{X}}) = -\mathrm{Tr}\left(\mathbf{\Sigma}_{\mathbf{X}}\log\left(\mathbf{\Sigma}_{\mathbf{X}}\right)\right)$$
(22)

Given that $\Sigma_{\mathbf{X}}$ is a symmetric positive definite matrix, we can perform an eigenvalue decomposition:

$$\Sigma_{\mathbf{X}} = \mathbf{U} \mathbf{\Lambda} \mathbf{U}^{\top} \tag{23}$$

where U is an orthogonal matrix composed of eigenvectors, and Λ is a diagonal matrix whose entries are the eigenvalues $\sigma_1, \sigma_2, \ldots, \sigma_D$. The logarithm of Σ_X can then be written as:

$$\log(\mathbf{\Sigma}_{\mathbf{X}}) = \mathbf{U}\log(\mathbf{\Lambda})\mathbf{U}^{\top}$$
(24)

where $\log(\Lambda)$ is a diagonal matrix whose elements are $\log(\sigma_1), \log(\sigma_2), \ldots, \log(\sigma_D)$. Substituting these into the entropy expression:

$$H(\mathbf{\Sigma}_{\mathbf{X}}) = -\mathrm{Tr}\left(\mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\top}\mathbf{U}\log(\mathbf{\Lambda})\mathbf{U}^{\top}\right)$$
(25)

Since $\mathbf{U}^{\top}\mathbf{U} = \mathbf{I}$, this simplifies to:

$$H(\mathbf{\Sigma}_{\mathbf{X}}) = -\mathrm{Tr}\left(\mathbf{\Lambda}\log(\mathbf{\Lambda})\right) \tag{26}$$

For a diagonal matrix, the trace is the sum of its diagonal elements. Therefore, we have:

$$H(\mathbf{\Sigma}_{\mathbf{X}}) = -\sum_{i=1}^{D} \sigma_i \log(\sigma_i)$$
(27)

This concludes the proof that the matrix entropy formula can be written as the sum of the eigenvalues of Σ_X .

905 Proof Lemma 3

908 **Proof.** Let $\mathbf{X} \in \mathbb{R}^{n \times p}$ be a matrix representing *n* observations and *p* variables. The covari-908 ance matrix $\Sigma_{\mathbf{X}}$ of \mathbf{X} is defined as:

$$\boldsymbol{\Sigma}_{\mathbf{X}} = \frac{1}{n-1} \mathbf{X}^{\top} \mathbf{X}$$
(28)

⁹¹² The goal is to determine the relationship between the rank of the matrix X and the rank of its ⁹¹³ covariance matrix Σ_X .

The rank of the matrix \mathbf{X} , denoted as rank(\mathbf{X}), is the number of linearly independent columns in \mathbf{X} , and it satisfies the inequality:

$$\operatorname{rank}(\mathbf{X}) \le \min(n, p) \tag{29}$$

Since the covariance matrix $\Sigma_{\mathbf{X}}$ is given by $\Sigma_{\mathbf{X}} = \frac{1}{n-1} \mathbf{X}^{\top} \mathbf{X}$, it is a $p \times p$ symmetric matrix. The rank of $\Sigma_{\mathbf{X}}$, denoted rank $(\Sigma_{\mathbf{X}})$, is determined by the product $\mathbf{X}^{\top} \mathbf{X}$. The rank of this product is bounded by the rank of \mathbf{X} , so we have the following inequality:

$$\operatorname{rank}(\mathbf{\Sigma}_{\mathbf{X}}) \le \operatorname{rank}(\mathbf{X})$$
 (30)

This shows that the rank of the covariance matrix $\Sigma_{\mathbf{X}}$ cannot exceed the rank of the original matrix X. In the case where the number of observations *n* is greater than or equal to the number of variables *p* (i.e., $n \ge p$), and the columns of X are linearly independent, the rank of X is equal to *p*, meaning rank(\mathbf{X}) = *p*. In this scenario, the matrix $\mathbf{X}^{\top}\mathbf{X}$ has full rank, which implies that the covariance matrix $\Sigma_{\mathbf{X}}$ will also have full rank. Therefore, we have rank($\Sigma_{\mathbf{X}}$) = *p*, and the rank of the covariance matrix is equal to the rank of the original matrix, i.e., rank($\Sigma_{\mathbf{X}}$) = rank(\mathbf{X}).

