Prepacking: A Simple Method for Fast Prefilling and Increased Throughput in Large Language Models

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Abstract

During inference for transformer-based large language models (LLM), prefilling is the computation of the key-value (KV) cache for input tokens in the prompt prior to autoregressive generation. For longer input prompt lengths, prefilling will incur a significant overhead on decoding time. In this work, we highlight the following pitfall of prefilling: for batches containing high-varying prompt lengths, significant computation is wasted by the standard practice of padding sequences to the maximum length. As LLMs increasingly support longer context lengths, potentially up to 10 million tokens, variations in prompt lengths within a batch become more pronounced. To address this, we propose *prepacking*, a simple yet effective method to optimize prefilling computation. To avoid redundant computation on pad tokens, prepacking combines prompts of varying lengths into a sequence and packs multiple sequences into a compact batch using a bin-packing algorithm. It then modifies the attention mask and positional encoding to compute multiple prefilled KV-caches for multiple prompts within a single sequence. On standard curated dataset containing prompts with varying lengths, we obtain a significant speed and memory efficiency improvements as compared to the default padding-based prefilling computation within Huggingface across a range of base model configurations and inference serving scenarios. Code is at: `https://github.com/siyan-zhao/prepacking`

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1 Introduction

Transformer-based large language models (LLMs) have emerged as a powerful general purpose tool to service natural language queries (Bai et al., 2022; Touvron et al., 2023; Achiam et al., 2023). As language models continue to grow in scale and their usage proliferates across various domains (Eloundou et al., 2023), the capability to generate tokens with optimal speed and efficiency becomes increasingly paramount.

The challenges of optimizing LLMs are unique compared to traditional software. LLMs are useful due to their generality, which means they can receive very diverse prompts, from short questions to long summarizing tasks. Due to the quadratic runtime of a Transformer, longer prompts require much more computation than short prompts. When long and short prompt queries are requested at the same time, the challenge of LLM inference is to route the queries in a manner that more computational resources are allocated where needed. In the current LLM paradigm, this poses a dilemma that worsens with increasing model scale due to longer, more compute-demanding queries. As an example, recent efforts are aimed at expanding the context window of LLMs to accommodate up to one million tokens and beyond (Reid et al., 2024). The increasing diversity and complexity of queries demand a more efficient approach to computational resource allocation than ever before.

The conventional approach to LLM inference with varied size inputs is inefficient, and it is exemplified by the Huggingface Transformers library (Wolf et al., 2020). The Huggingface library has seen widespread adoption in the NLP community. Despite its wide use, Huggingface handles prompts of varying lengths by padding all prompts to match the length of the longest sequence and processing the batch through a Transformer model in its entirety. This results in substantial memory utilization and computational inefficiency. While LLMs are compute-bound during prefilling, they are also memory-bound during generation (Kwon et al., 2023), so it is crucial to optimize memory and GPU

utilization to enable efficient inference and scalability.

In this work, we mitigate wasteful computation with an alternative pre-processing step called *prepacking*. Prepacking is specifically aimed at improving the speed and memory usage of LLM prefilling, which is the initial computation that populates the Key-Value cache (KV cache) preceding generation. Prepacking is conceptually simple; rather than padding every sequence to the same length, we pack multiple prompts together in place of padding tokens using an off-the-shelf bin-packing algorithm. This is made possible by custom attention masking and positional encoding that enable the computation of a batch within a single sequence. The positional encoding restarts its index for each prompt in the sequence and the mask prevents prompts from attending to previous prompts in the packed sequence (Figure 1). A forward pass on the pre-packed batch will populate a KV cache, which we can unpack to get the cache for the original prompts for next token generations.

We empirically demonstrate that prepacking leads to a **speedup of up to 6x** in prefilling and time-to-first-token (TTFT) compared to the full batching method used in Huggingface tested on NVIDIA A6000 GPUs. To evaluate prepacking's runtime performance under conditions representative of real-world user traffic, we tested it across six diverse language datasets, encompassing tasks such as question answering, summarization, instruction following, language modeling, and human preference modeling, with language models ranging from 1B to 13B parameters. Prepacking achieves greater speedup when the sequences within a batch exhibit more diverse length variations and when the batch size is large. Additionally, we demonstrate that prepacking is a simple method for increasing LLM throughput, especially in memory-constrained settings. Specifically, prepacking significantly reduces memory consumption by allowing up to **16x larger batch size** during prefilling.

2 Preliminaries

2.1 Transformer Architecture

The decoder-only Transformer (Vaswani et al., 2017; Radford et al., 2019) is ubiquitous in its use as the deep learning architecture for autoregressive LLMs. The core component of the Transformer is self-attention. Self-attention operates on input sequences $X \in \mathbb{R}^{n \times d}$ and is parameterized with matrices $W^Q, W^K, W^V \in \mathbb{R}^{d \times h}$. We can write self-attention as follows

$$\mathrm{SA}(X) = \mathrm{softmax}(A)XW^V.$$

where $A = \frac{(XW^Q)(XW^K)^\top}{\sqrt{d}}$ is an $n \times n$ attention matrix. Thus, a Transformer forward pass will have an $\mathcal{O}(n^2)$ runtime where n is the length of the input. To preserve autoregressive dependencies, an $n \times n$ mask M is applied to A such that "past" tokens cannot attend to "future" tokens. Finally, while attention itself is permutation-equivariant, the inputs X typically incorporate positional information through the use of positional embeddings.

2.2 Language Model Inference

Autoregressive sampling requires a forward pass through the Transformer for each new token generated. To avoid wastefully recomputing the attention matrix each forward pass, caching is standard practice at inference time. Sampling the $(n+1)$-th token autoregressively requires computing the attention matrix for n previous tokens. When we generate the $(n+2)$-th token, instead of computing an $(n+1) \times (n+1)$ attention matrix, we can cache the keys and values over the first n tokens to avoid redundant computation, and so on for $(n+j)$. This technique is known as KV caching (Pope et al., 2023).

Prefilling is the population of the KV cache on the initial forward pass. In a typical text generation inference framework, a model will be run on a batch of k prompts that, when tokenized, have lengths $l_1, ..., l_k$. Because a Transformer takes tensor input, the batch will be padded to the maximum length $m = \max_i l_i$. For the sake of simplicity, assume no parallelization over a batch. Although GPUs can parallelize computation over batches, we will argue in future sections that batch parallelization in practice has empirical limitations. Thus, under these assumptions the forward pass for prefilling will run in time $\mathcal{O}(km^2)$.

2.3 Performance Metrics

Key metrics for evaluating LLM serving (Miao et al., 2023) include latency measures such as Time-to-First-Token (TTFT), the time required for prefilling the KV cache and generating the first token, and Time-per-Output-Token (TPOT), the average time to generate each subsequent token. Together, these determine the total generation time. Throughput measures the number of requests processed per unit time. In this work, we focus on optimizing the prefilling stage by evaluating prefilling time and TTFT metrics. This is particularly important for assessing the overall responsiveness of any deployed system.

