CLUSTERGEN: TOKEN GENERATION IN SUBLINEAR TIME AND MEMORY WITH CLUSTERING KV CACHE

Amir Zandieh*
Google Research
zandieh@google.com

Insu Han*
KAIST
insu.han@kaist.ac.kr

Vahab Mirrokni
Google Research
mirrokni@google.com

Amin Karbasi
Yale University
amin.karbasi@yale.edu

ABSTRACT

Despite the significant success of large language models (LLMs), their extensive memory requirements pose challenges for deploying them in long-context token generation. The substantial memory footprint of LLM decoders arises from the necessity to store all previous tokens in the attention module, a requirement imposed by key-value (KV) caching. In this work, our focus is on developing an efficient compression technique for the KV cache. Empirical evidence indicates a significant clustering tendency within key embeddings in the attention module. Building on this key insight, we have devised a novel caching method with sublinear complexity, employing online clustering on key tokens and online ℓ_2 sampling on values. The result is a provably accurate and efficient attention decoding algorithm, termed CLUSTERGEN. Not only does this algorithm ensure a sublinear memory footprint and sublinear time complexity, but we also establish a tight error bound for our approach. Empirical evaluations on long-context question-answering tasks demonstrate that CLUSTERGEN significantly outperforms existing and state-of-the-art KV cache compression methods in terms of performance and efficiency.

1 INTRODUCTION

Large Language Models (LLMs) (Achiam et al., 2023; Touvron et al., 2023) play a crucial role in various natural language processing applications, including dialog systems (Taori et al., 2023; Chiang et al., 2023), coding assistance (Chen et al., 2021; Roziere et al., 2023), and image/video generations from text (Radford et al., 2021; Ho et al., 2022). All of these models rely on the transformer architecture, with the attention mechanism serving as the key component.

To fully harness the capabilities of LLMs, they must demonstrate both efficiency and accuracy in generating long sequences. In practical applications, deploying LLMs to generate tokens in an autoregressive manner involves a sequential decoding process, where attention is dynamically applied to each newly generated token. This process effectively constructs the output sequence in a streaming manner, one token at a time. Therefore, as the sequence grows, the model has to produce contextually relevant and coherent content.

A common method for autoregressive attention decoding involves the use of key-value (KV) caching, where key and value pairs from *all* preceding tokens are cached and reused to prevent redundant computations. However, this approach faces memory constraints, particularly when handling long sequences. In particular, the memory requirements and runtime for generating each new token increase linearly with context size, posing a significant challenge for efficient processing of extensive sequences. This linear scaling directly impedes practical applicability in real-world scenarios, such as chat systems, where large contexts are often encountered.

*Equal Contribution

We propose a novel approach designed to significantly reduce the memory and runtime complexity of token generation, moving from conventional linear growth to sublinear scale.

1.1 Streaming Attention Problem

Suppose a sequence of a vector pairs $(\boldsymbol{q}_1, \boldsymbol{k}_1, \boldsymbol{v}_1), (\boldsymbol{q}_2, \boldsymbol{k}_2, \boldsymbol{v}_2), \ldots$ is streamed where $\boldsymbol{q}_i, \boldsymbol{k}_i, \boldsymbol{v}_i \in \mathbb{R}^d$ are called by query, key and value, respectively. The objective of streaming attention problem is to compute the following:

$$\texttt{softmax}(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n = \frac{\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n}{\sum_{i \in [n]} \exp(\langle \boldsymbol{k}_i, \boldsymbol{q}_n \rangle)}, \tag{1}$$

where $\boldsymbol{K}_n := [\boldsymbol{k}_1, \ldots, \boldsymbol{k}_n]^\top$ and $\boldsymbol{V}_n := [\boldsymbol{v}_1, \ldots, \boldsymbol{v}_n]^\top \in \mathbb{R}^{n \times d}$ are matrices defined by stacking the keys and values in their respective rows. The output in Eq. (1) is often used for predicting the next $(n+1)$-th token and it is applied to a transformer model and introduces a new stream pair $(\boldsymbol{q}_{n+1}, \boldsymbol{k}_{n+1}, \boldsymbol{v}_{n+1})$ is generated. However, storing these values and keys requires $O(nd)$ memory, posing a significant space complexity challenge for long-context models with large n. In this work, we propose a novel approach designed to significantly reduce the memory and runtime complexity of token generation, moving from conventional linear growth to sublinear scale.

2 ClusterGen: Sublinear Time and Memory Algorithm

To compute the attention output in Eq. (1) we need to calculate two terms; (i) the matrix-vector product between $\boldsymbol{V}_n$ and $\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)$ and (ii) the partition function $\sum_{i \in [n]} \exp(\langle \boldsymbol{k}_i, \boldsymbol{q}_n \rangle)$. We will briefly give a high-level approach that approximates each.

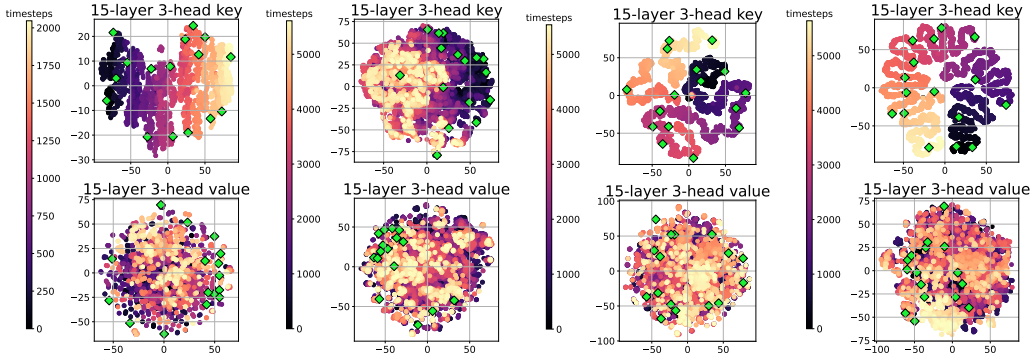
Matrix Vector Product. To efficiently approximate the matrix-vector product $\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n$, we make use of the row norm sampling approach (Drineas & Kannan, 2001; Cohen et al., 2016). Specifically, when multiplying two matrices $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{B} \in \mathbb{R}^{n \times p}$, we randomly sample an i.i.d. index $i \in [n]$ with probability proportional to the ℓ_2-norm of the i-th row in $\boldsymbol{B}$. Then, we estimate $\boldsymbol{A} \cdot \boldsymbol{B}$ by the average of the product between i-th column in $\boldsymbol{A}$ and i-th row in $\boldsymbol{B}$. With this approximation, we need only $O(\varepsilon^{-2} d \log n)$ samples to guarantee an ε multiplicative error in spectral norm for $\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n$. Luckily, it can be implemented in a streaming setting through a variant of reservoir sampling (Vitter, 1985).

More precisely, we maintain and update a list of s key-value pairs denoted by $\mathcal{M}$. Initially, $\mathcal{M}$ is filled with `null` values. After processing the first token tuple $(\boldsymbol{q}_1, \boldsymbol{k}_1, \boldsymbol{v}_1)$, this list is populated with s copies of the first key and value $(\boldsymbol{k}_1, \boldsymbol{v}_1)$. Then, we perform a variant of reservoir sampling upon observing any new token in the stream. At any iteration n of the stream, $\mathcal{M}$ is ensured to contain s i.i.d. samples chosen at random from $(\boldsymbol{k}_1, \boldsymbol{v}_1), \ldots, (\boldsymbol{k}_n, \boldsymbol{v}_n)$ with probabilities proportional to $\|\boldsymbol{k}_i\|_2^2$. In other words, for each $j \in [s]$ and $i \in [n]$ it holds that $\Pr[\mathcal{M}(j) = (\boldsymbol{k}_i, \boldsymbol{v}_i)] = \frac{\|\boldsymbol{v}_i\|_2^2}{\sum_{l \in [n]} \|\boldsymbol{v}_l\|_2^2}$.