930 931 On the other hand, when the number of observations is less than the number of variables (i.e., n < p), 932 the rank of X is constrained by the number of observations, such that rank(\mathbf{X}) $\leq n$. Consequently, 933 the rank of the covariance matrix $\Sigma_{\mathbf{X}}$ is also limited by n, meaning rank($\Sigma_{\mathbf{X}}$) $\leq n$. Since n < p in 934 this case, the covariance matrix is rank-deficient, and we have rank($\Sigma_{\mathbf{X}}$) < p.

In general, the rank of the covariance matrix $\Sigma_{\mathbf{X}}$ is less than or equal to the rank of the original matrix \mathbf{X} . Specifically, rank $(\Sigma_{\mathbf{X}}) = \operatorname{rank}(\mathbf{X})$ when the number of observations $n \ge p$ and the columns of \mathbf{X} are linearly independent. However, when n < p, the covariance matrix $\Sigma_{\mathbf{X}}$ will be rank-deficient, such that rank $(\Sigma_{\mathbf{X}}) < p$.

Proof Lemma 4

922 923

939 940

949 950

953 954 955

956 957 958 **Proof.** The entropy $H(\Sigma_{\mathbf{X}})$ of a set of singular values $\sigma_1, \sigma_2, \ldots, \sigma_D$ is given by the formula:

$$H(\sigma_1, \sigma_2, \dots, \sigma_D) = -\sum_{i=1}^D \sigma_i \log \sigma_i.$$
(31)

⁹⁴⁵ The trace of $\Sigma_{\mathbf{X}}$, Tr($\Sigma_{\mathbf{X}}$), is 1. Since entropy measures the uncertainty or disorder in a distribution, ⁹⁴⁶ we can establish certain bounds for the entropy based on the structure of the singular values.

First, we note that if the distribution is concentrated entirely at a single value (i.e., all but one of thesingular values are zero), then the entropy will be minimized at 0. Specifically:

$$H(1,0,\dots,0) = 0. \tag{32}$$

On the other hand, the entropy is maximized when the singular values are uniformly distributed. In
 the case of a uniform distribution over D singular values, we have:

$$\sigma_1 = \sigma_2 = \dots = \sigma_D = \frac{1}{D},\tag{33}$$

and the entropy in this case is:

$$H\left(\frac{1}{D}, \frac{1}{D}, \dots, \frac{1}{D}\right) = -D\left(\frac{1}{D}\log\frac{1}{D}\right) = \log D.$$
(34)

959 Thus, we have the inequality:

$$0 = H(1, 0, \dots, 0) \le H(\sigma_1, \sigma_2, \dots, \sigma_D) \le \log D.$$
(35)

The *effective rank* is defined as:

$$\operatorname{erank}(\mathbf{\Sigma}_{\mathbf{X}}) = \exp(H(\sigma_1, \sigma_2, \dots, \sigma_D)), \tag{36}$$

which quantifies the "effective" number of singular values that are significantly contributing to the rank of the matrix. Since $H(\sigma_1, \sigma_2, \dots, \sigma_D)$ is bounded by $\log D$, it follows that the effective rank is bounded by:

$$1 \le \operatorname{erank}(\boldsymbol{\Sigma}_{\mathbf{X}}) \le D. \tag{37}$$

Figure 26. Equality holds at the lower bound if and only if $(\sigma_1, \sigma_2, \dots, \sigma_D) = (1, 0, \dots, 0)$, that is, when all but one singular value is zero. In this case, the singular value vector is:

$$\sigma = (\|\sigma\|_1, 0, \dots, 0)^T,$$
(38)