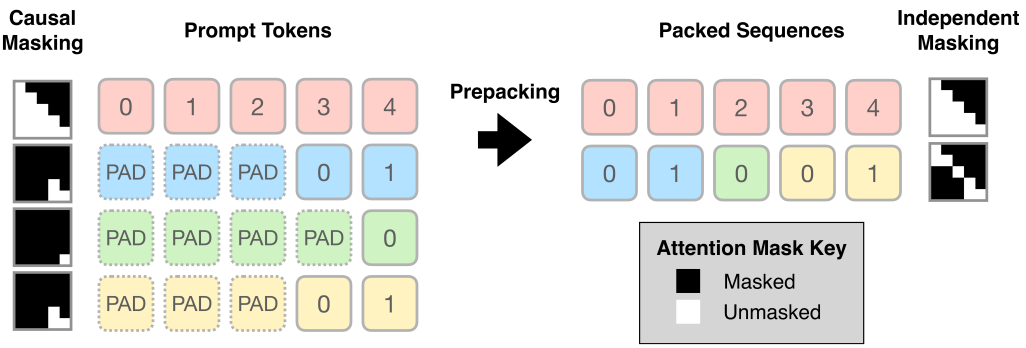


Figure 1: **Left:** The standard full batching approach (e.g., used in HuggingFace) pads shorter prompts to maximum prompt length in the batch. Each prompt has its own causal attention mask. **Right:** Prepacking combines multiple prompts into a single sequence using a bin-packing algorithm, and applies *independent masking* and *restart positional encodings* (numbers inside token boxes) to avoid prompts attending to other prompts. Both strategies are equivalent at decoding time, but prepacking is more compute efficient during prefilling.

3 Related Works

3.1 Accelerating Inference

Many advancements in accelerating LLM inference make architectural modifications that tradeoff quality with inference latency. These approaches include exploiting contextual sparsity (Liu et al., 2023), multiple decoding heads (Cai et al., 2024), model quantization (Xiao et al., 2023), and improved decoding algorithms such as speculative decoding which augments a base model with an "approximation model" (Leviathan et al., 2023). Packing has been applied to training to speed up training efficiency, while our work focuses on prefilling stage. Zheng et al. (2023) reduces padding by clustering the prompts with similar response lengths into mini batches for generation. Packing and using independent mask can also be used for pre-training to decrease the distraction between documents (Zhao et al., 2024). Another active area of research is speeding up inference by improving low-level compute scheduling (Aminabadi et al., 2022; Sheng et al., 2023). Our approach for improving LLM throughput differs from the aforementioned techniques because: (1) it does not require any architectural changes; (2) it can be fully implemented in PyTorch and is agnostic to the underlying hardware and cloud platforms.

3.2 LLM Serving

A relevant line of work takes a networking perspective on LLMs, in which a model must be "served" to clients that make requests. The core problem LLM serving addresses is the scheduling of inference, creating dynamic schedulers that optimize for throughput and latency. FasterTransformer (NVIDIA, 2021) increases decoding throughput but schedules at the request-level. To address this, Orca (Yu et al., 2022) proposes iteration-level scheduling which processes requests at finer granularity than a batch. PagedAttention in vLLM (Kwon et al., 2023) reduces KV-cache memory fragmentation with techniques inspired by virtual memory with paging. More recent and concurrent works such as Sarathi-Serve (Agrawal et al., 2024) and DistServe (Zhong et al., 2024) optimize a trade-off involving prefilling and decoding. In our work, we specifically target pre-filling only. As such, our work directly improves TTFT and is complementary to other works that seek to improve decoding efficiency and throughput while minimizing stalling. Our work also has great usability with easy implementation in pytorch, without the need of writting custom CUDA kernel operations such as ragged tensors operations (Fegade et al., 2022).

4 Prepacking

Although padding input prompts to the maximum length allows tensorized batch computation, the drawback is that significant computation is wasted on pad tokens. We propose a simple solution: insert more short prompts where padding was previously located. Because this method "packs" prompts together to speed up prefilling, we refer to this method as prepacking. In formal terms, we have a set of k prompts $p_1, \cdots, p_k$ of lengths $l_1, \cdots, l_k$, and our goal is to create a tensorized batch $B = (p'_1, ..., p'_r)$, where $p'_1, ..., p'_r$ are sequences that contain the original prompts such that $r \leq k$. The full algorithm is shown in Algorithm 1.

Algorithm 1 The *Prepacking* Algorithm for Efficient Pre-Filling

procedure PREPACKING(Prompts $p_1, \cdots, p_k$, Transformer-based Language Model π)
  Prompt Lengths $l_1, \cdots, l_k \leftarrow len(p_1, \cdots, p_k)$
  Maximum Length $m \leftarrow \max_i l_i$
  Packed sequences $p'_1, ..., p'_r$, bins $[idx]_{1:r} = \text{BINPACK}(l_1, \cdots, l_k, m)$ ▷ idx_i stores the start indices of the prompt(s) present in the packed sequence p'_i
  Batch $B \leftarrow \text{TENSORIZE}(p'_1, ..., p'_r)$
  Independent Masks $[M']_{1:r} \leftarrow \text{INDEPENDENT-MASK}([idx]_{1:r})$
  Restart Positional Encodings $[R]_{1:r} \leftarrow \text{RESTART-PE}([idx]_{1:r})$
  Caches $KVs \leftarrow \text{UNPACK}(\pi(B, [M']_{1:r}, [R]_{1:r}))$ ▷ π will return a KV Cache, which we unpack to obtain prompt-specific caches
  return KVs
end procedure

4.1 Bin Packing

The problem of packing prompts together can be cast as a bin packing problem, where a bin can contain tokens from several different sequences. The goal of prepacking is to efficiently concatenate prompts together such that original prompts with lengths $l_1, ..., l_k$ are placed into the smallest possible r bins, each of a fixed sized. It is guaranteed that $r \leq k$. We shall select m, where m is the maximum prompt length as previously defined, to be the fixed size of the bins. For sequences that do not completely reach size m after bin-packing, they will be padded to reach m. Note that we choose the smallest possible constant for our bin size because the bin size will incur quadratic running time. In general, bin packing is an NP-hard problem (Garey and Johnson, 1979), but many heuristic approaches exist obtain approximate solutions (Buljubašić and Vasquez, 2016). We use a First-Fit Decreasing bin packing heuristic as implemented by Maier (2021).

4.2 Prompt-wise Independent Masking and Restart Positional Encoding

Prepacking will concatenate multiple smaller prompts under a single bin. Simply using the KV-cache of this packed sequence will be incorrect, because every prompt within the bin will attend causally to previous prompts. As a remedy, we create a custom attention mask to prevent items from attending to each other. We refer to this masking strategy as *independent masking*. We describe our masking strategy below and illustrate it in Figure 1.