Partition Function. For the approximation of the partition function $\sum_{i \in [n]} \exp(\langle \boldsymbol{k}_i, \boldsymbol{q}_n \rangle)$, we construct a data structure (DS) that organizes the keys in the stream into a small number of clusters. Instead of keeping all keys in each cluster, we maintain only a random subset of t samples from each cluster. Such sampled keys in clusters can be used to estimate the partition function for any query vector. A key challenge is to guarantee runtime and memory in sublinear in length of the stream. To this end, we assume that the keys can be covered by a sublinear number of bounded diameter clusters which can be defined as below.

Definition 2.1 ((m, δ)-clusterability)**.** *For a positive integer m and a real-valued $\delta > 0$, a dataset of points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots \boldsymbol{x}_n \in \mathbb{R}^d$ is considered (m, δ)-clusterable if there exists a size-m partition $\mathcal{C}_1, \mathcal{C}_2, \ldots \mathcal{C}_m \subseteq \{\boldsymbol{x}_i\}_{i=1}^n$ satisfying that $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$ for every $i \neq j$ and $\bigcup_{j=1}^m \mathcal{C}_j = \{\boldsymbol{x}_i\}_{i=1}^n$ and for every $j \in [m]$ and every distinct pair $\boldsymbol{y}, \boldsymbol{z} \in \mathcal{C}_j$, $\|\boldsymbol{y} - \boldsymbol{z}\|_2 \leq \delta$.*

With the clusterability assumption, we can construct the DS for partition function as follows. First initialize the data structure $\mathcal{D}$ by an empty set. As new tokens in the stream are processed, new clusters get added to this set. Each cluster is characterized by a representative point, which is the



(a) `OPT-6.7B` (b) `MPT-7B` (c) `Llama-3.1-8B` (d) `Gemma-2-9B`

Figure 1: A t-SNE plot of cached keys (first row) and values (second row) embeddings from 4 open-source models; (a) `OPT-6.7B`, (b) `MPT-7B`, (c) `Llama-3.1-8B` and (d) `Gemma-2-9B` using TriviaQA dataset. Key embeddings are more clusterable than value ones. The green dots represent the centers from the greedy k-center algorithm (Dyer & Frieze, 1985) where k=16.

first key assigned to that cluster by our algorithm. Throughout stream processing, we compute the distance between the new key token and each existing cluster. Here the distance to an existing cluster is defined as the distance to the aforementioned representative of the cluster. If there is a cluster whose distance is less than δ, then the token is assigned to the nearest cluster, and we update our random samples of keys from this cluster using reservoir sampling. If the distance from all existing clusters is more than δ, we introduce a new cluster in $\mathcal{D}$, and the new key becomes the representative of this new cluster. At any point in the stream, this algorithm identifies at most m clusters if the keys so far are (m, δ)-clusterable. If m grows sublinearly in the stream length n, the memory and update time of our algorithm will be sublinear as well.

End-to-end Guarantee. Putting altogheter we are able to analyze the end-to-end performance. Our main result is as follows:

Theorem 2.2. *For any $\delta, r, \varepsilon > 0$ and any sequence of $(\boldsymbol{q}_1, \boldsymbol{k}_1, \boldsymbol{v}_1), \ldots, (\boldsymbol{q}_n, \boldsymbol{k}_n, \boldsymbol{v}_n)$ where $\boldsymbol{q}_i, \boldsymbol{k}_i, \boldsymbol{v}_i \in \mathbb{R}^d$ for all $i \in [n]$, assume that $\|\boldsymbol{q}_n\|_2 \leq r$. If we choose $t = \Omega\left(\varepsilon^{-2} \cdot e^{2\delta \cdot r} \cdot \log n\right)$ and $s = \Omega(\varepsilon^{-2} \cdot d)$, then with probability at least 0.99 we can compute a vector $\boldsymbol{z}_n \in \mathbb{R}^d$ that satisfies*

$$\|\boldsymbol{z}_n - \mathrm{Attn}(\boldsymbol{q}_n, \boldsymbol{K}_n, \boldsymbol{V}_n)\|_2 \leq \varepsilon \, \|\mathtt{softmax}(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)\|_2 \, \|\boldsymbol{V}_n\|_{\mathrm{op}} . \tag{2}$$

Furthermore, if the keys $\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots \boldsymbol{k}_n$ are (m, δ)-clusterable as per Theorem B.1, then both the total memory of the algorithm and its runtime during the n-th iteration is bounded by $O(d \cdot (mt + s))$.

Theorem B.4 demonstrates that if the keys can be clustered into some sublinear number $m = n^{1-\Omega(1)}$ of clusters with diameters at most δ, and the queries have bounded ℓ_2-norms of at most r such that $\delta r = o(\log n)$, then both memory and runtime can be $O\left(\varepsilon^{-2} \cdot mdn^{o(1)}\right) = O\left(\varepsilon^{-2} \cdot dn^{1-\Omega(1)}\right)$. A full proof of the theorem can be found in the supplementary material.

3 Ablation Study: Clusterability on Key and Value Embeddings

We demonstrate the clusterability of KV cache from long-range tokens. We collect key and value embeddings from 4 popular open-source language models; `OPT-6.7B`, `MPT-7B`, `Llama-3.1-8B` and `Gemma-2-9B`, where each adopts different positional encoding methods across absolute positional encoding (AbsPE), Attention with Linear Biases (ALiBi) (Press et al., 2021) and Rotational Positional Encodding (RoPE) (Su et al., 2024). We use prompts from TriviaQA dataset in LongBench (Li et al., 2023), and the length of input tokens is approximately 5,600 tokens, except for `OPT-6.7B`, which has a maximum sequence length of 2048. We then visualize the cached embeddings (at randomly selected layer/head) using t-SNE (Van der Maaten & Hinton, 2008), identifying cluster center points through the greedy k-center algorithm (Dyer & Frieze, 1985). The results are shown in Fig. 1.

	$n = 5$k		$n = 7$k		$n = 9$k	
Algorithm	Cache Size (GB)	Accuracy	Cache Size (GB)	Accuracy	Cache Size (GB)	Accuracy
Exact	2.351	0.98	3.488	1.0	4.613	0.68
Sink (Xiao et al., 2023)	1.511 (35% ↓)	0.56	2.012 (42% ↓)	0.56	2.262 (50% ↓)	0.38
H2O (Zhang et al., 2023)	1.511 (35% ↓)	0.66	2.012 (42% ↓)	0.58	2.262 (50% ↓)	0.38
CLUSTERGEN (our)	1.512 (35% ↓)	**0.86**	2.012 (42% ↓)	**0.66**	2.262 (50% ↓)	**0.44**

Table 1: Results on accuracy of line retrieval from LongEval (Li et al., 2023) dataset with context length ranging 5k to 9k. Under the sublinear cache budgets in terms of the sequence length, the proposed approach based on greedy k-center outperforms other methods over all sequence lengths.

Algorithm	Single-QA	Multi-QA	Summurization	Fewshot	Code
Exact	70.05	56.00	56.67	190.44	108.41
Sink (Xiao et al., 2023)	54.19	51.91	53.47	184.94	96.15
CLUSTERGEN (our)	55.96	48.52	47.24	181.57	96.18

Table 2: Results on generation tasks for long-range prompts from LongBench (Li et al., 2023) datasets. The prompt length is at most 20k and the cache size budget is set to 2k, i.e., $\ell = k = 1{,}024$.

