Draft & Verify: Lossless Large Language Model Acceleration via Self-Speculative Decoding

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Abstract

We present a novel inference scheme, self-speculative decoding, for accelerating Large Language Models (LLMs) without the need for an auxiliary model. This approach is characterized by a two-stage process: drafting and verification. The drafting stage generates draft tokens at a slightly lower quality but more quickly, which is achieved by selectively skipping certain intermediate layers during drafting. Subsequently, the verification stage employs the original LLM to validate those draft output tokens in one forward pass. This process ensures the final output remains *identical* to that produced by the unaltered LLM. Moreover, the proposed method requires no additional neural network training and no extra memory footprint, making it a plug-and-play and cost-effective solution for inference acceleration. Benchmarks with LLaMA-2 and its variants demonstrated a speedup up to 1.99×.[1]

1 Introduction

Transformer-based Large Language Models (LLMs), such as GPT-3/4, PaLM, and LLaMA, have been widely adopted in various real-world applications (Bommasani et al., 2021; Liang et al., 2022; Brown et al., 2020; Min et al., 2022; Chan et al., 2022; Touvron et al., 2023). However, their inference costs have raised significant concerns, especially for latency-sensitive scenarios (Pope et al., 2022). The main efficiency bottleneck is the *autoregressive decoding* process. This process decodes each output token sequentially, leading to a high number of Transformer calls; furthermore, each Transformer call is typically memory bandwidth-bound, resulting in low computation utility and thus longer wall-clock time (Shazeer, 2019). For instance, decoding 128 tokens autoregressively using LLaMA-2-13B on an A100 GPU can take up to 100× longer than a sequence-level forward pass on the same number of tokens, highlighting the substantial inefficiency inherent in the current decoding process.

Established model compression techniques such as quantization (Han et al., 2015), pruning (Molchanov et al., 2016), and distillation (Hinton et al., 2015) have been employed to alleviate these costs. While these solutions have proven extremely effective, they usually require changing the model architecture, changing the training procedure, retraining or fine-tuning the models, and do not maintain identical outputs.

In parallel to model compression, *speculative execution* is being explored to accelerate the autoregressive decoding process (Leviathan et al., 2023; Chen et al., 2023). These methods train an auxiliary **draft model** that can quickly generate some draft output tokens. Subsequently, the original LLM, referred to as the **verify model**, then checks the acceptability of these draft tokens with one single forward pass. This verification step ensures that the outputs are derived from the original LLM's probability distribution.

However, an essential issue of existing speculative execution methods is the need to identify or train a suitable draft model that can generate outputs consistent with the verify model. It becomes more tricky when the LLM is already a fine-tuned model, e.g. LLaMA-2-Chat (Touvron et al., 2023), CodeLLaMA (Rozière et al., 2023). How to find or train a draft model that can effectively mimic the outputs of such a tailored model is a formidable task, with no straightforward or guaranteed solutions. Furthermore, the introduction of an additional draft model escalates the GPU memory overhead, increasing deployment challenges particularly on devices with restricted memory capacity.

In this paper, we present *self-speculative decoding*, a novel approach to accelerate the inference of LLMs. This method builds on the principles of

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[1]Code is available at https://github.com/dilab-zju/self-speculative-decoding.

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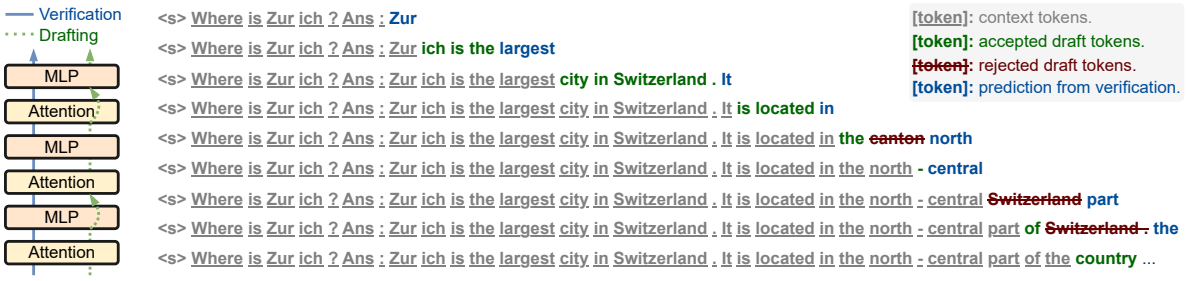


Figure 1: Visualization of the self-speculative decoding process. The verification stage evaluates all drafted tokens in a single forward pass, with accepted tokens marked in green and rejected tokens highlighted in red. Each verification step also predicts one more token, which is denoted in blue.