Formally, consider a causal (lower triangular) attention mask M , where entry $M_{i,j} = 1$ signifies that token t_i can attend to t_j and $i \geq j$. An independent mask M' is a mask such that for all indices a, b that mark the start and end of a prompt, $M'_{a:b,a:b} = 1$, with all other entries 0. Creating the attention mask and extracting the resultant KV-cache requires a certain amount of bookkeeping for tracking lengths of sequences and indices, but these operations contribute an insignificant (linear) overhead compared to the Transformer forward pass.

Lastly, we need to modify the positional encodings for the packed sequences. In general, the Transformer architecture is permutation equivariant (Naseer et al., 2021), so the purpose of positional encodings (PE) is to give the model information about the position of a token in a sequence. Thus, in a prepacked sequence, we must edit the PEs for the tokens such that it is the same as it was in the unpacked prompts. This leads to positions that "restart" in the packed sequence at the beginning of any new prompt, hence the name *restart positional encoding*. With packed batches, independent masks, and restart PEs, we can compute and prefill the KV cache for each prompt and use it for autoregressive generation using any decoding algorithm.

4.3 Runtime Analysis

With Algorithm 1, we are guaranteed to compute the *exact* KV caches as a padded, full-batching method. Next, we analyze the gains during the prefilling stage using our approach. Let the sum of prompt lengths over the batch be denoted by $L = \sum_i l_i$. In the best case scenario, our bin packing algorithm is able to pack every prompt into bins with no additional padding. Then we can express the number of bins as $r = L/m$. We can now find the runtime of prefilling a batch with prepacking and compare it to the naive method.

$$\begin{aligned} \mathcal{O}(rm^2) &= \mathcal{O}((L/m)m^2) = \mathcal{O}(Lm) \\ &= \mathcal{O}(km(L/k)) \leq \mathcal{O}(km^2) \end{aligned} \tag{1}$$

The final inequality holds because the average length must be less than or equal to the maximum length. Also note that the prepacking algorithm itself runs in $\mathcal{O}(k \log k)$ time which is insignificant toward the overall runtime. Thus, we find that prepacking will

outperform the naive padding approach in the best case scenario. In the worst case scenario, we cannot reduce the number of bins from the original batch size and $r = k$ will lead to the same runtime. We shall show in our experiments that datasets tend to have enough length variation such that $r < k$ is a comfortable assumption in practice, and the differences between the naive method and prepacking can be stark.

Limitations of GPU Batch Parallelization Note that the above analysis assumes no parallelization over a batch. With perfect batch parallelization, prepacking will have better memory performance but no time improvement. We show empirically that GPUs cannot parallelize over batches without limitation. To show this, we sample a tensor of dimension (k, m), that is batch size k and prompt length m. In Figure 2, we demonstrate that for a fixed m, increasing k results in a higher latency. As the batch size grows, constraints such as memory bandwidth and synchronization overhead become more pronounced (Yuan et al., 2024). Prepacking exploits this by reducing batch size for a fixed sequence length m. Figure 3 illustrates an actual packing done by prepacking which greatly reduces paddings.

5 Experiments

We empirically show the significant throughput improvements and GPU memory savings achieved by prepacking across real-world datasets with diverse length distributions. Our comprehensive evaluation spans language models of varying architectures and scales, ranging from 1.3B to 13B parameters. With constraints on our academic budget, all experiments are conducted on a single NVIDIA 48GB A6000 GPU connected to a Colfax CX41060s-EK9 4U Rackmount Server with AMD EPYC (Genoa) 9124 processors.

5.1 Datasets and Models

To profile prepacking's runtime performance under conditions representative of real-world user traffic, we evaluate on a diverse suite of datasets spanning question answering, summarization, instruction following, language modeling, and human preference modeling. Specifically, we use the MMLU (Hendrycks et al., 2021a), SamSum (Gliwa et al., 2019), Alpaca (Taori et al., 2023), Wikitext (Merity et al., 2016), and Anthropic HH RLHF (Bai et al., 2022) datasets. While not actually evaluating task performance, we leverage the variety of formats and prompt length distributions present in these datasets to simulate the diverse input queries a LLM may encounter from user requests in production environments. Due to computational constraints, we subsample 1000 prompts from each dataset, and the lengths statistics are presented in Table 5. We profile a range of language models to comprehensively assess runtime impacts of scale and architecture choices: the 1.3B Sharded LLAMA (Xia et al., 2023), 7B LLAMA 2 (Touvron et al., 2023) and Mistral (Jiang et al., 2023), and 13B LLAMA 2 (Touvron et al., 2023) spanning 1.3B to 13B parameters with varying configurations shown in Appendix Table 6. We profile them with 4 bit or 8 bit quantization due to computational constraints. Since prepacking aims to reduce wasted computation and memory on padding within batches, for fair evaluation, we do not manually construct batches. Instead, we use actual datasets to randomly sample batches and obtain aggregate metrics with respect to diverse prompt lengths. This also reflects a more realistic setting in which the flow of queries cannot be controlled.

5.2 Baselines

(1)***Full Batching*:** As implemented by Huggingface, this method first determines the maximum prompt length across the batch and appends special padding tokens to shorter prompts until they match the maximum length. It then generates corresponding attention masks to ensure that the language model disregards the padded tokens during computation. Huggingface's inference framework (Wolf et al., 2020) employs this approach for handling prompts of variable lengths, serving as the basis for this baseline's profiling.

(2)***Length-Ordered Batching*:** This baseline assumes access to the full set of user requests, serving as an oracle baseline that can first sort the inputs according to their lengths and sample batches in order to minimize the padding required when using the Full Batching. This method reduces computational overhead on paddings. However, it is not practical in real-world scenarios where user requests arrive in an unpredictable order, and the entire set of requests is not available upfront. In contrast, prepacking does not rely on this assumption, making it more suitable for handling dynamic and continuous streams of input prompts.

These baselines represent the standard practices in widely used LLM inference frameworks like HuggingFace Transformers (Wolf et al., 2020), which do not rely on custom CUDA kernels. Our method is a high-level PyTorch implementation aimed at broad applicability and ease of integration. Comparing against methods that require custom CUDA kernels, such as paged attention in vLLM (Kwon et al., 2023), would not provide a fair comparison, as they involve hardware-specific optimizations beyond the scope of our approach.