960 961 962

963 964

972 where $\|\sigma\|_1 = 1$. Hence, erank $(\Sigma_X) = 1$. 973

974 Next, suppose that only k singular values of A are non-zero for some $k \in \{1, 2, ..., D\}$. In this 975 case, the rank of A is given by rank(A) = k, and the entropy only depends on the non-zero singular 976 values. Thus, we have:

$$H(\sigma_1, \sigma_2, \dots, \sigma_D) = H(\sigma_1, \sigma_2, \dots, \sigma_k), \tag{39}$$

where $\sigma_1, \sigma_2, \ldots, \sigma_k$ are the non-zero singular values. Since entropy is maximized when these non-zero singular values are uniformly distributed, we have:

$$H(\sigma_1, \sigma_2, \dots, \sigma_k) \le \log k. \tag{40}$$

981 Hence, the effective rank satisfies:

$$\operatorname{erank}(\mathbf{\Sigma}_{\mathbf{X}}) \le \operatorname{rank}(\mathbf{\Sigma}_{\mathbf{X}}) \le D, \tag{41}$$

with equality $\operatorname{erank}(\Sigma_{\mathbf{X}}) = \operatorname{rank}(\Sigma_{\mathbf{X}})$ if and only if the non-zero singular values are uniformly distributed, i.e.,

$$(\sigma_1, \dots, \sigma_k, \sigma_{k+1}, \dots, \sigma_D) = \left(\frac{1}{k}, \dots, \frac{1}{k}, 0, \dots, 0\right),$$
(42)

or equivalently:

977

979 980

982 983

984

985 986 987

988 989

990

991 992

993 994

$$\sigma = (\|\sigma\|_1/k, \dots, \|\sigma\|_1/k, 0, \dots, 0)^T.$$
(43)

In this case, the effective rank coincides with the actual rank of the matrix, since the singular values contribute equally to the rank.

D ABLATION STUDY

D.1 NUMBER OF HEAD GROUPS

	Llama2-7B	-chat-hf, KV	V size=384				
Group num	KV size in different groups	Qasper	HotpotQA	QMSum	SAMSum	Lee	Average
2 groups	32/736	18.23	30.96	19.82	40.05	57.13	33.24
3 groups	32/384/736	18.90	30.53	19.95	40.04	58.29	33.54
4 groups	32/266/502/736	19.29	30.48	20.10	41.03	59.37	34.05
5 groups	32/208/384/560/736	19.58	31.17	20.72	40.61	58.93	34.20
8 groups	32/132/232/332/436/536/636/736	19.34	31.04	20.16	40.92	59.48	34.19
2 groups	256/512	19.67	30.98	20.20	39.36	60.28	34.10
3 groups	256/384/512	19.45	31.29	20.24	39.63	59.63	34.05
4 groups	256/342/427/512	19.20	30.99	20.10	39.33	59.71	33.87
5 groups	256/320/384/448/512	19.71	30.95	20.22	39.60	59.99	34.09
8 groups	256/296/332/368/404/440/476/512	19.55	31.02	20.59	39.10	59.39	33.93

Table 6: Multiple group comparison

In this section, we analyze the impact of the number of groups on performance. As illustrated in the Table 6, when the KV size is set to 384 and the difference between the maximum and minimum KV sizes within each group is minimal, the number of groups has a small effect on overall performance, with the maximum observed variation being only 0.23%. However, when there is a significant disparity between the maximum and minimum KV sizes, increasing the number of groups tends to enhance performance, with a maximum observed improvement of 0.96%. This indicates that the number of groups is highly correlated with the distribution of KV sizes within groups, impacting the experimental results.

1007

1008

1018 D.2 TRUNCATION STRATEGY

In this section, we examine truncation strategies, with a focus on evaluating the effectiveness of elbow points. We conduct tests using various elbow points by selecting different top k eigenvalues and compared the results to cases where no elbow points are applied. As demonstrated in Table 7, the results demonstrate a 0.70% performance gap between the truncated and untruncated settings, highlighting the efficacy of our approach.