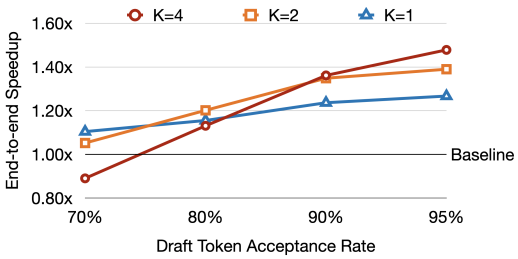


Figure 2: Impact of the number of draft tokens (K) and acceptance rate on end-to-end speedup. The draft model is assumed to be 2× faster than the verify model.

speculative execution, but with a unique twist: it utilizes one LLM for both drafting and verification stages. The key insight driving our approach is the observation that skipping certain layers in LLMs does not significantly compromise the generation quality (Liu et al., 2023). As such, by selectively bypassing some intermediate layers, we can use the LLM itself to generate draft tokens. These tokens are then verified by the original LLM in a single forward pass. Figure 1 illustrates this two-stage decoding process. The blue arrow indicates the inference path of the original model, while the green arrow depicts the inference path during the drafting stage. Notably, both inference paths share the same model so we do not need a standalone draft model with extra memory overhead.

Implementing self-speculative decoding poses two main challenges: (a) determining which layers and the number of layers to skip during drafting, and (b) deciding the timing to stop generating draft tokens. To tackle the first challenge, we formulate it as an optimization problem, which accepts the combinations of layers to bypass as input and aims to minimize the average inference time per token. We employ Bayesian optimization (Jones et al., 1998) to solve this problem. The optimization is performed offline at the model level, and the searched layer combinations are fixed. The second challenge pertains to determining the optimal number of draft tokens (K) to generate. As shown in Figure 2, the choice of K significantly influences the end-to-end speedup: for an acceptance rate below 80%, $K = 1$ is optimal, and for rates above 80%, a larger K is necessary. This observation underscores that a static K is not universally applicable. To tackle this variability, we introduce an adaptive draft-exiting mechanism, which stops generating draft tokens once its confidence level drops below a threshold. This intervention prevents unnecessary computation and potential discard of additional draft tokens, thereby enhancing efficiency.

To summarize, our main contributions are: (1) *Inference scheme*: we propose self-speculative decoding, a practical, plug-and-play solution for inference acceleration that does not require further neural network training and avoids additional memory overhead; (2) *Optimization strategies*: we adopt Bayesian optimization to select which layers to skip during drafting and propose a simple yet effective method to adaptively determine the number of draft tokens; (3) *Evaluation*: we evaluate our method on text summarization and code generation tasks, and the experimental results indicate that our method can achieve up to 1.99× in end-to-end speedup.

2 Related Work

Transformer-based LLM inference. As LLMs continue to evolve rapidly, we are seeing a surge of systems specifically engineered for LLM inference, including Faster Transformer (NVIDIA), Orca (Yu et al., 2022), LightSeq (Wang et al., 2021), PaLM inference (Pope et al., 2022), TurboTransformers (Fang et al., 2021), Deepspeed Inference (Aminabadi et al., 2022), FlexGen (Sheng et al., 2023), Text Generation Inference (HuggingFace, 2023), etc. The token generation phase typically takes up

the majority of the end-to-end inference time compared to the prompting encoding phase. Despite the introduction of system optimizations by those state-of-the-art systems to improve the inference speed, there is still a gap in the careful co-design of algorithms and systems. This is necessary to fully harness the potential of hardware efficiency during LLM inference computation.

Model Compression. Various model compression methods have been studied for model inference. For example, quantization (Han et al., 2015; Jacob et al., 2018; Nagel et al., 2019; Zhao et al., 2019; Yao et al., 2022; Park et al., 2022; Dettmers et al., 2022; Xiao et al., 2022; Frantar et al., 2022), pruning or sparsification (Molchanov et al., 2016; Liu et al., 2018; He et al., 2019; Hoefler et al., 2021; Frantar and Alistarh, 2023; Liu et al., 2023; Bansal et al., 2022), and distillation (Hinton et al., 2015; Cho and Hariharan, 2019; Tang et al., 2019; Touvron et al., 2021) have been applied to speed up the inference of the machine learning model, particularly LLMs. While these solutions are extremely effective, they often necessitate modifications to the model architecture and the training procedure. This usually involves re-training or fine-tuning the models. And it is important to note that these methods do not result in identical outputs.

Speculative Execution. Speculative execution (Burton, 1985; Hennessy and Patterson, 2011) is employed in computer architecture where a system performs some task in advance if that task is known to be required after the previous task. Speculative decoding (Chen et al., 2023; Leviathan et al., 2023) has been proposed as an effective strategy to boost the inference speed of LLMs. Previously, (Stern et al., 2018) proposed to use block-wise parallel decoding to accelerate greedy decoding of attention models. However, these methods need to train or select a high-quality draft model, and also result in increased memory overhead. Yang et al. (2023) proposed to copy the reference text tokens and validate them in a forward pass. However, this method relies on the repetitiveness assumption, and thus does not apply to general scenario generation. In contrast, our approach does not incur additional memory overhead and does not hinge on explicit assumptions about data distribution.

Early Exit. Early exit allows the model to choose different calculation paths based on the input during the inference process to achieve acceleration.