Observe that the key embeddings (first rows in Fig. 1) exhibit a higher degree of clusterability compared to value embeddings. Furthermore, we note that the cluster centers (indicated by green dots) corresponding to the key embeddings are evenly distributed across the entire embedding space. In particular, the key embeddings demonstrate significant dispersion across different time steps, and their cluster centers are distributed over the entire embedding space. Similar results are observed across various layers and heads and can be founded in supplementary material.

4 EXPERIMENTS

Line Retrieval. We first evaluate our proposed algorithm on long-context line retrieval task in LongEval (Li et al., 2023) benchmark. The task involves long-context line retrieval from extensive documents, each comprising multiple lines, complete with line numbers and topics. The objective is to precisely retrieve a specified number of lines corresponding to a target topic. We vary the number of lines, representing the number of targets, to 200, 300, and 400 and they correspond to sequence lengths of n =5,000, 7,000, and 9,000, respectively. Each dataset contains 50 distinct questions, and we systematically extract the number from the generated answers and compute accuracies. The answers are generated employing the `longchat-7B` model[1], which is a fine-tuned version of the Llama-2-7B model with long-range context length.

We compare our method to two KV cache compression algorithms; H2O (Zhang et al., 2023) and AttentionSink (Xiao et al., 2023). To leverage this insight, we integrate it with our clustering approach; retain the most recent ℓ embeddings, in addition to k centers selected from the remaining tokens. We apply the greedy k-center clustering algorithm once to compress the entire KV caches. To make comparisons fair, we set cache memory budgets of all algorithms identical (i.e., $\ell + k$) We set the compression ratio $(\ell + k)/n$ to fixed number, e.g., 0.35 for $n = 5$k, and report the highest accuracy among all combinations of (r, k) where $r \in \{2048, 3072\}$ as long as r does not exceed the compressed length.

The results are reported in Table 1. We observe that our clustering-based method consistently outperforms other algorithms across all sequence lengths. For instance, we achieve an accuracy of 44% while utilizing only half of the cached KV embeddings with a length of 9k tokens, whereas both H2O and AttentionSink can achieve accuracies 10% lower. This finding suggests that maintaining the embedding information holds greater significance in sustaining the performance of LLMs compared to attention scores and positional information.

[1] `https://huggingface.co/lmsys/longchat-7b-v1.5-32k`

Text Generation on Long-range Inputs. We evaluate our method on various tasks from LongBench (Li et al., 2023) datasets including summarization, single/multi-document question-answering, few-shot learning, and code completion. Similar to the above we choose `longchat-7B` model and apply AttentionSink and CLUSTERGEN to the token generation process. The generated texts are evaluated using metrics from the original code Li et al. (2023). We set the maximum input length to 20,000 for all datasets and truncate the middle prompts when it overflows (i.e., first and last 10,000 tokens are appended). We fix hyperparameters ℓ, r to $1{,}024$ for all datasets and both cache methods. The results are summarized in Table 1. As a result, our algorithm shows better performance scores on single-document QA and code completion tasks.

REFERENCES

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.

Josh Alman and Zhao Song. Fast attention requires bounded entries. *Neural Information Processing Systems (NeurIPS)*, 2023.

Jimmy Lei Ba. Layer normalization. *arXiv preprint arXiv:1607.06450*, 2016.

Mark Chen, Jerry Tworek, Heewoo Jun, Qiming Yuan, Henrique Ponde de Oliveira Pinto, Jared Kaplan, Harri Edwards, Yuri Burda, Nicholas Joseph, Greg Brockman, et al. Evaluating large language models trained on code. *arXiv preprint arXiv:2107.03374*, 2021.

Wei-Lin Chiang, Zhuohan Li, Zi Lin, Ying Sheng, Zhanghao Wu, Hao Zhang, Lianmin Zheng, Siyuan Zhuang, Yonghao Zhuang, Joseph E Gonzalez, et al. Vicuna: An open-source chatbot impressing gpt-4 with 90%* chatgpt quality. 2023. URL `https://vicuna.lmsys.org`.

Michael B Cohen, Jelani Nelson, and David P Woodruff. Optimal Approximate Matrix Product in Terms of Stable Rank. In *International Colloquium on Automata, Languages, and Programming (ICALP)*, 2016.

Petros Drineas and Ravi Kannan. Fast Monte-Carlo algorithms for approximate matrix multiplication. In *Foundations of Computer Science (FOCS)*, 2001.

Martin E Dyer and Alan M Frieze. A simple heuristic for the p-centre problem. *Operations Research Letters*, 1985.

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.

Jonathan Ho, William Chan, Chitwan Saharia, Jay Whang, Ruiqi Gao, Alexey Gritsenko, Diederik P Kingma, Ben Poole, Mohammad Norouzi, David J Fleet, et al. Imagen video: High definition video generation with diffusion models. *arXiv preprint arXiv:2210.02303*, 2022.

Ke Hong, Guohao Dai, Jiaming Xu, Qiuli Mao, Xiuhong Li, Jun Liu, Kangdi Chen, Hanyu Dong, and Yu Wang. Flashdecoding++: Faster large language model inference on gpus. *arXiv preprint arXiv:2311.01282*, 2023.

Dacheng Li, Rulin Shao, Anze Xie, Ying Sheng, Lianmin Zheng, Joseph Gonzalez, Ion Stoica, Xuezhe Ma, and Hao Zhang. How Long Can Context Length of Open-Source LLMs truly Promise? In *NeurIPS 2023 Workshop on Instruction Tuning and Instruction Following*, 2023.

Zichang Liu, Aditya Desai, Fangshuo Liao, Weitao Wang, Victor Xie, Zhaozhuo Xu, Anastasios Kyrillidis, and Anshumali Shrivastava. Scissorhands: Exploiting the Persistence of Importance Hypothesis for LLM KV Cache Compression at Test Time. *Neural Information Processing Systems (NeurIPS)*, 2023a.

Zichang Liu, Jue Wang, Tri Dao, Tianyi Zhou, Binhang Yuan, Zhao Song, Anshumali Shrivastava, Ce Zhang, Yuandong Tian, Christopher Re, et al. Deja vu: Contextual sparsity for efficient llms at inference time. In *International Conference on Machine Learning (ICML)*, 2023b.

Colin McDiarmid. Concentration. In *Probabilistic methods for algorithmic discrete mathematics*. Springer, 1998.

Ofir Press, Noah A Smith, and Mike Lewis. Train short, test long: Attention with linear biases enables input length extrapolation. *arXiv preprint arXiv:2108.12409*, 2021.

Alec Radford, Jong Wook Kim, Chris Hallacy, Aditya Ramesh, Gabriel Goh, Sandhini Agarwal, Girish Sastry, Amanda Askell, Pamela Mishkin, Jack Clark, et al. Learning transferable visual models from natural language supervision. In *International Conference on Machine Learning (ICML)*, 2021.

Baptiste Roziere, Jonas Gehring, Fabian Gloeckle, Sten Sootla, Itai Gat, Xiaoqing Ellen Tan, Yossi Adi, Jingyu Liu, Tal Remez, Jérémy Rapin, et al. Code llama: Open foundation models for code. *arXiv preprint arXiv:2308.12950*, 2023.

Tamas Sarlos, Xingyou Song, David Woodruff, and Qiuyi Zhang. Hardness of low rank approximation of entrywise transformed matrix products. In *Thirty-seventh Conference on Neural Information Processing Systems*, 2023.

Ying Sheng, Lianmin Zheng, Binhang Yuan, Zhuohan Li, Max Ryabinin, Beidi Chen, Percy Liang, Christopher Ré, Ion Stoica, and Ce Zhang. Flexgen: High-throughput generative inference of large language models with a single gpu. In *International Conference on Machine Learning (ICML)*, 2023.

Jianlin Su, Murtadha Ahmed, Yu Lu, Shengfeng Pan, Wen Bo, and Yunfeng Liu. Roformer: Enhanced transformer with rotary position embedding. *Neurocomputing*, 2024.