Llama-	2-7B-cha	t-hf, KV	size=384	
Top k Qasper	QMSum	SAMSur	n Lcc Average	
top 16 19.28	20.38	39.45	59.72 34.71	
top 32 19.34	20.51	39.35	59.93 34.78	
top 64 18.75	20.43	39.36	59.86 34.60	
top all 18.14	20.14	38.52	59.51 34.08	

Table 7: Truncation strategy

¹⁰¹⁷

1026 D.3 RANDOM PARTITION

1028 In this section, we evaluate the validity of our layer 1029 partitioning approach. For this analysis, Llama2-1030 7B-chat-hf is selected as our base model, where the KV size per layer is configured to 64. the attention 1031 heads are divided into two distinct groups: one group 1032 with a KV size of 96 and another with a KV size of 1033 32. As demonstrated in Table 8, the performance 1034 gains achieve through our method are substantial, 1035 highlighting the effectiveness of our partitioning ap-1036 proach. 1037

	Ours-group	Random-group
Qasper	15.40	11.70
Musique	6.96	4.47
GovReport	14.88	7.31
TREC	55.50	32.50
PCount	5.00	3.97
Lcc	50.00	32.50
Avg.	24.62	15.49

Table 8: Random groups condition

D.4 COMPRESSION RATIO ALLOCATION BETWEEN HEAD GROUPS

1040 In this section we discuss the allocation of compress-1041 ibility between groups. Using the same experimen-1042 tal setup as the previous section, we only exchange 1043 the KV size between the two groups, and find that 1044 the text generation exhibits abnormal changes. As 1045 demonstrated in Table 9, the results in the table in-1046 dicate that text generation exhibited abnormalities in several datasets, with the overall average accuracy 1047 decreasing to 5.89%. This suggests that assigning 1048 smaller KV sizes to lower-rank groups is effective. 1049 Conversely, allocating smaller KV sizes to higher-1050 rank groups leads to significant information loss. 1051

	Ours-group	Random-group
Qasper	15.40	2.32
Musique	6.96	0.13
GovReport	14.88	1.01
TREC	55.50	19.00
PCount	5.00	0.33
Lcc	50.00	12.50
Avg.	24.62	5.89

Table 9. Complessionity distribution	Table 9:	Compressibility	v distribution
--------------------------------------	----------	-----------------	----------------

D.5 MATRIX ENTROPY AND VARIANCE

	Single	e-Docume	nt QA	Mult	i-Docume	nt QA	Su	mmariza	tion	Few	-shot Lea	rning	Synt	hetic	Co	ode	
Methods	NUNQA	Qasper	MFen	HotpotQ!	2WikiMQ	Musique	GovRepor	0MSum	MultiNews	TREC	TriviaQA	SAMSum	PCount	pre	Lee	RB.P	Avg.
Variance KV (384)	16.75	18.15	32.09	32.42	27.29	8.50	19.46	20.42	22.94	62.50	84.65	38.64	5.50	12.00	58.59	52.98	32.06
Uncomp (384)	17.33	19.34	34.16	31.54	28.23	10.04	20.38	20.51	23.33	63.00	84.11	39.35	5.50	9.50	59.93	54.87	32.57
Variance KV (64)	8.75	13.58	12.24	20.27	13.38	3.89	8.76	15.73	13.98	29.50	56.22	30.35	5.00	5.45	37.10	30.47	19.04
Uncomp (64)	14.05	15.40	25.56	26.28	21.96	6.96	14.88	18.83	17.58	55.50	81.61	34.74	5.00	5.00	50.00	45.55	27.43

Table 10: Comparison of entropy and variance of truncated matrices

In this section we discuss the grouping policy. We provide the compression rate estimates based on the variance of attention scores in Table 10, evaluated under two KV Cache sizes, 384 and 64. The results clearly highlight our advantages, especially under the budget of 64. This suggests that solely relying on compression rate estimation based on attention is unreasonable, as attention itself is subject to biases such as the attention sink(Xiao et al., 2023) and recency bias(Peysakhovich & Lerer, 2023). It is necessary to introduce additional metrics to measure unbiased compression estimation methods.

1071 D.6 ATTENTION SCORE MATRIX SELECTION FOR HIDDEN STATES



Table 11: Using the attention of the current layer and the attention of the previous layer on Long-Bench

1052 1053 1054

1055 1056 1057

1038

1039

1080 We designed an experiment to demonstrate that using the attention scores from the previous layer to predict the compression strategy for the current layer is reasonable, as shown in the Table11. 1082 The performance difference between the two methods is minimal, but using the current layer for prediction results in inference being twice as slow and more computationally expensive. Therefore, 1084 Our method remains efficient while achieving good performance.