Algorithm 1 Autoregressive Decoding (Greedy)

1: Given model $p(x|x_1, ..., x_t)$, prompt $x_1, ..., x_t$ and target sequence length T.
2: **for** i = t, ..., T-1 **do**
3: $\quad x_{i+1} \leftarrow \arg\max p(x|x_1, ..., x_i)$
4: **return** $x_1, ..., x_T$

Various early exit techniques for encoder-only Transformers (Devlin et al., 2019) have been proposed (Xin et al., 2020b; Schwartz et al., 2020; Liu et al., 2020; Xin et al., 2020a; Hou et al., 2020; Zhou et al., 2020; Liao et al., 2021; Zhu, 2021; Li et al., 2021; Sun et al., 2022). Recently, (Schuster et al., 2022) further verified the effectiveness of early exit on the encoder-decoder LLM (Raffel et al., 2020). Inspired by these works, we opt to skip certain intermediate layers during drafting.

3 Method

In this section, we first go through the standard autoregressive decoding. Subsequently, we provide a detailed depiction of our proposed method, including selectively skipping layers during drafting, and adaptively determining the number of draft tokens.

3.1 Standard Autoregressive Decoding

Existing LLMs typically follow an autoregressive decoding process. Given a prompt sequence $x_1, ..., x_t$, the model calculates the probability distribution of the next token $p(x|x_1, ..., x_t)$. We present a greedy decoding process in Algorithm 1. In practice, instead of choosing the token with the highest probability (as in greedy decoding), we can sample tokens based on their probability distribution, which introduces some randomness and generates more diverse outputs.

Ideally, the computational cost of autoregressive decoding is comparable to that of sequence-level forward processing for an equivalent number of tokens.[2] However, this decoding process is significantly bounded by the memory bandwidth of the device. When decoding each token, all the model parameters need to pass through the accelerator chip. So the model size divided by the memory bandwidth gives a hard ceiling on the decoding speed, resulting in a much longer inference time.

[2]In fact, due to the causal nature of language modeling, autoregressive decoding could potentially save some attention computation.

Algorithm 2 Self-Speculative Decoding (Greedy)

LLM $p(x|\boldsymbol{z}^*, x_1, ..., x_t)$ where $x_1, ..., x_t$ is the prompt, $\boldsymbol{z}^*$ is a vector that represents the specific layers to bypass; target sequence length T; max draft tokens to generate K. The $p(x|\vec{0}, x_1, ..., x_t)$ denotes original LLM, where $\vec{0}$ is a zero vector, indicating all layers are used in inference.
$i \leftarrow t$
while $i < T$ **do**
  for $j \leftarrow i, ..., i + K$ **do** ▷ Drafting Stage
    $x_{j+1} \leftarrow \arg\max p(x|\boldsymbol{z}^*, x_1, ..., x_j)$
    if need to exit drafting (§3.4) **then**
      Break
  for $i \leftarrow i, ..., j$ **do** ▷ Verification Stage
    if $x_{i+1} \neq \arg\max p(x|\vec{0}, x_1, ..., x_i)$ **then**
      $x_{i+1} \leftarrow \arg\max p(x|\vec{0}, x_1, ..., x_i)$
      Break
  $i \leftarrow i + 1$
  If all draft tokens are accepted, generate next token $x_{i+1} \leftarrow \arg\max p(x|\vec{0}, x_1, ..., x_i)$ and $i \leftarrow i + 1$
return $x_1, ..., x_T$

3.2 Self-Speculative Decoding

To mitigate the inherent inefficiency of autoregressive decoding, speculative decoding can be employed to enhance the inference speed of LLMs. This strategy involves two models: an LLM that we want to optimize, and a draft model that runs faster, albeit potentially at a lower quality. Speculative decoding can be explained as a two-stage process: (1) drafting: the draft model first generates K draft tokens from a given prompt sequence $x_1, ..., x_i$, denoted as $x_{i+1}, ..., x_{i+K}$. (2) verification: following the drafting stage, the original LLM is then employed to validate these draft tokens. This validation is accomplished in a single forward pass, where the LLM predicts the probability distributions for each draft token and assesses whether they align with the draft tokens. Once a draft token x_j is not validated, we use the original LLM's prediction to override x_j, and start the next round of drafting beginning from token x_{j+1}.

The above process is based on the observation that computing the forward pass of a short continuation of tokens in parallel is not much slower than that of a single token. Consequently, the verification stage could be significantly more efficient than decoding tokens using the original LLM in standard autoregressive decoding.

In contrast to existing methods that use a standalone draft model to obtain draft tokens, our paper proposes a novel 'self-speculative' approach. We employ the original LLM itself for both the drafting and verification stages. During the drafting stage, the LLM selectively skips some of its intermediate layers so as to generate draft tokens quicker. Subsequently, these draft tokens are verified by the original LLM. Algorithm 2 presents a detailed description of the greedy decoding process. A complete sampling-based decoding process is elaborated in Appendix L.

Despite the simplicity of the main idea of self-speculative decoding, it poses several challenges:

Challenge 1: First, it is non-trivial to determine which layers and the number of layers to skip during drafting. If an excessive number of layers are skipped, the quality of the draft could be significantly compromised. This could result in a low acceptance rate in the verification stage, consequently increasing the overall inference time. On the other hand, if fewer layers are skipped, it ensures a higher acceptance, but also caps the maximum speedup that could be achieved.