Rohan Taori, Ishaan Gulrajani, Tianyi Zhang, Yann Dubois, Xuechen Li, Carlos Guestrin, Percy Liang, and Tatsunori B. Hashimoto. Stanford alpaca: An instruction-following llama model. `https://github.com/tatsu-lab/stanford_alpaca`, 2023.

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 foundation and fine-tuned chat models. *arXiv preprint arXiv:2307.09288*, 2023.

Laurens Van der Maaten and Geoffrey Hinton. Visualizing data using t-SNE. *Journal of Machine Learning Research (JMLR)*, 2008.

Jeffrey S Vitter. Random sampling with a reservoir. *ACM Transactions on Mathematical Software (TOMS)*, 1985.

Guangxuan Xiao, Yuandong Tian, Beidi Chen, Song Han, and Mike Lewis. Efficient streaming language models with attention sinks. *arXiv preprint arXiv:2309.17453*, 2023.

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 Generative Inference of Large Language Models. *Neural Information Processing Systems (NeurIPS)*, 2023.

A Related Work

Recent studies have underscored the need for efficient token generation, particularly with the rise of long-range context datasets. Several recent works have developed efficient strategies for compressing the KV cache. Zhang et al. (2023) proposed a greedy-type eviction algorithm that dynamically keeps at most $k \ll n$ token embeddings based on the accumulated attention scores where they refer to the Heavy Hitter Oracle (H2O). Liu et al. (2023a) empirically observed that tokens with initially high attention scores tend to stay high during the future generation process. Motivated by this observation, the authors proposed a strategy that only keeps the most recent and pivotal tokens whose attention scores are higher than a threshold. Ge et al. (2023) proposed an adaptive method of KV cache compression which identifies the intrinsic structures of attention heads and uses them to determine the optimal compression policy. Xiao et al. (2023) observed that a simple eviction mechanism that keeps only first few and last few tokens does not degrade much the decoding quality. They additionally proposed a fine-tuning method to solve performance degradation from their method. Liu et al. (2023b) developed an algorithm that reduces the generation latency by exploiting contextual sparsity. In addition to algorithmic acceleration, there has also been a line of work optimizing hardware resource configurations (Sheng et al., 2023; Hong et al., 2023). However, to the best of our knowledge, none of these works have achieved an efficient method for KV cache with fully sublinear-time memory space.

On the lower bound side, achieving subquadratic amortized runtime for producing output embeddings for n tokens in the worst-case instances is likely impossible without making assumptions about the input tokens (Alman & Song, 2023; Sarlos et al., 2023). Therefore, to achieve fast runtime, it is necessary to rely on certain assumptions about the input tokens.

B Details of Section 2

Note that our goal is to approximate the attention output in Eq. (1) with a space complexity that is sublinear in context length n. To achieve this objective, we aim to design the following data structure (DS) for efficiently approximating the streaming attention mechanism:

B.1 Streaming Attention Data Structure

For every positive integer n and every stream of token triplets $(\boldsymbol{q}_1, \boldsymbol{k}_1, \boldsymbol{v}_1), \ldots, (\boldsymbol{q}_n, \boldsymbol{k}_n, \boldsymbol{v}_n)$ where $\boldsymbol{q}_i, \boldsymbol{k}_i, \boldsymbol{v}_i \in \mathbb{R}^d$, we aim to construct an efficient DS with the following properties:

- The required memory space is sublinear in n, i.e., $o(n)$.
- Upon the arrival of a new triplet $(\boldsymbol{q}_{n+1}, \boldsymbol{k}_{n+1}, \boldsymbol{v}_{n+1})$ in the stream, the time complexity to update is sublinear in n, i.e., $o(n)$.
- Given such data structure, there exists an algorithm that outputs an estimator $\boldsymbol{z}_n \in \mathbb{R}^d$ in sublinear time $o(n)$ such that:

$$\left\| \boldsymbol{z}_n - \mathtt{softmax}(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n \right\|_2 \leq \varepsilon \left\| \mathtt{softmax}(\boldsymbol{K}_n \cdot \boldsymbol{q}_n) \right\|_2 \left\| \boldsymbol{V}_n \right\|_{\mathrm{op}}. \tag{3}$$

In the rest of this section, our focus is on developing an algorithm to satisfy the above properties. Note that the attention output in Eq. (1), using the definition of softmax, is equivalent to the following expression:

$$\mathrm{Attn}(\boldsymbol{q}_n, \boldsymbol{K}_n, \boldsymbol{V}_n) = \frac{\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n}{\sum_{i \in [n]} \exp(\langle \boldsymbol{k}_i, \boldsymbol{q}_n \rangle)}.$$

Thus, to compute the attention output we need to calculate:

1. The matrix-vector product between $\boldsymbol{V}_n$ and $\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)$.
2. The partition function $\sum_{i \in [n]} \exp(\langle \boldsymbol{k}_i, \boldsymbol{q}_n \rangle)$.

Thus, our DS needs to efficiently approximate each of these two operations. The matrix-vector product $\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n$ can be approximated efficiently using standard sampling-based techniques. Specifically, we make use of the row norm sampling approach (Drineas & Kannan, 2001; Cohen

et al., 2016). When multiplying two matrices $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ and $\boldsymbol{B} \in \mathbb{R}^{n \times p}$, we randomly sample an i.i.d. index $i \in [n]$ with probability proportional to the ℓ_2 norm of the i-th row in $\boldsymbol{B}$. Then, we estimate $\boldsymbol{A} \cdot \boldsymbol{B}$ by the average of the product between i-th column in $\boldsymbol{A}$ and i-th row in $\boldsymbol{B}$. With this approximation, we need only $O(\varepsilon^{-2} d \log n)$ samples to guarantee an ε multiplicative error in spectral norm for $\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n$. Luckily, it can be implemented in a streaming setting through a variant of reservoir sampling (Vitter, 1985).

The more challenging task is the sublinear-time approximation of the partition function $\sum_{i \in [n]} \exp(\langle \boldsymbol{k}_i, \boldsymbol{q}_n \rangle)$. We construct a DS for computing this under the assumption that the keys in the token stream are organized into $o(n)$ of clusters. To be more precise, we introduce the following notion of clusterability:

Definition B.1 (Clusterability)**.** *For a positive integer m and a real-valued $\delta > 0$, a dataset of points $\boldsymbol{x}_1, \boldsymbol{x}_2, \ldots \boldsymbol{x}_n \in \mathbb{R}^d$ is considered (m, δ)-clusterable if there exists a size-m partition $\mathcal{C}_1, \mathcal{C}_2, \ldots \mathcal{C}_m \subseteq \{\boldsymbol{x}_i\}_{i=1}^n$ of the dataset satisfying the following conditions:*

- *$\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$ for every $i \neq j$ and $\bigcup_{j=1}^m \mathcal{C}_j = \{\boldsymbol{x}_i\}_{i=1}^n$.*
- *for every $j \in [m]$ and every distinct pair $\boldsymbol{y}, \boldsymbol{z} \in \mathcal{C}_j$, $\|\boldsymbol{y} - \boldsymbol{z}\|_2 \leq \delta$.*

We demonstrate that under the assumption that the stream of keys $\boldsymbol{k}_1, \boldsymbol{k}_2, \ldots \boldsymbol{k}_n$ is (m, δ)-clusterable as defined in Theorem B.1, with the number of clusters scaling sublinearly in stream length ($m = o(n)$), it is possible to construct a DS with sublinear memory space. The procedure for this DS is presented in Algorithm 1 which we refer to as CLUSTERGEN.

To verify this in the practical settings, we plot key embeddings from open-source LLMs in Fig. 1 and observe that they are indeed well clusterable on their embedding space. This motivates us to utilize an efficient stream clustering algorithm on key embeddings. In the remainder of this section, we provide a detailed explanation for the execution of the algorithm while simultaneously analyzing it through a series of lemmas.