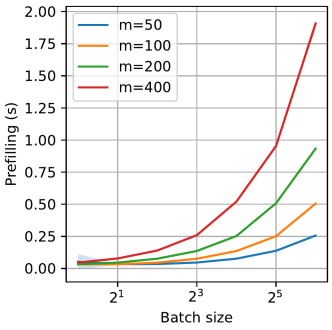
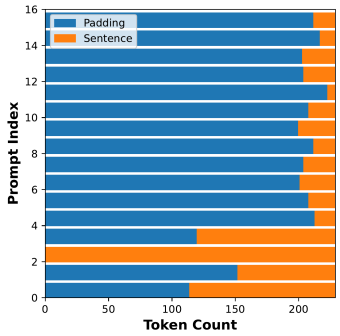


Figure 2: Prefilling latency scaling with batch size k highlights GPU parallelization limits. Results averaged over 100 runs.



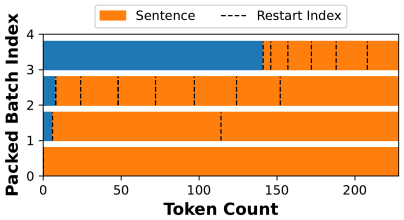


Figure 3: An actual example of one batch sampled from the MMLU dataset shows how a batch of 16 prompts is packed into a compact packed batch. Restart indices denote the point at where independent mask and position encoding are reset to preserve the semantics of each individual prompt.

5.3 Prefilling Time and TTFT

We compare the prefilling time and Time-to-First-Token (TTFT) between prepacking and Full Batching across datasets and models in Figure 4. TTFT measures the total time required for prefilling the KV cache and generating the first token. For our method, TTFT additionally includes an overhead which is the unpacking phase, where we unpack the prompts to their original order for generation. This unpacking phase has a linear time complexity in the number of prompts, which is dominated by the quadratic computational complexity of prefilling. Prepacking consistently outperforms Full Batching with less prefilling time and TTFT, enhancing speed ranging from 1.6x to 3.5x. Moreover, Prepacking has lower inference time standard deviations, attributed to reduced padding overhead, enabling more reliable and predictable performance suitable for applications demanding consistent LLM serving. As shown in Table 1, prepacking significantly reduces the padding ratios across datasets, while the overhead introduced by packing is minimal.

Table 1: Padding ratios (ratio of padding tokens to all tokens) decreased significantly after packing across all datasets, with the packing time overhead being minimal (less than 2.1% of TTFT) with batch size = 32.

Dataset	Unpacked (Padding / Total)	Packed (Padding / Total)	Packing Time (% of TTFT)
MMLU	0.61	0.11	1.28
Wiki256	0.76	0.12	2.03
Wiki512	0.76	0.12	1.55
RLHF	0.67	0.06	1.58
Alpaca	0.60	0.09	1.46
SamSum	0.67	0.06	2.08

5.4 GPU Memory Saving and Utilization

We evaluate Prepacking's GPU memory efficiency, stemming from reduced computation on padded tokens, against other baselines in Figure 6. Prepacking consistently exhibits lower peak memory consumption, which directly translates to the ability to process larger batch sizes without encountering out-of-memory errors. For instance, with the Llama2-1.3B model on the MMLU dataset, prepacking can accommodate batch sizes up to 16x larger during prefilling compared to Full Batching before encountering OOM. This has significant implications for deploying models in resource-constrained environments, where maximizing hardware utilization is crucial. Consequently, as shown in Appendix Figure 13, Prepacking also exhibits lower GPU utilization when operating with the same batch size as the baselines, owing to its reduced computational overhead. A recent work known as FlexAttention (He and Liang, 2024) allows significant memory and performance improvements for sparse attention masks. We demonstrate even compatibility with FlexAttention in Appendix E.

5.5 Enhanced Speedup with Increasing Batch Sizes

In realistic situations, the distribution of batch sizes encountered during language model inference can fluctuate due to non-uniform user requests arrival patterns. To evaluate our method's effectiveness in handling this variability, we conducted experiments across a range of batch sizes for the Llama2-7B and Llama2-1.3B models. The results shown in Figure 7 demonstrate substantial speedup gains achieved by our approach over Full Batching. Larger batch sizes exhibit greater performance improvements with our method, up to **4.5x** and **6x** speedup for the 7B and 1.3B Llama2 models, respectively. This trend stems from the increased likelihood of diverse prompt lengths within larger batches, which

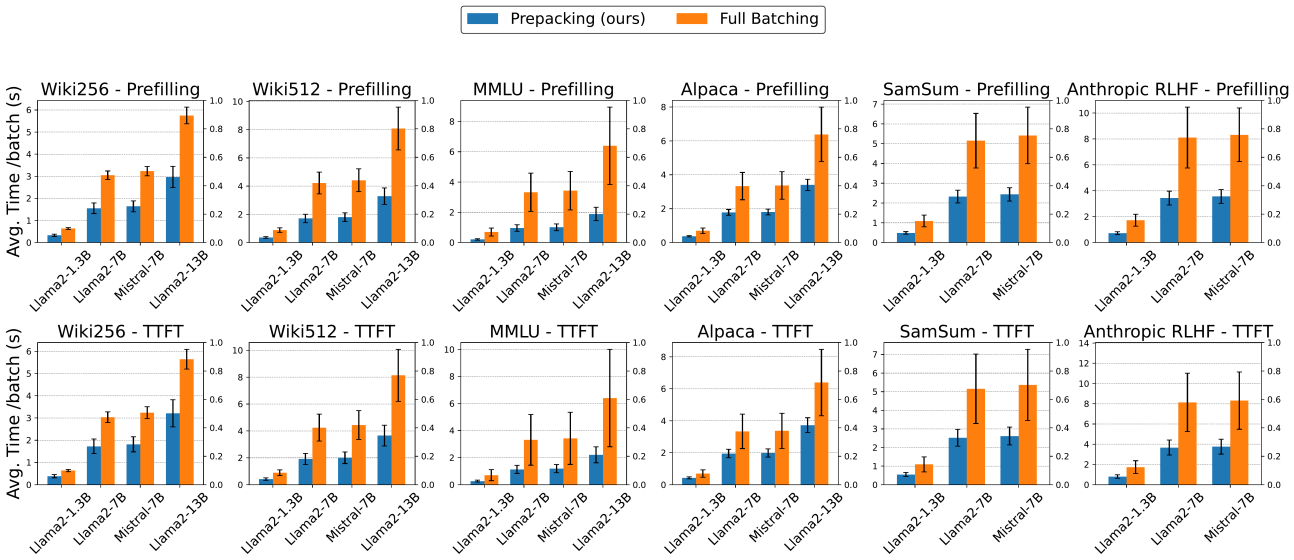


Figure 4: Average inference time per batch for various language models using prepacking and Full Batching, with a batch size of 16. The comparison is conducted across multiple datasets with two metrics, Prefilling Time and TTFT (Time-to-First-Token). Error bars represent the standard deviation of inference times across batches and seed runs. The results show that prepacking consistently leads to reduced inference times compared to Full Batching and exhibits reduced variability, as evidenced by smaller standard deviation errors, indicating more reliable and predictable inference times when adopting prepacking.

leads to more padding overhead for Full Batching. In contrast, our method efficiently handles variable-length prompts via bin-packing, mitigating this overhead.