Challenge 2: It is hard to decide when to stop the generation of draft tokens. As shown in Figure 2, the choice of the number of draft tokens to generate significantly influences the end-to-end speedup. In speculative decoding, if a draft token is rejected, all subsequent draft tokens will be discarded. Therefore, generating an excessive number of draft tokens could lead to unnecessary computation, thereby increasing the inference time.

In Sections 3.3 and 3.4, we will detail our approach to address these two challenges respectively.

3.3 Selection of Skipped Layers

The selection of skipped layers is essential in our method, shaping the configuration of the draft model and, consequently, the speedup achieved via self-speculative decoding. This selection process must carefully balance two key factors: the draft model's 'effectiveness' and 'efficiency.' Both are intrinsically linked to the selection of skipped layers and significantly influence the overall performance of our method. Specifically:

(1) The 'effectiveness' of the draft model is quantified by the acceptance rate, which measures the agreement between the draft and verify models. However, we note that an exclusive focus on optimizing the acceptance rate could lead to no layers being skipped, i.e. the draft model identical to the verify model, resulting in an acceptance rate of 100%, but without any speedup.

(2) On the other hand, the 'efficiency' of the draft model can be quantified by the number of layers in the draft model. Indeed, minimizing the number of layers can reduce the inference latency of the draft

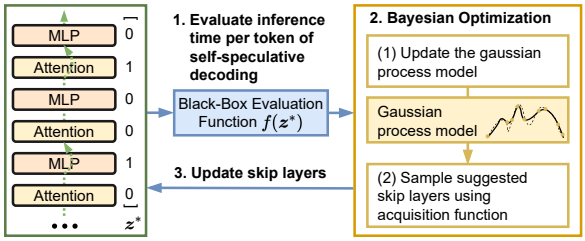


Figure 3: Illustration of using Bayesian optimization to search the best combination of skip layers that results in the lowest average token inference time.

model, but an extreme setup where all layers are skipped would result in the draft model generating low-quality tokens. This would drastically lower the acceptance rate, negating any potential speedup.

In this section, we frame the layer selection process as an optimization problem, our primary objective is to optimize the *average inference time per verified token*. This metric provides a comprehensive measure of the end-to-end inference time, including both drafting and verifying stages, normalized by the number of verified tokens.

Objective Function. This metric is a function of the selection of layers to be skipped in the draft model. The function, represented as $f(\boldsymbol{z})$, takes the selection of layers ($\boldsymbol{z}$) as input and returns the average inference time per *verified* token on a development set. Here, $\boldsymbol{z}$ is a vector that represents the layers to be skipped.

Optimization Problem. The optimization problem's goal is to find the input $\boldsymbol{z}^*$ that minimizes the objective function $f(\boldsymbol{z})$. This problem can be formally expressed as:

$$\boldsymbol{z}^* = \arg\min_{\boldsymbol{z}} f(\boldsymbol{z}), \quad s.t.\ \boldsymbol{z} \in \{0,1\}^L. \tag{1}$$

While a brute force search could find the globally optimal solution for smaller models with a manageable solving space, it becomes prohibitively expensive for larger language models with many layers (e.g., $L = 160$ for LLaMA-2-70B).

To tackle this, we employ Bayesian optimization (Jones et al., 1998). As shown in Figure 3, it iteratively selects new inputs $\boldsymbol{z}^*$ for evaluation, based on a surrogate model of the objective function, i.e. Gaussian process (Rasmussen et al., 2006), and an acquisition function. The latter balances exploration (testing inputs where the model's prediction is uncertain) and exploitation (testing inputs where the model anticipates a favorable result). This procedure continues until a predetermined number of iterations is reached. We use the obtained $\boldsymbol{z}^*$ to accelerate text generation, and $\boldsymbol{z}^*$ is fixed for each model (i.e., generating draft model at model-level) without further updating. When the draft model's target tasks vary significantly, task-level optimization is more appropriate to achieve good performance. Specifically, building the development set of optimization process from a single data source to mitigate inter-task interference.

In addition, while we here adopt skipping intermediate layers as a simple yet effective strategy to expedite the drafting stage, our scheme can be integrated with quantization (Dettmers et al., 2022) and sparsification (Sun et al., 2023) to further reduce resource consumption, as detailed in Appendix G.

3.4 Adaptive Draft-Exiting Mechanism

Our self-speculative decoding approach incorporates an adaptive draft-exiting mechanism to enhance computational efficiency during the drafting stage. In speculative decoding, if a draft token is rejected, all subsequent draft tokens will be discarded accordingly. The draft-exiting mechanism prevents the wasteful allocation of computational resources toward draft tokens that are less likely to be accepted in the verification stage.

Specifically, it compares the predicted probability of each draft token against a threshold γ. If the predicted probability falls below γ such that $p(x_{t+1}|x_1, ..., x_t) < \gamma$, indicating low confidence, it immediately stops drafting. This approach ensures a better use of computing by focusing on the generation and verification of high-quality tokens, thereby improving the overall efficiency.