E THROUGHPUT ANALYSIS

1087 1088

108 109

1104 1105

batch_size	C	Ours-group-stage		Ours-group		FullKV
	ms/token	max memory used(MB)	ms/token	max memory used(MB)	ms/token	max memory used(MB)
1	28.055	23492	28.536	23080	25.691	24690
4	7.910	37526	8.504	37516	13.806	44220
8	4.822	59014	5.436	59036	11.823	72444
10	5.340	69802	5.887	69780	-	Out-of-Memory
12	3.994	80514	4.567	80522	-	Out-of-Memory
		Llama2-7B-chat-hf	f, KV Size = 3	84, Prompt+Generate is 403	32+64	
batch size	C	Ours-group-stage		Ours-group		FullKV
	ms/token	max memory used(MB)	ms/token	max memory used(MB)	ms/token	max memory used(MB
1	34.782	24298	39.231	24312	36.596	24240
4	13.671	41180	18.458	41170	23.952	41146
8	10.186	66560	15.074	66580	21.944	66532
0	0.007	70108	14 603	79206	21.482	79168
10	9.907	/9198	1 11000			

Table 12: Throughput analysis

1106 To ensure the accuracy of performance analysis, we conduct experiments on a NVIDIA A100 80G 1107 GPU. We randomly sample 96 data points from the Wikitext-2 dataset, with strict control over the 1108 token lengths for both the prompt and generation phases. Detailed analyses of memory usage and throughput are provided in the Table 12. From the table, we can see that in the long-prompt, short-1109 generate scenario, our method achieves up to 2.96x throughput. 1110

1111 In addition to the configurations outlined in the table, we conduct experiments under the 2048+8096 1112 setting too. The results demonstrate that our method supports a batch size of 32, whereas FullKV is 1113 limited to a batch size of 6. Notably, in this scenario, FullKV requires 15.67ms per token generation, 1114 while our approach reduces this to only 2.45ms. Our methods leads to a throughput that is up to 6.4 1115 times that of FullKV.

1116 In this experiment, for the Ours-group-stage method, S_{min} was set to 512, and the layers were 1117 divided into five groups: layers 0 to 1, layers 2 to 14, layers 15 to 25, layers 26 to 30, and layer 31. 1118 The reserved sizes for these groups were set to 4096, 3200, 2304, 1408, and 512, respectively. The 1119 attention heads were divided into two groups: one group with a KV size of 512, and the other with 1120 a KV size of 256. The final KV cache length retained by each layer was 384.

1121

1122 F SUPPLEMENTARY DATASET COMPARISO 1123

1124 F.1 RULER 1125

1126 RULER(Hsieh et al., 2024) is a novel synthetic benchmark designed to comprehensively evaluate the 1127 capabilities of long-context language models (LMs). Unlike the traditional Needle-in-a-Haystack 1128 (NIAH) test, which focuses solely on retrieval tasks, RULER provides flexible configurations to 1129 support customized sequence lengths and task complexities. It extends the vanilla NIAH test by introducing diverse variations in the types and quantities of "needles" and adding new task categories, 1130 such as multi-hop tracing and aggregation, to assess capabilities beyond simple context search. Re-1131 sults are showed at Table 13, where the Llama-3-8B-Instruct model is used, and other Settings are 1132 consistent with the previous section A.3. The experiments are implemented on a single A100 80G 1133 GPU.