5.6 Dataset Prepacking vs Length-Ordered Batching

In the previous experiments, we apply prepacking on randomly sampled batches from each dataset. However, this assumes the inability to control the contents of each batch. Given the ability to determine batches, a method to padding inefficiency would be to sort the dataset by length and batch accordingly. We refer to this baseline as *Length-Ordered Batching*. Alternatively, we can create batches after performing prepacking on the dataset as a whole and apply prepacking, i.e. *Dataset Prepacking*. We find that even in this scenario, where one might expect length-ordered batching to have a near optimal runtime by reducing the number of pad tokens, we observe prepacking still exhibits improvements as shown in Figure 5, where we compare the prefilling time per prompt.

5.7 How does the performance gain scale with characteristics of lengths within a batch?

Previously in Section 4.3, we find the runtime of full batching is $\mathcal{O}(km^2)$. Prepacking is $\mathcal{O}(rm^2)$, where k is the original batch size, r is the batch size after prepacking, and m is the maximum prompt length. Therefore, we can estimate the speedup as a function of r/k (Batch Size Reduction). Because in practice it is difficult to predict r from the dataset statistics alone, we can also estimate the speedup as a function of $m - L/k$ (Max Absolute Deviation), which is how much the maximum length of a batch deviates from the mean length. We conduct the analysis on 5000 synthetic prompts with lengths uniformly distributed from 1 to 512, using the Llama2 1.3B model with batch size of 32. As can be seen in Figure 8, these metrics can predict the speedup obtained by using prepacking over full batching. We show more plots with different model and batch size in Appendix D.

5.8 Is Prepacking Compatible With Existing LLM Inference Optimizations?

While we have demonstrated substantial efficiency improvements over prefilling with vanilla Attention over fixed batch sizes, we also consider how prepacking can be used to improve inference in tandem with:

- FlashAttention 2 Dao (2023)
- Continuous Batching Yu et al. (2022)
- PagedAttention Kwon et al. (2023)

While full integration with LLM serving systems that utilize these optimizations, such as vLLM, is infeasible,

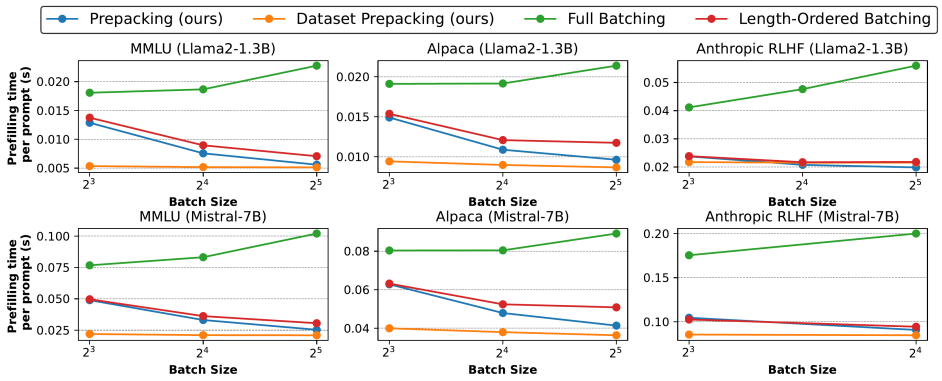


Figure 5: Comparison of prefilling time per prompt. The Dataset prepacking and Length-Ordered Batching benefit from access to the entire dataset, in contrast to Batch prepacking and Full Batching, which operate on a per-batch basis. Dataset prepacking further minimizes prefilling latency through packing when provided with full dataset access. Results are averaged over 5 runs.

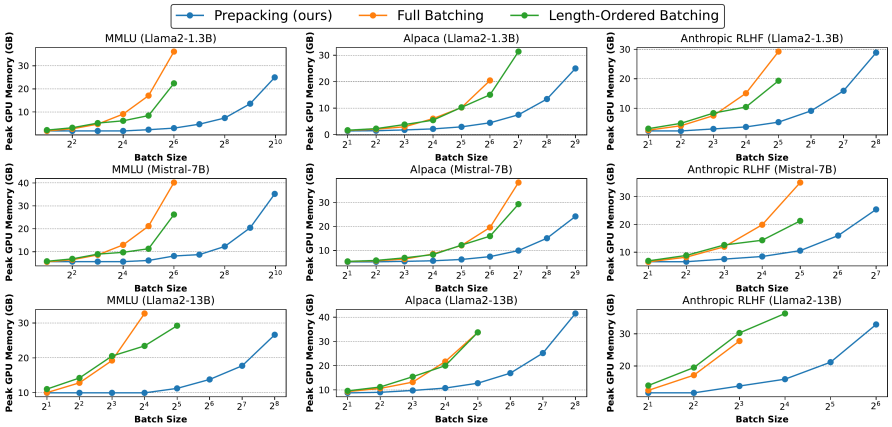


Figure 6: Peak GPU memory usage comparison across models and datasets on a single GPU. Absent data points indicate out-of-memory errors. Prepacking achieves lower peak GPU memory usage and allows for up to **16x larger batch sizes** in prefilling computations than Full Batching and Length-Ordered Batching.

we conduct experiments to showcase that prepacking can be beneficial and complementary to each method in isolation.

FlashAttention 2

Table 2: Performance comparison of Full-batching vs. Prepacking with FlashAttention 2 on average prefill time per batch (s) and max GPU memory (MB).

Method	Avg prefill time	Max GPU Memory
Full-batching + FA2	2.05 ± 1.03	16468.39 ± 0.00
Prepacking + FA2	**0.22 ± 0.06**	**3478.37 ± 0.00**

Surprisingly, we found that FA2 performs worse than vanilla eager attention in the prefilling phase for batches with significant padding. This occurs because the current FlashAttention 2 implementation does not natively support computing attention scores with padding tokens, as documented in the Hugging Face Transformers repository[1]. Our experiments, shown in Table 2, demonstrate that prepacking with FA2 dramatically reduces both prefilling time and GPU memory usage compared to standard batching with FA2. This significant improvement occurs because prepacking substantially reduces the number of padding tokens that create overhead for FlashAttention 2, effectively addressing a known limitation in FA2's handling of padded sequences during inference.