Moreover, it is worth noting that a static threshold may not accurately reflect the actual acceptance rate between the drafting and verification stages. For example, more challenging examples with a lower acceptance rate would be better served by a higher γ. To avoid the need for case-by-case threshold determination, we use an adaptive threshold that adjusts dynamically according to an updating rule, thereby allowing for an accurate reflection of the acceptance rate and better handling of examples in different difficulties. We denote the acceptance rate (AR) at e-th drafting stage as AR_e. Consequently, the update rule is defined as follows:

$$AR \leftarrow \beta_1 AR + (1-\beta_1) AR_e, \tag{2}$$

$$\tilde{\gamma} = \begin{cases} \gamma + \epsilon, & \text{if } AR \leq \alpha \\ \gamma - \epsilon, & \text{otherwise} \end{cases}, \tag{3}$$

$$\gamma \leftarrow \beta_2 \gamma + (1-\beta_2)\tilde{\gamma}, \tag{4}$$

where α represents a target acceptance rate (another anchor is discussed in Appendix K), ϵ is the update step-size, and β_1 and β_2 are factors designed to mitigate fluctuations of γ and AR respectively. Notably, when e is 1, $\beta_1 = 0$. We update γ after each verification stage. This updating rule ensures that the acceptance rate remains in close proximity to a target acceptance rate α.

4 Evaluation

4.1 Setup

We evaluate a diverse range of models including LLaMA-2-13B, LLaMA-2-13B-Chat, CodeLLaMA-13B, and LLaMA-2-70B. Detailed setup can be found in Appendix B. We perform Bayesian optimization[3] (BO) for 1000 iterations to select the skipped layers in the drafting stage[4]. Results of tuning the number of BO iterations are reported in Appendix D. The datasets include CNN/Daily Mail (CNN/DM), Extreme Summarization (XSum), and HumanEval. These tasks cover the evaluation of text and code generation capabilities. Appendix H shows effectiveness on more diverse tasks such as solving math problems and open-domain chitchat. We perform 1-shot evaluation for CNN/DM and XSum, and compare the ROUGE-2 (Lin, 2004). We compare pass@1 and pass@10 (Kulal et al., 2019) for HumanEval. We randomly sample 1000 instances from the testset for CNN/DM and XSum.

4.2 Main Results

We evaluate the performance of our decoding scheme, denoted as 'Self-Speculative', with both greedy decoding (temperature = 0.0) and random sampling (temperature = 0.2/0.6), across text and code generation. The baseline is 'Autoregressive', which uses the original model to perform standard autoregressive decoding. The experiments involve various scales of LLaMA-2 and its fine-tuned models. The results can be found in Tables 1 and 2. We visualize the layer skipping distribution for different models in Section 4.8.

For text generation tasks, Table 1 shows that our method, when applied with temperature settings of 0.0 and 0.2 achieves considerable speedups ranging from 1.210× to **1.992**×. Another important observation from these results is the minimal to nonexistent loss in ROUGE-2[5], which verifies a core advantage of our decoding scheme, namely *consistent output quality*. In Appendix J.1, we compare the ROUGE-2 with other mainstream LLMs and evaluate the various metrics (ROUGE-1 and ROUGE-L) to quantitatively show our output quality. Moreover, the case study in Appendix J.2 qualitatively presents consistent output examples. In particular, our approach can be effectively applied on LLaMA-2-13B-Chat, a fine-tuned LLaMA-2-13B for conversation scenarios, indicating the compatibility of our method with fine-tuned models. This effectively addresses the dependency of the original speculative decoding method on high-quality draft models, which can be challenging to train and obtain, especially for fine-tuned models. Furthermore, the higher speedup achieved on LLaMA-2-70B suggests that larger models introduce more redundancy. This allows the drafting stage to skip a larger percentage of intermediate layers, thereby enhancing the overall speedup.

We also tested CodeLLaMA-13B, another fine-tuned LLaMA-2-13B for code generation. The performance on larger CodeLLaMA-34B is presented in Appendix I. We used the HumanEval benchmark. Table 2 shows that we achieve speedups of 1.345× and 1.456×, respectively, while maintaining similar task scores in terms of pass@1 and pass@10. This further validates the compatibility of our scheme for coding.

4.3 Impact of Skipped Layer Selection

To investigate the impact of skipped layer selection, we conduct experiments on LLaMA-2-13B, which comprises 80 layers. Throughout the BO process, we track the number of layers skipped, denoted as $||z^*||$, and the speedup relative to the autoregressive baseline. Figure 4 shows the results, where the dashed line indicates the maximum speedup for runs that skip the same number of layers.

These results reveal that: (1) The peak end-to-end speedup is observed when about half of the layers are skipped during the drafting stage; (2) The specific combination of layers skipped also plays a significant role. In particular, an inappropriate combination of skipped layers can actually result in a decrease in the end-to-end inference speed. (3) There is a noticeable drop in speedup when more than 42 layers are skipped. This suggests that the

[3] https://github.com/bayesian-optimization/BayesianOptimization (MIT License) is used.

[4] Appendix B reports the offline BO time at model-level.

[5] We attribute any slight differences observed in the case of greedy decoding to numerical rounding errors.