1134	RULER(8k)	niah_single_1	niah_single_2	niah_single_3	niah_multikey_1	niah_multikey_2	niah_multikey_3	niah_multivalue	niah_multique	ery vt	cwe	fwe	qa_1	qa_2	average
1135	FullKV 8k	100.00	100.00	100.00	98.80	88.20	97.60	95.40	99.40	98.60	97.74	83.93	67.40	50.80	90.61
1100	uncomp	100.00	99.80	3.80	99.40	72.80	0.00	81.55	74.75	93.88	20.78	53.93	64.40	49.60	62.67
1136	snapkv pyramidkv	100.00 100.00	99.80 98.40	1.60 0.00	98.80 98.40	72.60 66.00	0.00 0.00	78.00 63.60	71.05 42.55	94.36 81.96	21.16 8.16	49.60 41.00	64.80 65.00	50.00 48.60	61.67 54.90
1137	chai h2o	35.00 2.80	22.80 3.80	23.40 5.80	22.00 5.40	3.80 4.00	0.60 3.00	23.40 4.60	23.80 5.20	11.24 4.60	0.66 34.60	7.00 85.87	25.80 42.00	21.80 39.60	17.02 18.56
1138	RULER(4k)	niah_single_1	niah_single_2	niah_single_3	niah_multikey_1	niah_multikey_2	niah_multikey_3	niah_multivalue	niah_multique	ery vt	cwe	fwe	qa_1	qa_2	average
1120	FullKV 4k	100.00	100.00	100.00	99.40	100.00	98.80	99.15	99.85	99.72	99.80	94.20	81.40	58.00	94.64
1139	uncomp	100.00	99.80	18.80	95.60	98.80	0.00	93.00	93.00	95.84	56.06	78.07	81.40	57.20	74.43
1140	snapkv pyranikv	100.00	99.60 99.40	8.00 0.60	99.40 98.60	97.40 91.80	0.00	88.30 65.85	87.70 49.40	95.80 78.84	52.86 10.50	76.33 66.20	81.40 81.00	56.60 55.40	61.35
1141	chai h2o	44.40 10.40	54.00 12.60	46.60 13.00	36.60 14.60	14.00 9.20	7.20 7.00	53.40 12.25	52.60 13.15	17.16 8.64	13.00 82.94	25.60 93.00	59.40 81.80	30.20 40.00	34.94 30.66

Table 13: Performance comparison of methods on RULER benchmark across different context lengths. The first section shows results for an 8k context, while the second section highlights 4k context performance.

F.2 INFINITEBENCH

Method	En.Sum	En.QA	En.MC	En.Dia	Zh.QA	Code.Debug	Code.Run	Math.Calc	Math.Find	Retrieve.PassKey	Retrieve.Number	Retrieve.KV	Average
FullKV	12.55	0.27	42.79	1.00	4.04	22.34	0.00	0.00	38.57	6.27	6.44	4.80	14.38
uncomp	11.74	0.23	44.98	3.80	3.00	21.57	0.00	0.00	38.57	6.27	6.44	0.00	14.77
snapkv	11.59	0.28	42.36	1.00	4.01	21.83	0.00	0.00	38.29	6.27	6.61	0.00	14.22
pyramidkv	11.34	0.23	40.61	2.50	4.03	22.08	0.00	0.00	38.57	6.27	6.78	0.00	14.26
chai	9.69	0.37	34.06	8.00	3.26	24.97	0.00	0.00	27.43	4.58	5.93	1.20	12.79
h2o	10.99	0.18	44.98	3.50	3.98	22.08	0.00	0.00	37.71	1.69	1.69	0.00	14.24

Table 14: Performance comparison of various methods on InfiniteBench across different tasks, in-cluding summarization, QA, mathematical reasoning, and code-related benchmarks. The "Average" column represents the overall average performance.

InfiniteBench(Zhang et al., 2024b) is a state-of-the-art benchmark designed to evaluate language models' ability to process, understand, and reason over extremely long contexts exceeding 100k tokens. By pushing context lengths 10 times beyond traditional datasets, InfiniteBench aims to advance applications of LLMs and enable high-level interactions in scenarios requiring extensive context comprehension. Results are showed at Table 14, where the Llama-3-8B-Instruct model is used, and other Settings are consistent with the previous section A.3.