[1]This limitation is documented at: `https://github.com/huggingface/transformers/issues/26990`

Continuous Batching

Table 3: Performance comparison of continuous batching with and without prepacking

Avg Time (s)	Llama 1.3B	Llama 2 7B
Continuous Batching	39.49	139.48
Continuous Batching + Prepacking	**35.58**	**117.38**

We integrate prepacking into a continuous batching framework to speed up prefilling. Since our implementation is PyTorch-based, we follow a PyTorch-based continuous batching framework. In continuous batching, there are 2 stages that require prefilling: the initial prefilling of the first batch, and when new requests

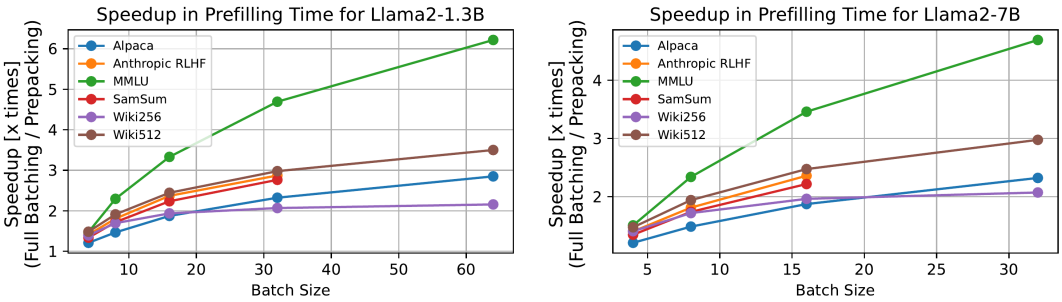


Figure 7: Speed up across various batch sizes for Llama2-1.3B and Llama2-7B. Speed up is calculated as the ratio of the prefilling time with full batching to that of prepacking. Missing data points for Anthropic RLHF and SamSum are due to out-of-memory issues as these two datasets have larger mean prompt length.

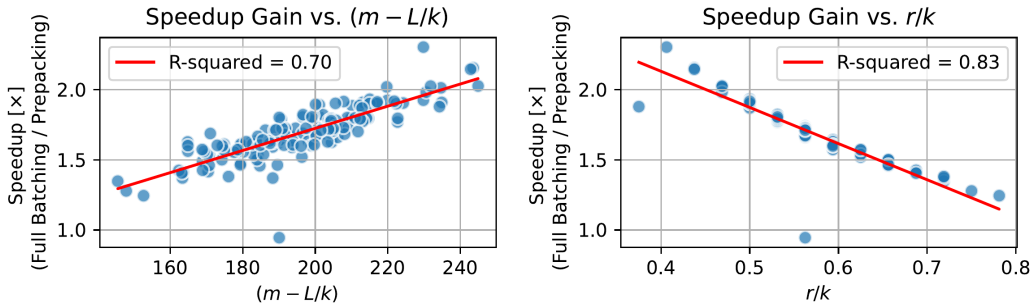


Figure 8: We show that speedup can be predicted from two dataset statistics: Max Absolute Deviation $(m - L/n)$ and Batch Size Reduction (r/n). We perform a linear regression and observe a high correlation between these statistics and observed speedup.

arrive, prefilling for the new batch. Our method can be utilized to speed up both of these prefilling runs. We compared continuous batching with and without prepacking and found that prepacking speeds up continuous batching as shown in Table 3, where we simulated a range of incoming requests with varying sizes and generation lengths (where we randomly generate 200 requests with input lengths up to 512 and max generation length of 50).

Paged Attention

To implement PagedAttention in PyTorch, we replace the typical Huggingface LLM attention call with `flash_attn_with_kvcache`. This function is the same attention mechanism used in vLLM. Although Flash Attention has not implemented sparse masking, we can obtain a lower bound in the speedup that does not exploit the sparsity of independent masking used for prepacking. We implement a simple cache manager, and since we are only measuring prefill time, the cache manager does not need active updating during decoding. Table 4 shows the results with PagedAttention for Llama 1.3B. Thus, prepacking also demonstrates great promise when combined with PagedAttention.

Table 4: Performance comparison of Paged Attention (PA) with and without prepacking on Llama 1.3B

Method	Prefill Time (s)	GPU Utilization (%)
PA + Full batching	0.909	78.306
PA + Prepacking	**0.405**	**54.246**

6 Conclusion

We proposed prepacking, a simple and effective approach to optimize the prefilling computation for LLMs during inference. Our evaluation on typical datasets with varying prompt lengths demonstrates significant speedups compared to standard prefilling computation in Huggingface's implementation. As language models continue to scale and support longer context lengths, addressing the inefficiencies associated with prefilling computation becomes crucial for optimizing inference speed and computational resource allocation. Prepacking provides a promising solution to this challenge, enabling more efficient inference for prompts with varying lengths. In the future, it would be interesting to explore more complex decoding strategies post-prefilling that also incorporate bin packing for further increase in throughput.

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Checklist

1. For all models and algorithms presented, check if you include:
   (a) A clear description of the mathematical setting, assumptions, algorithm, and/or model. [Yes]
   (b) An analysis of the properties and complexity (time, space, sample size) of any algorithm. [Yes]
   (c) (Optional) Anonymized source code, with specification of all dependencies, including external libraries. [Yes/No/Not Applicable]

2. For any theoretical claim, check if you include:
   (a) Statements of the full set of assumptions of all theoretical results. [Not Applicable]
   (b) Complete proofs of all theoretical results. [Not Applicable]
   (c) Clear explanations of any assumptions. [Not Applicable]

3. For all figures and tables that present empirical results, check if you include:
   (a) The code, data, and instructions needed to reproduce the main experimental results (either in the supplemental material or as a URL). [No]
   (b) All the training details (e.g., data splits, hyperparameters, how they were chosen). [Yes]
   (c) A clear definition of the specific measure or statistics and error bars (e.g., with respect to the random seed after running experiments multiple times). [Yes]
   (d) A description of the computing infrastructure used. (e.g., type of GPUs, internal cluster, or cloud provider). [Yes]

4. If you are using existing assets (e.g., code, data, models) or curating/releasing new assets, check if you include:
   (a) Citations of the creator If your work uses existing assets. [Yes]
   (b) The license information of the assets, if applicable. [Yes]
   (c) New assets either in the supplemental material or as a URL, if applicable. [Not Applicable]
   (d) Information about consent from data providers/curators. [Not Applicable]
   (e) Discussion of sensible content if applicable, e.g., personally identifiable information or offensive content. [Not Applicable]

5. If you used crowdsourcing or conducted research with human subjects, check if you include:
   (a) The full text of instructions given to participants and screenshots. [Not Applicable]
   (b) Descriptions of potential participant risks, with links to Institutional Review Board (IRB) approvals if applicable. [Not Applicable]
   (c) The estimated hourly wage paid to participants and the total amount spent on participant compensation. [Not Applicable]