B.2 MATRIX PRODUCT DATA STRUCTURE

Here, we focus on the UPDATEMATRIXPRODUCT primitive and establish its correctness by introducing invariants that are maintained throughout the stream processing. This primitive maintains and updates a list of s elements denoted by $\mathcal{M}$ in CLUSTERGEN (Algorithm 1). Initially, this list is filled with `null` values. After processing the first token tuple $(\boldsymbol{q}_1, \boldsymbol{k}_1, \boldsymbol{v}_1)$, this list is populated with s copies of the first key and value $(\boldsymbol{k}_1, \boldsymbol{v}_1)$. The procedure UPDATEMATRIXPRODUCT performs a variant of reservoir sampling upon observing any new token in the stream. At any iteration n of the stream, $\mathcal{M}$ is ensured to contain s i.i.d. samples chosen at random from $(\boldsymbol{k}_1, \boldsymbol{v}_1), \ldots, (\boldsymbol{k}_n, \boldsymbol{v}_n)$ with probabilities proportional to $\|\boldsymbol{k}_i\|_2^2$. More precisely, the following invariants hold:

Lemma B.2 (Correctness of UPDATEMATRIXPRODUCT)**.** *For any positive integer s, at any iteration n of the stream in Algorithm 1 the following properties are maintained:*

1. *$\mu = \sum_{i \in [n]} \|\boldsymbol{v}_i\|_2^2$.*
2. *$\mathcal{M}$ is a list of s i.i.d. samples from $\{(\boldsymbol{k}_1, \boldsymbol{v}_1), \ldots, (\boldsymbol{k}_n, \boldsymbol{v}_n)\}$ where the probability distribution for each element $j \in [s]$ and $i \in [n]$ is $\Pr[\mathcal{M}(j) = (\boldsymbol{k}_i, \boldsymbol{v}_i)] = \frac{\|\boldsymbol{v}_i\|_2^2}{\sum_{l \in [n]} \|\boldsymbol{v}_l\|_2^2}$.*

Proof. The first property is trivial because μ is initialized at zero and is updated in line 6 of the algorithm by adding the squared norms of $\boldsymbol{v}_i$'s. The proof of the second invariance is by induction. The base of induction holds for $n = 1$ because after processing the first token by procedure UPDATEMATRIXPRODUCT we have $\Pr[\mathcal{M}(j) = (\boldsymbol{k}_1, \boldsymbol{v}_1)] = \frac{\|\boldsymbol{v}_1\|_2^2}{\|\boldsymbol{v}_1\|_2^2} = 1$ for $j \in [s]$.

Now suppose that the inductive hypothesis holds for n and we prove it must also hold for $n + 1$. For any $j \in [s]$ in line 24 of Algorithm 1 with probability $p = \frac{\|\boldsymbol{v}_{n+1}\|_2^2}{\mu + \|\boldsymbol{v}_{n+1}\|_2^2}$, $\mathcal{M}(j)$ gets updated to

Algorithm 1 CLUSTERGEN: Sublinear Streaming Attention via Clustering

inputs: stream of token embeddings $(\boldsymbol{q}_n, \boldsymbol{k}_n, \boldsymbol{v}_n)$, parameter $\delta > 0$, positive integers s, t
Initialize $\mu \leftarrow 0$, $\mathcal{D} \leftarrow \emptyset$, $\mathcal{M} \leftarrow \left[\texttt{null}, \ldots^{\times s} \ldots\right]$
repeat
  $\mathcal{D} \leftarrow$ UPDATESOFTMAXNORMALIZER$(\mathcal{D}, \delta, t, \boldsymbol{k}_n)$
  $\mathcal{M} \leftarrow$ UPDATEMATRIXPRODUCT$(\mathcal{M}, s, \mu, \boldsymbol{k}_n, \boldsymbol{v}_n)$
  $\mu \leftarrow \mu + \|\boldsymbol{v}_n\|_2^2$
  $\boldsymbol{z}_n \leftarrow$ QUERYSTREAMATTN$(\mathcal{D}, \mathcal{M}, s, t, \mu, \boldsymbol{q}_n)$
  $n \leftarrow n + 1$
  output $\boldsymbol{z}_n$
until Token stream ends

Procedure UPDATESOFTMAXNORMALIZER $(\mathcal{D}, \delta, t, \boldsymbol{k})$
Initialize $\mathcal{D} \leftarrow \{(\boldsymbol{x}_i, \mathcal{S}_i, n_i) : i \in [m]\}$ and $i^* \leftarrow \arg\min_{i \in [m]} \|\boldsymbol{x}_i - \boldsymbol{k}\|_2$
if $\|\boldsymbol{k} - \boldsymbol{x}_{i^*}\|_2 \leq \delta$ **then**
  $n_{i^*} \leftarrow n_{i^*} + 1$
  Suppose $\mathcal{S}_{i^*}$ is a list of t vectors in $\mathbb{R}^d$
  for $j \in [t]$ **do**
    Flip a coin and with probability $p = \frac{1}{n_{i^*}}$, update the j^{th} entry of $\mathcal{S}_{i^*}$ as $\mathcal{S}_{i^*}(j) \leftarrow \boldsymbol{k}$
  end for
else
  $\mathcal{S}' \leftarrow \left[\boldsymbol{k}, \ldots^{\times t} \ldots\right]$ (contains t copies of $\boldsymbol{k}$)
  $\mathcal{D} = \mathcal{D} \cup \{(\boldsymbol{k}, \mathcal{S}', 1)\}$
end if
return $\mathcal{D}$

Procedure UPDATEMATRIXPRODUCT $(\mathcal{M}, s, \mu, \boldsymbol{k}, \boldsymbol{v})$
Suppose $\mathcal{M}$ is a list of s tuples of vectors in $\mathbb{R}^d$
for $i \in [s]$ **do**
  Flip a coin and with probability $p = \frac{\|\boldsymbol{v}\|_2^2}{\mu + \|\boldsymbol{v}\|_2^2}$, update the i^{th} entry of $\mathcal{M}$ as $\mathcal{M}(i) \leftarrow (\boldsymbol{k}, \boldsymbol{v})$
end for
return $\mathcal{M}$

Procedure QUERYSTREAMATTN $(\mathcal{D}, \mathcal{M}, s, t, \mu, \boldsymbol{q})$
$\boldsymbol{z} \leftarrow \sum_{(\boldsymbol{k}, \boldsymbol{v}) \in \mathcal{M}} \frac{\mu}{s \cdot \|\boldsymbol{v}\|_2^2} \cdot \exp(\langle \boldsymbol{q}, \boldsymbol{k} \rangle) \cdot \boldsymbol{v}$
$\tau \leftarrow \sum_{(\boldsymbol{x}, \mathcal{S}, n') \in \mathcal{D}} \frac{n'}{t} \cdot \sum_{\boldsymbol{k} \in \mathcal{S}} \exp(\langle \boldsymbol{q}, \boldsymbol{k} \rangle)$
return $\boldsymbol{z}/\tau$

$(\boldsymbol{k}_{n+1}, \boldsymbol{v}_{n+1})$. Since we showed that $\mu = \sum_{i \in [n]} \|\boldsymbol{v}_i\|_2^2$ we have:

$$\Pr[\mathcal{M}(j) = (\boldsymbol{k}_{n+1}, \boldsymbol{v}_{n+1})] = \frac{\|\boldsymbol{v}_{n+1}\|_2^2}{\sum_{l \in [n+1]} \|\boldsymbol{v}_l\|_2^2}.$$