Model	Method	Temp.	CNN/DM		XSum	
			ROUGE-2	Speedup	ROUGE-2	Speedup
LLaMA-2-13B	Autoregressive	0.0	0.106	1.000×	0.124	1.000×
LLaMA-2-13B	Self-Speculative	0.0	0.108	1.572×	0.125	1.429×
LLaMA-2-13B	Autoregressive	0.2	0.111	1.000×	0.117	1.000×
LLaMA-2-13B	Self-Speculative	0.2	0.111	1.529×	0.117	1.377×
LLaMA-2-13B-Chat	Autoregressive	0.0	0.144	1.000×	0.109	1.000×
LLaMA-2-13B-Chat	Self-Speculative	0.0	0.143	1.409×	0.109	1.224×
LLaMA-2-13B-Chat	Autoregressive	0.2	0.143	1.000×	0.106	1.000×
LLaMA-2-13B-Chat	Self-Speculative	0.2	0.145	1.383×	0.108	1.210×
LLaMA-2-70B	Autoregressive	0.0	0.130	1.000×	0.118	1.000×
LLaMA-2-70B	Self-Speculative	0.0	0.130	1.992×	0.118	1.598×
LLaMA-2-70B	Autoregressive	0.2	0.131	1.000×	0.108	1.000×
LLaMA-2-70B	Self-Speculative	0.2	0.131	1.964×	0.110	1.560×

Table 1: Evaluation on text generation tasks. 'Speedup' represents the acceleration of average inference time per token compared to the 'Autoregressive' baseline on the same setting.

Model	Method	HumanEval		Speedup
CodeLLaMA-13B	Autoreg.	pass@1	0.311	1.000×
CodeLLaMA-13B	Self-Spec.	pass@1	0.317	1.456×
CodeLLaMA-13B	Autoreg.	pass@10	0.659	1.000×
CodeLLaMA-13B	Self-Spec.	pass@10	0.659	1.345×

Table 2: Evaluation on code generation tasks. We use greedy decoding for pass@1 and random sampling with a temperature of 0.6 for pass@10.

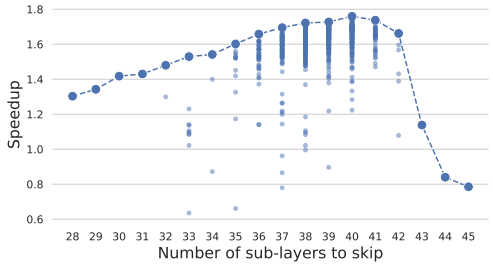


Figure 4: Speedup vs the number of skipped layers. These results are derived from the BO process.

quality of drafting significantly deteriorates when an excessive number of layers are omitted.

These findings indicate the importance of layer selection in the implementation of self-speculative decoding. However, alternative layer skipping strategies do not achieve satisfactory speedup compared to BO, as detailed in Appendix C.

Performance degradation in drafting may be compensated by adopting *aggressive skipping* strategy and further training the draft model on a small amount of data, as described in Appendix E. This finding aligns with the Sheared-LLaMA (Xia et al., 2023), which shows the effectiveness of pruning followed by fine-tuning on a small corpus.

4.4 Effectiveness of Draft-Exiting

Here we explore the effectiveness of the adaptive draft exit mechanism, specifically whether a threshold is needed and whether a static threshold is sufficient. Our settings are LLaMA-2-13B, CNN/DM, and greedy decoding.

Fixed Number of Draft Tokens. We evaluated a self-speculative decoding variant where the draft model generates a constant number K of tokens. As Table 3 shows, speedup initially increases with K, then decreases. This pattern arises as a large K (e.g., $K = 8$) produces many tokens likely to fail verification, wasting computation in drafting.

While an appropriate K, e.g. $K = 4$, can partially alleviate this issue, a static setting limits the draft model's potential and achieves only a modest speedup (1.44×). This is because a static K does not adapt to the complexity of different instances. Ideally, we should use a larger K for simpler instances and a smaller K for challenging ones.

Moreover, Table 3 reveals that the acceptance rate and speedup do not have a direct proportionality. For instance, when $K = 2$, the acceptance rate peaks at 0.924, yet the speedup is only 1.37×. This discrepancy is due to the overly conservative $K = 2$, which underutilizes the draft model's capacity. By generating fewer draft tokens, we miss opportunities to produce more valid draft tokens, thus limiting the overall speedup.

Draft-Exiting with Static Threshold. Another variant is to stop generating draft tokens if the confidence score falls below a predefined static threshold. Table 4 shows that different static thresholds have large differences in acceleration (1.38×~1.58×). This highlights the importance of adaptively determining the appropriate threshold to optimize the speedup. Specifically, we observe that high thresholds (γ=0.8) tend to underestimate the capabilities of the drafting model. Despite a

K	2	4	6	8	Adaptive
ROUGE-2	0.107	0.107	0.107	0.107	**0.108**
AR	**0.924**	0.865	0.807	0.748	0.919
Speedup	1.37×	1.44×	1.42×	1.36×	**1.57**×

Table 3: Drafting with different K values.