A Mean GPU utilization comparison

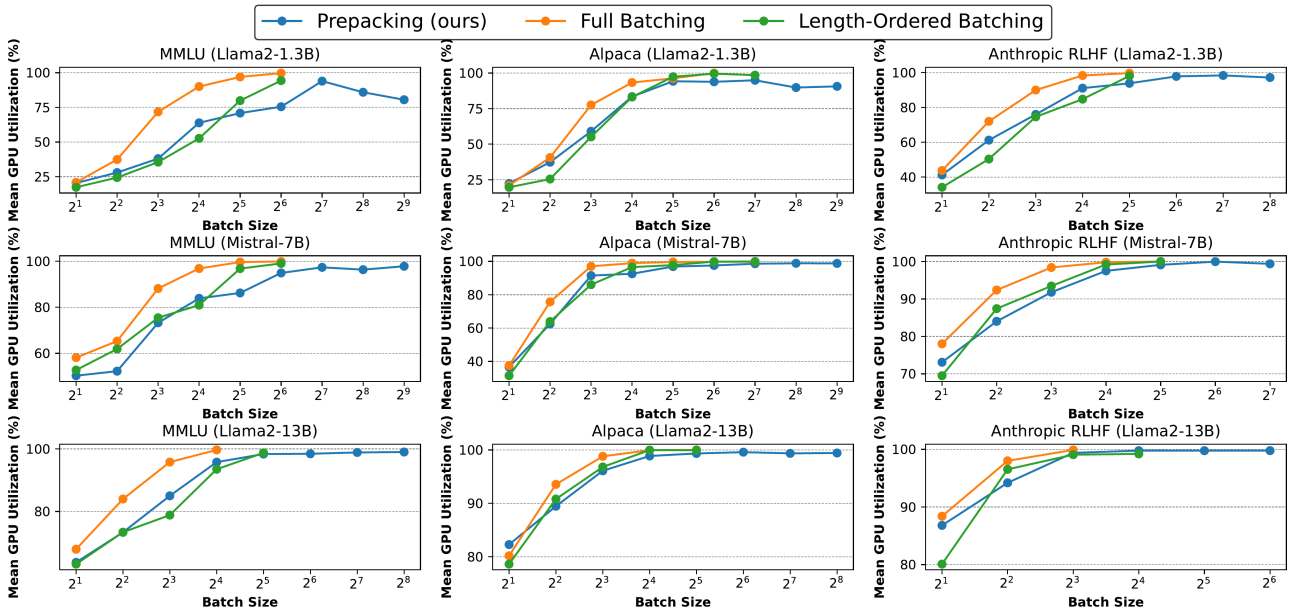

Figure 9: Mean GPU utilization for prefilling the prompts in datasets, sampled with a fixed batch size. Prepacking achieves lightest GPU utilization when the batch size is the same for every method.

B Dataset length distribution statistics

Table 5: Evaluation Datasets Length Statistics. Due to computational resources constraints, we choose subsets from these datasets for evaluation.

Dataset name	Subset Min. / Mean / Max. SeqLength
Wikitext Max SeqLen 256 (Wiki256) (Merity et al., 2016)	1 / 73 / 256
Wikitext Max SeqLen 512 (Wiki512) (Merity et al., 2016)	6 / 120 / 512
MMLU (Hendrycks et al., 2021b)	4 / 64 / 1102
Anthropic HH RLHF (Bai et al., 2022)	22 / 247 / 1620
Alpaca (Taori et al., 2023)	43 / 126 / 527
SamSum (Gliwa et al., 2019)	21 / 169 / 942

C Model details

Table 6: Model architecture used in the evaluations

Model	Num Params	Num layers	Hidden dim	Num heads
Sheared LLAMA 1.3B (Xia et al., 2023)	1.3B	24	2048	16
LLAMA 2 7B (Touvron et al., 2023)	7B	32	4096	32
Mistral 7B (Jiang et al., 2023)	7B	32	4096	32
LLAMA 2 13B (Touvron et al., 2023)	13B	40	4096	40

D How does the performance gain scale with characteristics of lengths within a batch?

We extend our runtime analysis from section 5.7, evaluating prepacking's speedup across various settings using a synthetic dataset with prompt lengths uniformly distributed. The experiments, conducted with the Llama2

1.3B and Llama2 7B, aim to quantify the efficiency gains through Batch Size Reduction (r/k) and Max Absolute Deviation ($m - L/k$). These findings, presented in detailed plots, offer insights into prepacking's performance scalability.

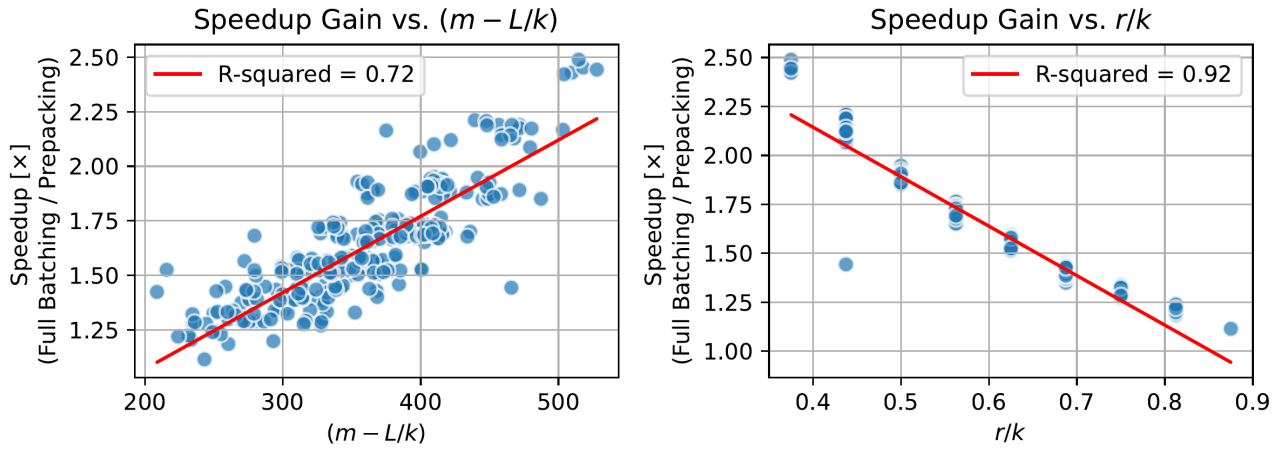

Figure 10: Speedup gains relative to full batching, with respect to Batch Size Reduction (r/k) and Max Absolute Deviation ($m - L/k$), conducted on Llama2 1.3B with batch size 16 and 5000 prompts.