Moreover with probability $1 - p = \frac{\mu}{\mu + \|\boldsymbol{v}_{n+1}\|_2^2}$, $\mathcal{M}(j)$ keeps its previous value. Using the inductive hypothesis we have that for every $i \in [n]$:

$$\Pr[\mathcal{M}(j) = (\boldsymbol{k}_i, \boldsymbol{v}_i)] = \frac{\|\boldsymbol{v}_i\|_2^2}{\sum_{l \in [n]} \|\boldsymbol{v}_l\|_2^2} \cdot \frac{\sum_{l \in [n]} \|\boldsymbol{v}_l\|_2^2}{\sum_{l \in [n+1]} \|\boldsymbol{v}_l\|_2^2} = \frac{\|\boldsymbol{v}_i\|_2^2}{\sum_{l \in [n+1]} \|\boldsymbol{v}_l\|_2^2}.$$

This completes the proof of Theorem B.2. □

B.3 SOFTMAX NORMALIZER (PARTITION FUNCTION) DS

Here we delve into a detailed discussion of the UPDATESOFTMAXNORMALIZER primitive. This primitive constructs and maintains a DS denoted by $\mathcal{D}$, enabling accurate approximation of the

partition function in the softmax denominator for any query. A crucial requirement for the efficiency of this primitive is that the key tokens must be (m, δ)-clusterable, as per Theorem B.1. Our algorithm locates and stores a subsampled representation of each cluster in $\mathcal{D}$ in a small memory. Particularly, to achieve sublinear memory complexity, instead of keeping all keys in each cluster which would require $O(n)$ memory space, we maintain only a random subset of t samples from each cluster.

Initially, $\mathcal{D}$ is an empty set. As new tokens in the stream are processed, new clusters get added to this set. Each cluster is characterized by a representative point, which is the first key assigned to that cluster by our algorithm. Throughout stream processing, we compute the distance between the new key token and each existing cluster. Here the distance to an existing cluster is defined as the distance to the aforementioned representative of the cluster. If there is a cluster whose distance is less than δ, then the token is assigned to the nearest cluster, and we update our random samples of keys from this cluster using reservoir sampling. If the distance from all existing clusters is more than δ, we introduce a new cluster in $\mathcal{D}$, and the new key becomes the representative of this new cluster. At any point in the stream, this algorithm identifies at most m clusters if the keys so far are (m, δ)-clusterable. If m grows sublinearly in the stream length n, the memory and update time of our algorithm will be sublinear as well. Formally, we prove that the following invariant holds:

Lemma B.3 (Correctness of UPDATESOFTMAXNORMALIZER)**.** *For any $\delta > 0$, any positive integer t, at any iteration n of the stream in Algorithm 1 the following properties are maintained. $\mathcal{D}$ is a set of m items of the form $\mathcal{D} = \{(\boldsymbol{x}_i, \mathcal{S}_i, n_i) : i \in [m]\}$, where there exists a partition of keys into m disjoint subsets $\mathcal{C}_1, \mathcal{C}_2, \ldots \mathcal{C}_m \subseteq \{\boldsymbol{k}_i\}_{i=1}^n$ satisfying $\bigcup_{j=1}^m \mathcal{C}_j = \{\boldsymbol{k}_i\}_{i=1}^n$ and $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$ for every $i \neq j$, such that for every $i \in [m]$:*

1. $\boldsymbol{x}_i \in \mathcal{C}_i$,
2. $n_i = |\mathcal{C}_i|$,
3. $\|\boldsymbol{x}_i - \boldsymbol{k}'\|_2 \leq \delta$ *for every* $\boldsymbol{k}' \in \mathcal{C}_i$,
4. $\|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2 > \delta$ *for every* $i \neq j$,
5. $\mathcal{S}_i$ *is a set of* t *i.i.d. uniform samples from the set* $\mathcal{C}_i$.

Proof. The proof is by induction on the stream length n. The base of induction trivially holds for $n = 0$, where $\mathcal{D}$ is an empty set. To prove the inductive step suppose that the inductive hypothesis holds for some n. Specifically, suppose that $\mathcal{D}$ is a set of m items of the form $\mathcal{D} = \{(\boldsymbol{x}_i, \mathcal{S}_i, n_i) : i \in [m]\}$ and there exists a partition of keys into m disjoint subsets $\mathcal{C}_1, \mathcal{C}_2, \ldots \mathcal{C}_m \subseteq \{\boldsymbol{k}_i\}_{i=1}^n$ as per in the lemma statement, such that for every $i \in [m]$: **(1)** $\boldsymbol{x}_i \in \mathcal{C}_i$, **(2)** $n_i = |\mathcal{C}_i|$, **(3)** $\|\boldsymbol{x}_i - \boldsymbol{k}'\|_2 \leq \delta$ for every $\boldsymbol{k}' \in \mathcal{C}_i$, **(4)** $\|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2 > \delta$ for every $i \neq j$, and **(5)** $\mathcal{S}_i$ is a set of t i.i.d. uniform samples from the set $\mathcal{C}_i$. Given this assumption, we prove that the inductive step also holds for after processing the $(n+1)$-th key in the stream $\boldsymbol{k}_{n+1}$.

In the next iteration, specifically in line 12 of UPDATESOFTMAXNORMALIZER, the algorithm finds the index $i^* \in [m]$ such that $\|\boldsymbol{x}_{i^*} - \boldsymbol{k}_{n+1}\|_2$ is minimized. Two cases arise:

Case 1: $\|\boldsymbol{x}_{i^*} - \boldsymbol{k}_{n+1}\|_2 \leq \delta$**.** In this case, the algorithm increments $n_{i^*} \leftarrow n_{i^*} + 1$ in line 14. Consider the new partitioning of the keys defined as $\mathcal{C}'_i = \mathcal{C}_i$ for $i \neq i^*$ and $\mathcal{C}'_{i^*} = \mathcal{C}_{i^*} \cup \{\boldsymbol{k}_{n+1}\}$. It follows from the inductive hypothesis that for every $i \in [m]$: **(1)** $\boldsymbol{x}_i \in \mathcal{C}'_i$, **(2)** $n_i = |\mathcal{C}'_i|$, **(3)** $\|\boldsymbol{x}_i - \boldsymbol{k}'\|_2 \leq \delta$ for every $\boldsymbol{k}' \in \mathcal{C}'_i$, and **(4)** $\|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2 > \delta$ for every $i \neq j$ hold after the $n+1$-th iteration. Furthermore, since the algorithm does not alter the lists $\mathcal{S}_i$ for $i \neq i^*$, we have that **(5)** $\mathcal{S}_i$ is a set of t i.i.d. uniform samples from the set $\mathcal{C}'_i$ for any $i \neq i^*$. On the other hand, the algorithm in line 17 performs reservoir sampling on the set $\mathcal{S}_{i^*}$ with new element $\boldsymbol{k}_{n+1}$ which implies that $\mathcal{S}_{i^*}$ is a set of t i.i.d. uniform samples from the set $\mathcal{C}'_{i^*}$. This completes the inductive step in the first case.