γ	0.2	0.4	0.6	0.8	Adaptive
ROUGE-2	0.107	0.107	0.107	0.107	**0.108**
AR	0.749	0.852	0.909	**0.935**	0.919
Speedup	1.38×	1.52×	**1.58**×	1.55×	1.57×

Table 4: Static draft-exiting threshold γ with $K = 12$.

high acceptance rate (AR=0.935), this does not necessarily result in the best speedup due to a reduced number of drafting tokens (1.55×). Conversely, a lower threshold (γ=0.2) tends to overestimate the drafting model's capabilities, leading to a significantly lower acceptance rate (AR=0.749), wasting computational resources during the drafting stage, and thereby leading to slower inference speed (1.38×).

Draft-Exiting with Adaptive Threshold. To address the issue of optimal threshold determination, we propose an adaptive draft-exiting mechanism. Specifically, we evaluate the acceptance rate and compare it to a target acceptance rate. The threshold is updated with an updating rule depicted in Section 3.3. Table 4 shows that the speedup achieved by our adaptive threshold update method (1.57×) is comparable to, if not superior to, the speedup achieved with careful tuning of static thresholds. This indicates that dynamic threshold updating yields efficient and stable inference acceleration. This is mainly because the acceptance rate gets closer to the target AR by adjusting the γ value in a timely manner for instances of varying difficulties. Also, Appendix F reveals the adaptive draft-exiting is insensitive to changes in K.

4.5 Evolution of Draft-Exiting Threshold

Figure 5 captures the evolution of the draft-exiting threshold across different models and datasets over approximately 5,000 drafting and verification iterations. We can observe that our strategy adeptly adjusts the threshold, facilitating effective acceleration. However, the substantial variability across different models and datasets confirms the limitation of static threshold settings and the necessity for adaptive updates.

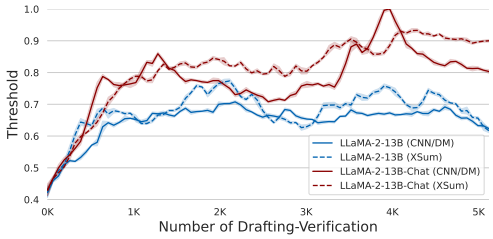


Figure 5: Threshold γ varies with models and data. We calculate a moving average for every 64 cycles and plot the standard deviation. The initial γ is set to 0.4.

Operation	Autoregressive	Self-Speculative
Drafting	-	**25.5±1.14 ms**
- Attention	-	14.6±0.65 ms
- MLP	-	9.46±0.42 ms
Verification	-	10.7±2.81 ms
- Attention	-	7.55±1.91 ms
- MLP	-	2.73±0.80 ms
γ update	-	0.61±0.14 µs
Latency *	56.3±1.23 ms	36.8±3.23 ms
- Attention	39.7±0.91 ms	22.2±2.33 ms
- MLP	14.3±0.29 ms	12.2±1.22 ms

Table 5: Breakdown of computation. * denotes the average inference latency per token for 10 instances sampled from CNN/DM test set on LLaMA-2-13B.

4.6 Breakdown of Computation

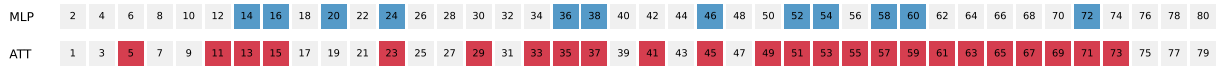
Table 5 presents a computation breakdown comparing the baseline with our 'Self-Speculative' decoding method. Our approach exhibits a significant speedup in average inference time per token compared to 'Autoregressive'. This speedup is primarily attributed to two key techniques: the selection of skipped layers and the adaptive draft-exiting. Notably, the drafting stage consumes the majority of inference latency, highlighting the need for draft model optimizations to improve overall inference speedup. Importantly, our adaptive exit mechanism (γ update) incurs negligible computational cost as it does not involve neural network calculations.

4.7 Impact of Target Acceptance Rate

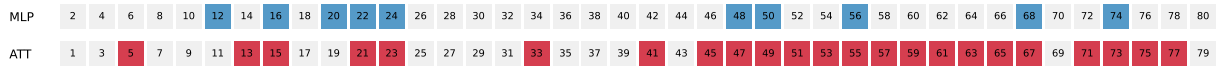
Here, we explore the impact of the target acceptance rate α on LLaMA-2-13B and CNN/DM. As shown in Table 6, the results reveal several insights. As the target acceptance rate increases, the inference speed acceleration ratio initially increases and then decreases. A higher predefined acceptance rate can enhance generation speed. Additionally, we find that at higher acceptance rates (greater than 0.8), the speedup ratio remains relatively stable, indicating that setting the target acceptance rate is straightforward.