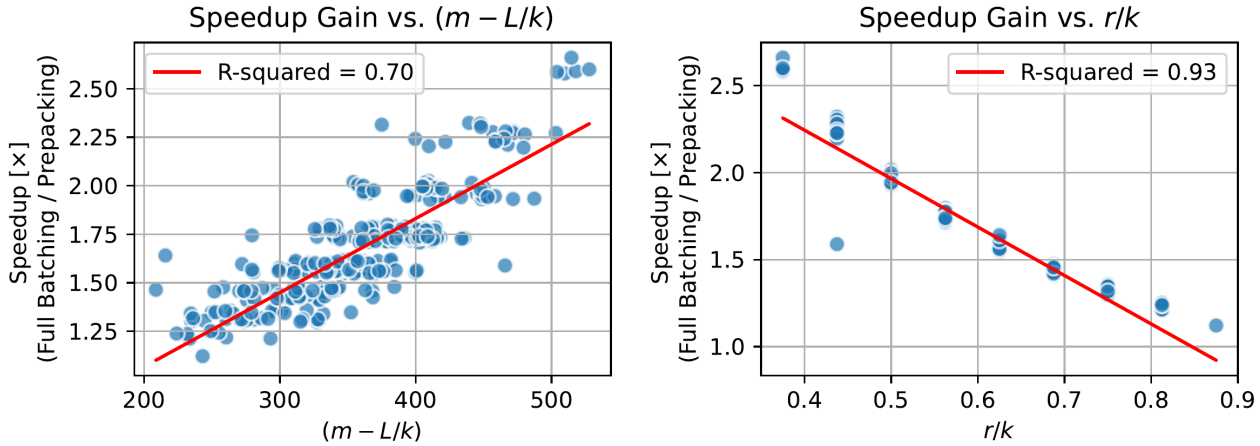

Figure 11: Speedup gains relative to full batching, with respect to Batch Size Reduction (r/k) and Max Absolute Deviation ($m - L/k$), conducted on Llama2 7B with batch size 16 and 2500 prompts.

E Use FlexAttention To Speed Up Prepacking

Table 7 presents preliminary results of implementing Prepacking with FlexAttention (He and Liang, 2024), a novel PyTorch API that enables efficient and flexible attention variants. FlexAttention compiles customized masking operations into kernels through torch.compile, allowing for performance competitive with handwritten implementations. Our initial findings demonstrate that FlexAttention yields improved speed compared to our primary PyTorch implementation. This approach suggests potential for further performance gains and increased adaptability in Prepacking through the use of FlexAttention.

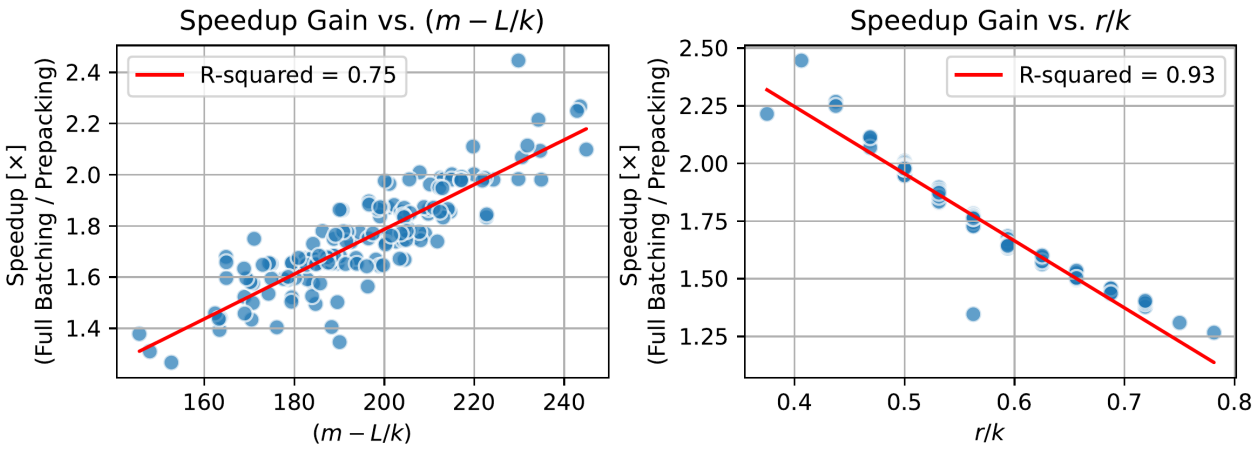

Figure 12: Speedup gains relative to full batching, with respect to Batch Size Reduction (r/k) and Max Absolute Deviation ($m - L/k$), conducted on Llama2 7B with batch size 32 and 5000 prompts.

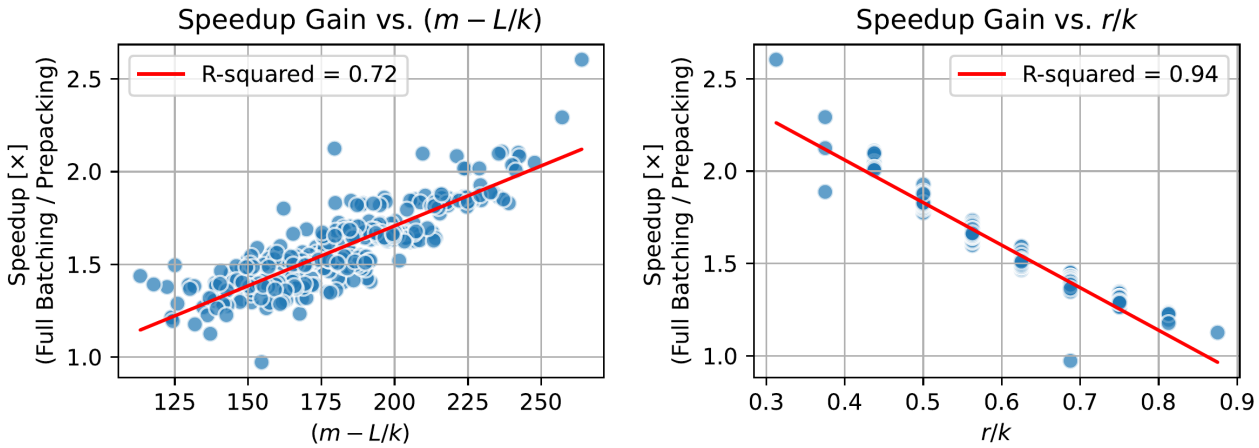

Figure 13: Speedup gains relative to full batching, with respect to Batch Size Reduction (r/k) and Max Absolute Deviation ($m - L/k$), conducted on Mistral 7B with batch size 16 and 5000 prompts.

Method	Avg prefill Time /batch (s)	Max GPU Memory (MB)
Full-batching	0.888 ± 0.365	17488.229 ± 0.000
Prepacking + PyTorch	0.531 ± 0.155	3375.934 ± 0.000
Prepacking + FlexAttn	0.491 ± 0.120	3860.999 ± 0.000

Table 7: Comparison of methods on MMLU dataset (batch size = 32, model = llama1b)

F Limitations

Our prepacking algorithm is currently only used for the prefilling stage. After prepacking, our current approach is to repack and then generate normally. This is suboptimal as it involves extra bookkeeping and rearrangement in the memory space. Extending the prepacking algorithm to the generation stage will be an interesting and efficient future direction.

Additionally, we did not compare our method with hardware-aware approaches or CUDA kernel approaches, which can be more efficient than prepacking. However, we do not consider this a major limitation as we demonstrate

the usability of our algorithm, which can be fully implemented in PyTorch.