Case 2: $\|\boldsymbol{x}_{i^*} - \boldsymbol{k}_{n+1}\|_2 > \delta$**.** In this case, the algorithm adds a new element to $\mathcal{D}$, thus, the updated set is $\mathcal{D}' = \{(\boldsymbol{x}_i, \mathcal{S}_i, n_i) : i \in [m+1]\}$ with $\boldsymbol{x}_{m+1} = \boldsymbol{k}_{n+1}$ and $n_{m+1} = 1$. If we consider the new partitioning of keys to be $\mathcal{C}_1, \mathcal{C}_2, \ldots \mathcal{C}_m, \mathcal{C}_{m+1}$, where $\mathcal{C}_{m+1} = \{\boldsymbol{k}_{n+1}\}$, we can use the inductive hypothesis to deduce that for any $i \in [m+1]$: **(1)** $\boldsymbol{x}_i \in \mathcal{C}_i$, **(2)** $n_i = |\mathcal{C}_i|$, **(3)** $\|\boldsymbol{x}_i - \boldsymbol{k}'\|_2 \leq \delta$ for every $\boldsymbol{k}' \in \mathcal{C}_i$, and **(4)** $\|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2 > \delta$ for every $i \neq j$ hold after the $n+1$-th iteration of the stream. Furthermore, $\mathcal{S}_{m+1}$ is defined to be a list of t copies of $\boldsymbol{k}_{n+1}$, thus, **(5)** $\mathcal{S}_i$ is

a set of t i.i.d. uniform samples from the set $\mathcal{C}_i$ for any $i \in [m+1]$. This completes the inductive step in this case and also concludes the proof of Theorem B.3. □

B.4 STREAMING ATTENTION: MAIN THEOREM

Now we are ready to analyze the end-to-end performance of CLUSTERGEN and prove the main theorem. We show that, given the data structures created throughout the stream and analyzed in Theorem B.2 and Theorem B.3, the primitive QUERYSTREAMATTN can efficiently output an accurate approximation to the streaming attention, satisfying Eq. (1).

Our analysis unfolds in two steps. First, we establish that the data structures created by UPDATESOFTMAXNORMALIZER and UPDATEMATRIXPRODUCT can be stored in small memory and updated very quickly if the sequence of keys is clusterable into a sublinear number of clusters. Then we show that the QUERYSTREAMATTN can use these data structures to produce an accurate attention output for any given query. Our main result is as follows:

Theorem B.4 (Efficiency and Correctness of Algorithm 1)**.** *For any $\delta, r, \varepsilon > 0$, any positive integers n, d, and any sequence of tokens $(\boldsymbol{q}_1, \boldsymbol{k}_1, \boldsymbol{v}_1), (\boldsymbol{q}_2, \boldsymbol{k}_2, \boldsymbol{v}_2), \dots (\boldsymbol{q}_n, \boldsymbol{k}_n, \boldsymbol{v}_n)$ where $\boldsymbol{q}_i, \boldsymbol{k}_i, \boldsymbol{v}_i \in \mathbb{R}^d$, suppose that the followings hold*

- $t = \Omega\left(\varepsilon^{-2} \cdot e^{2\delta \cdot r} \log n\right)$,
- $s = \Omega(\varepsilon^{-2} \cdot d)$,
- $\|\boldsymbol{q}_n\|_2 \leq r$.

Then, CLUSTERGEN *(Algorithm 1) at n-th step of the stream processing outputs a vector $\boldsymbol{z}_n \in \mathbb{R}^d$ that satisfies Eq.* (1) *with probability at least* 0.99*. Furthermore, if the keys $\boldsymbol{k}_1, \boldsymbol{k}_2, \dots \boldsymbol{k}_n$ are (m, δ)-clusterable as per Theorem B.1, then both the total memory of the algorithm and its runtime during the n-th iteration is bounded by $O(d \cdot (mt + s))$.*

Proof. We start the correctness proof by observing that all preconditions of Theorem B.3 are satisfied, allowing us to invoke this lemma. Let the partition of keys into disjoint subsets be denoted by $\mathcal{C}_1, \mathcal{C}_2, \dots \mathcal{C}_{m'} \subseteq \{\boldsymbol{k}_i\}_{i=1}^n$ satisfying $\bigcup_{j=1}^{m'} \mathcal{C}_j = \{\boldsymbol{k}_i\}_{i=1}^n$ and $\mathcal{C}_i \cap \mathcal{C}_j = \emptyset$ for every $i \neq j$ as per Theorem B.3 for some positive integer m'. Rewriting the partition function in the attention denominator gives:

$$\sum_{j \in [n]} \exp(\langle \boldsymbol{k}_j, \boldsymbol{q}_n \rangle) = \sum_{i \in [m']} \sum_{\boldsymbol{k}' \in \mathcal{C}_i} \exp(\langle \boldsymbol{k}', \boldsymbol{q}_n \rangle).$$

Now by property **(3)** in Theorem B.3 and triangle inequality, for every $i \in [m']$ and every $\boldsymbol{k}', \boldsymbol{k}'' \in \mathcal{C}_i$ we have:

$$\|\boldsymbol{k}' - \boldsymbol{k}''\|_2 \leq \|\boldsymbol{k}' - \boldsymbol{x}_i\|_2 + \|\boldsymbol{k}'' - \boldsymbol{x}_i\|_2 \leq 2\delta.$$

Therefore, using the precondition of the theorem on $\|\boldsymbol{q}_n\|_2 \leq r$ we have

$$\exp(\langle \boldsymbol{k}', \boldsymbol{q}_n \rangle) / \exp(\langle \boldsymbol{k}'', \boldsymbol{q}_n \rangle) \leq e^{2\delta \cdot r}.$$

Using the above inequality and the assumption in the theorem statement regarding $t = \Omega\left(\varepsilon^{-2} \cdot e^{2\delta \cdot r} \log n\right)$ combined with the properties **(2)** and **(5)** proved in Theorem B.3, we can invoke Chernoff-Hoeffding inequality (see e.g., McDiarmid (1998)) along with union bound to conclude that the following holds simultaneously for all $i \in [m']$ with probability at least $1 - \frac{1}{\text{poly}(n)}$:

$$\frac{n_i}{t} \cdot \sum_{\boldsymbol{k}' \in \mathcal{S}_i} \exp(\langle \boldsymbol{q}_n, \boldsymbol{k}' \rangle) \in (1 \pm \varepsilon/3) \cdot \sum_{\boldsymbol{k}' \in \mathcal{C}_i} \exp(\langle \boldsymbol{k}', \boldsymbol{q}_n \rangle)$$

Since the terms above are positive, by summing up the given inequality for all $i \in [m']$, we find that the quantity τ computed in line 27 of Algorithm 1 satisfies the following:

$$\Pr\left[\tau \in (1 \pm \varepsilon/3) \sum_{j \in [n]} \exp(\langle \boldsymbol{k}_j, \boldsymbol{q}_n \rangle)\right] \geq 0.995 \tag{4}$$

Next, we invoke Theorem B.2 to derive an error bound on the approximate matrix-vector product between the softmax vector and the matrix of values $\boldsymbol{V}_n$. By leveraging well-established techniques in approximate matrix products, such as the standard result from Drineas & Kannan (2001), and using the conclusion of Theorem B.2 regarding $\mathcal{M}$ as a list of $s = \Omega(\varepsilon^{-2} \cdot d)$ i.i.d. sample from the probability distribution $\Pr[\mathcal{M}(j) = (\boldsymbol{k}_i, \boldsymbol{v}_i)] = \frac{\|\boldsymbol{v}_i\|_2^2}{\sum_{l\in[n]}\|\boldsymbol{v}_l\|_2^2}$ for $i \in [n]$ for $i \in [n]$ and $j \in [s]$, we have that vector $\boldsymbol{z}$ computed in line 26 of Algorithm 1 satisfies the following inequality with a probability of at least 0.995:

$$\left\|\boldsymbol{z} - \exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n\right\|_2 \leq \frac{\varepsilon}{3} \left\|\exp(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)\right\|_2 \|\boldsymbol{V}_n\|_{op}$$

Now by combining inequalities in Eq. (4) and Eq. (5) using union bound and triangle inequality we find that the output of Algorithm 1 computed in line 28 as $\boldsymbol{z}/\tau$ satisfies the following with probability at least 0.99

$$\left\|\boldsymbol{z}/\tau - \texttt{softmax}(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)^\top \cdot \boldsymbol{V}_n\right\|_2 \leq \varepsilon \left\|\texttt{softmax}(\boldsymbol{K}_n \cdot \boldsymbol{q}_n)\right\|_2 \|\boldsymbol{V}_n\|_{op}.$$

This completes the correctness proof of Theorem B.4. □

Memory and Runtime. First, note that the memory requirement for storing the list $\mathcal{M}$ in Algorithm 1 is $O(sd)$ because it contains s pairs of d-dimensional vectors. Next, to bound the memory requirement for storing $\mathcal{D}$ we need to bound the size of this set which we denoted by m'. According to properties **(1)** and **(4)** in Theorem B.3, for every $i \in [m']$ there exist $\boldsymbol{x}_i \in \{\boldsymbol{k}_1, \boldsymbol{k}_2, \dots \boldsymbol{k}_n\}$ such that $\|\boldsymbol{x}_i - \boldsymbol{x}_j\|_2 > \delta$ for $i \neq j$. Given the assumption in the theorem statement that keys are (m, δ)-clusterable, by the definition of clusterability in Theorem B.1 along with the pigeonhole principle, we must have $m' \leq m$. Therefore storing $\mathcal{D}$ will require $O(m'td) = O(mtd)$ because it is a set of m' elements, and each element of this set is a list of t vectors in dimension d.