G SUPPLEMENTARY METHOD COMPARISON

	Single-Do	ocument QA	Multi-Document QA		Summarization		Few-shot Learning			Synthetic		Code	
Methods	NtrvQA Qas	per MF-en	HotpotQA 2WikiMC	Musique	jovReport OMS	um MultiNet	NS TREC	riviaQA	SAMSum	PCount	PRe	Lec	RB-P A
FullKV	19.34 18.	89 35.19	30.66 28.26	10.05	25.27 20.2	2 25.86	63.00	83.62	41.70	5.00	10.00	61.40	55.41 33
StreamLLM(Xiao et al., 2023)	13.71 13.	68 19.40	26.97 28.03	6.78	15.13 18.8	7 18.27	46.50	80.02	40.85	4.50	5.00	56.84	51.56 27
Double-Sparse+key(Yang et al., 2024)	17.27 19.	85 32.30	29.45 28.54	9.90	20.88 19.8	4 25.38	61.50	83.48	40.56	5.25	8.00	52.27	51.97 31
Double-Sparse+query(Yang et al., 2024)	17.99 19.1	27 31.93	30.83 27.91	9.25	23.68 20.5	4 26.10	62.00	84.60	41.75	4.75	8.00	58.27	55.49 32
Quest(Tang et al., 2024)	17.31 19.	55 32.18	30.25 27.20	9.48	22.82 19.2	5 25.99	62.50	83.26	40.37	5.00	5.25	58.81	53.24 32
UNComp+key	17.04 19.	11 34.03	30.73 28.73	9.61	20.38 20.3	4 23.48	63.00	84.14	38.63	5.50	10.00	59.89	53.93 32
UNComp+query	17.33 19.	34 34.16	31.54 28.23	10.04	20.38 20.5	1 23.33	63.00	84.11	39.35	5.50	9.50	59.93	54.87 32

Table 15: The supplementary baseline is uniformly compared with a kv cache size of 384. The base model is Llama2-7B-chat-hf. "(Method) + key" uses the features of the key matrix for model param-eter pruning, while "(method) + query" uses the features of the query matrix for model parameter pruning. We conducted experiments using the default hyperparameters from the open-source code repository.

Double-sparse and our method achieved the best performance when using query-based sparse prun-ing, surpassing our method by 0.08%. However, when using the key matrix as the criterion for sparse pruning, its performance was worse than ours.

PYRAMIDKV WITH UNCOMP Η

190										
191		Single-Document QA		Multi-Document QA		Summarizatio	n Few-shot	Few-shot Learning		Code
1192	Methods	NITY QA Dasp	er MF-en	aotpotQA	1A Musique	ovReport ONSum	News TREC Trivie	QA SAMSum	Count PRe	Lee RB-P Avg.
1193	PyramidKV±Uncomp Group32 head	× 42 × 18 21 18 5	9 34 22	30.66 28.20	9.10	20.04.20.19.22	84 63 00 84 3	9 39 46	5 50 5 00	58 89 52 86 31 95
1194	PyramidKV+Uncomp Group8 heads	17.74 18.0	0 34.48	31.26 28.21	9.20	20.04 20.19 22 20.41 20.38 23	.23 63.00 84.2	21 40.30	5.50 8.50	59.38 53.65 32.34
1195	PyramidKV+Uncomp Group3 heads PyramidKV+Uncomp Group2 heads	17.32 18.2	4 33.78 3 33.25	31.60 27.50 30.70 27.62	9.05	20.03 20.23 22 20.19 20.84 22	.97 63.00 83.9 .79 63.00 84.0)3 38.35	5.50 10.50 5.50 9.50	59.16 53.18 32.22 59.23 53.10 32.02
1196	PyramidKV	16.86 18.2	6 31.01	31.59 27.93	8.69	19.88 20.15 22	.43 62.00 83.8	36 38.98	5.50 10.00	58.94 52.80 31.81

Table 16: The impact of PyramidKV's dynamic sparsity ratio when applied in UNComp. The comparison of dynamic sparsity ratios between this method and PyramidKV.

Based on PyramidKV+Uncomp Group8 heads, which applies PyramidKV using our method of setting different compression rates for different heads, our method can bring greater improvements to PyramidKV if an appropriate number of groups is chosen. This is because different heads can be categorized as streaming heads and retrieval heads (Xiao et al., 2024). It is reasonable for retrieval heads to compress fewer tokens with their groups. Setting finer-grained groups for compression might harm the performance of retrieval heads.

Ι ANALYSIS ABOUT MATRIX ENTROPY OF HIDDEN STATES



Figure 6: Matrix entropy of hidden states across different layers of Wikitext2 datasets

Figure 6 shows the matrix entropy trend of 6 samples of the Wikitext2 data set. It can be seen that the matrix entropy of hidden states increases layer by layer, which means that the token information becomes more and more abundant as the number of layers increases. This provides strong support to decrease the number of tokens retained by hidden states layer by layer.