Three major operations dominate the runtime of the n-th iteration. Firstly, executing UPDATESOFTMAXNORMALIZER requires computing m' distances in line 12 that takes $O(md)$ time. Additionally, the for loop in line 16 takes $O(td)$ time. Secondly, UPDATEMATRIXPRODUCT has a runtime bounded by $O(sd)$. Thirdly, running QUERYSTREAMATTN involves $O(sd)$ operations in line 26 and $O(m'td) = O(mtd)$ operations in line 27. As a result, the total runtime of Algorithm 1 in n-th iteration is $O(mtd + sd)$.

Theorem B.4 demonstrates that if the keys can be clustered into some sublinear number $m = n^{1-\Omega(1)}$ of clusters with diameters at most δ, and the queries have bounded ℓ_2 norms of at most r such that the product of the cluster diameter and maximum ℓ_2 norm of queries is bounded by $\delta r = o(\log n)$, then Algorithm 1 operates with sublinear $O\left(\varepsilon^{-2} \cdot mdn^{o(1)}\right) = O\left(\varepsilon^{-2} \cdot dn^{1-\Omega(1)}\right)$ memory and runtime. We summarize this in the following corollary:

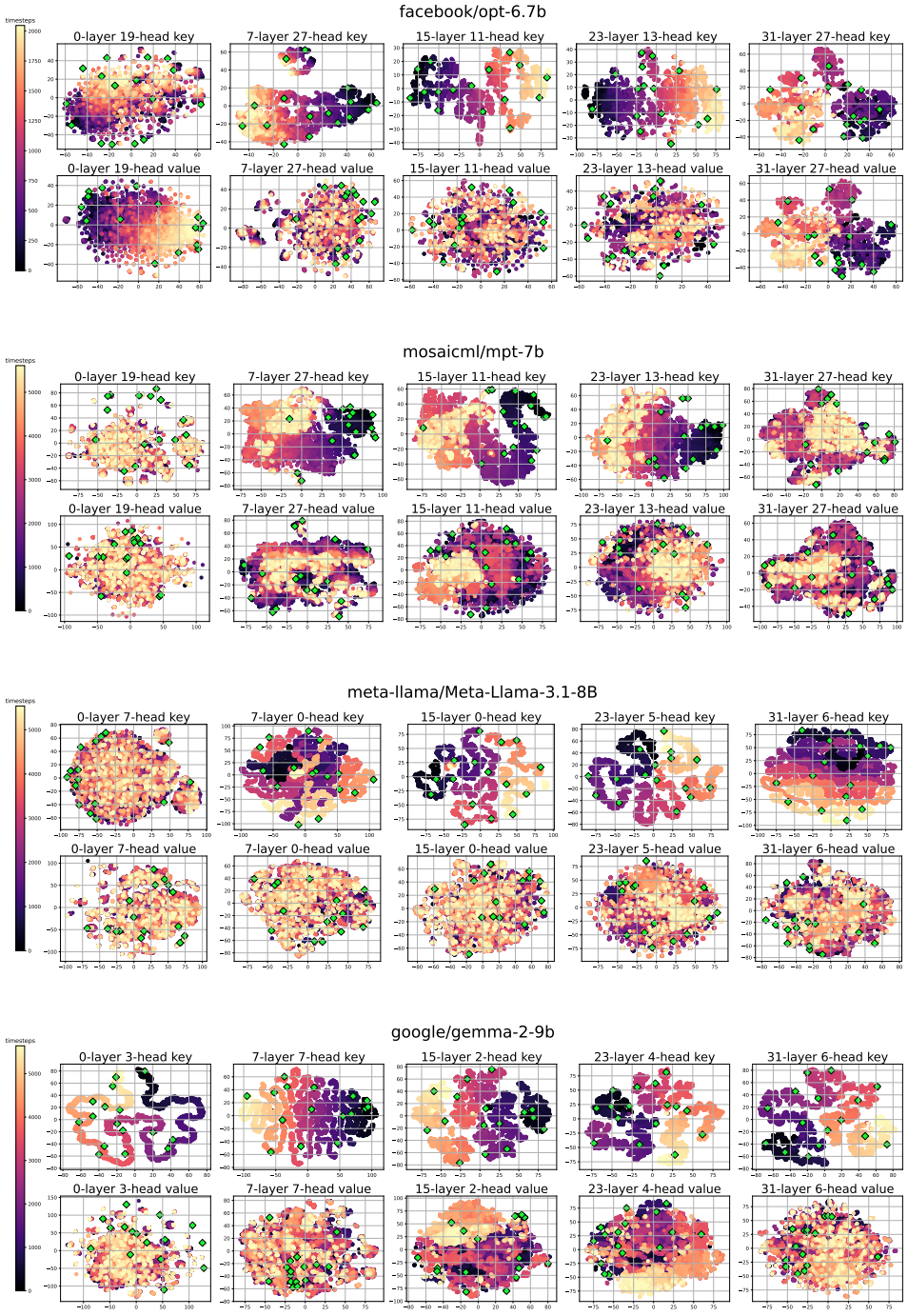
Corollary B.5. *Suppose the preconditions of Theorem B.4 hold. If the diameter of key token clusters δ and the maximum ℓ_2 norm of queries r satisfy $\delta r = o(\log n)$, then the total memory and runtime of Theorem B.4 are bounded by $O\left(\varepsilon^{-2} \cdot dmn^{o(1)}\right)$. Moreover, if the number of key token clusters m grows as a sublinear function of n, i.e., as $m = n^{1-\Omega(1)}$, then the memory and runtime are bounded by $O\left(\varepsilon^{-2} \cdot dn^{1-\Omega(1)}\right)$.*

The above results require that the key embeddings are well clusterable in their space, and the cluster centers should cover all keys with a small radius. In the next section, we empirically explore distributions on key and value embeddings and verify that the keys are indeed distributed in their embedding space. This supports that our assumption of clusterability on keys is reasonable in practical settings.

C ADDITIONAL EXPERIMENTS

C.1 BOUNDED NORM ON QUERY EMBEDDINGS

We additionally investigate assumption on the upper bound of query embeddings in Theorem B.4, i.e., $\|\boldsymbol{q}_n\|_2 \leq r$ for some constant $r > 0$. Essentially, query embeddings are obtained by multiplying weights by the input embeddings, and they are typically passed through the Layer Normalization (Ba, 2016). Therefore, entries of query embeddings are expected to be small assuming the weight matrices have small eigenvalues, and the norms of query embeddings in our case after Layer Normalization are expected to be small constants.



C.2 CLUSTERABILITY

We additionally provide t-SNE plots of key (first rows) and value (second rows) with more diverse layers and heads, and similar results discussed in **??** are observed; a higher degree of clusterability on the key embeddings compared to value ones.