α	0.20	0.40	0.60	0.80	0.85	0.90	0.95
ROUGE-2	0.107	**0.108**	**0.108**	**0.108**	**0.108**	**0.108**	**0.108**
AR	0.677	0.713	0.772	0.851	0.880	0.910	**0.934**
Speedup	1.25×	1.31×	1.40×	1.50×	**1.53**×	**1.53**×	1.51×

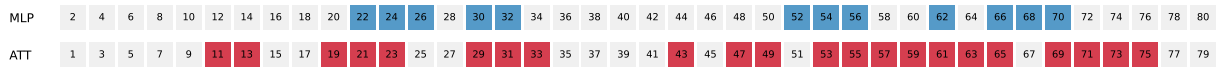
Table 6: Drafting with different α values.



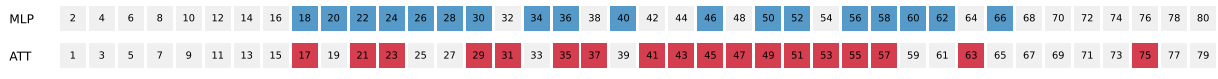
(a) LLaMA-2-13B



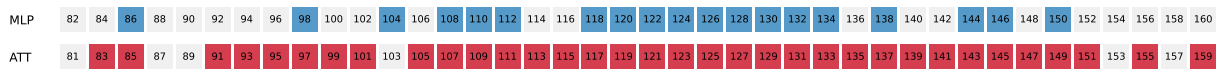
(b) LLaMA-2-13B-Chat



(c) CodeLLaMA-13B



(d) The first half of LLaMA-2-70B



(e) The second half of LLaMA-2-70B

Figure 6: Visualization of layer skip distributions in draft models for various base models. Gray squares indicate retained layers, red squares denote skipped attention layers, and blue squares signify skipped MLP layers.

4.8 Which Layers Are Skipped?

Figure 6 visualizes the distinct base models corresponding to layer skip distributions within the draft model. Two key observations are made as follows:

First, we observe that there are more skips in the attention layer compared to the MLP layer, suggesting the attention layer is more effective for reducing inference time. This is reinforced by the results in Table 5, where the time spent in the attention layer significantly contributes to the average inference latency per token.

Second, regardless of whether it is the MLP layer or the attention layer, the skipped layers tend to cluster in the latter half of the model. This pattern suggests that most tokens can be accurately predicted in the first half of the model, leaving the second half of the model relatively redundant.

5 Conclusion

In this paper, we introduced self-speculative decoding, a novel and efficient inference scheme that accelerates Transformer-based LLMs. Our method does not depend on additional neural network training and incurs no extra device memory, making it a highly practical and cost-effective solution for inference acceleration. Moreover, we used Bayesian optimization to search for layers to skip in drafting and proposed an adaptive draft-exiting mechanism to improve the end-to-end inference speed. Benchmark tests with LLaMA-2 and its fine-tuned models demonstrated a speedup of up to 1.99×. For future work, we aim to explore more sophisticated model compression strategies to further accelerate the drafting stage for low-resource scenarios.

6 Acknowledgements

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7 Ethical Considerations

In compliance with ethical considerations, we emphasize that the entirety of our research revolves around open-source datasets, models, and tools. Notably, we exclusively focus on improving model inference efficiency and do not engage in any commercial usage or ethical implications.

8 Limitations

While our self-speculative decoding scheme presents benefits for accelerating LLMs, there are a few limitations to consider. Firstly, the utilization of Bayesian optimization to determine the layers to be skipped during the drafting stage may require several hours. Nonetheless, this limitation is not critical, as this process is a one-time, offline execution at the model level. Secondly, our method does not involve any neural network training, which imposes a constraint on the number of layers that can be skipped. An excessive reduction in layers could result in a significant drop in the acceptance rate, thereby diminishing the achieved speedup. Although fine-tuning the draft model–a sub-graph of the original model–could potentially mitigate this issue and yield a better speedup, as shown in Appendix E, it incurs additional memory overhead since the draft model no longer shares the same parameters with the original model. In addition, we can refer to FlashAttention (Dao, 2023) and vLLM (Kwon et al., 2023) and similar works to further adapt our technique for batched decoding.

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A Data

The datasets that we have selected for evaluation are CNN/Daily Mail (CNN/DM), Extreme Summarization (XSum), and HumanEval. These tasks cover a broad spectrum of language processing capabilities, including text and code generation capabilities. We perform 1-shot evaluation for CNN/DM and XSum, and compare the ROUGE-2. We compare pass@10 for HumanEval. For the results of efficiency, we randomly sample 1000 instances from the testset for CNN/DM and XSum.

CNN/Daily Mail (CNN/DM): This task involves summarizing news articles from the CNN and Daily Mail websites. The models are required to generate a concise summary of each article, testing their ability to understand and condense complex information.

Extreme Summarization (XSum): In the XSum task, models are asked to produce a single-sentence summary of a news article. This task tests the models' capability to extract the most salient information from a text and express it in a single, coherent sentence.

HumanEval: The HumanEval task is a benchmark for Python programming. This task challenges the models with a variety of coding problems that require a wide range of skills, from basic programming to complex problem-solving abilities. It serves to evaluate the models' understanding of Python syntax, their ability to implement algorithms, and their proficiency in problem-solving using code. This benchmark provides a unique perspective on the models' capabilities in the realm of programming, complementing the language-focused tasks.

B Setup

We present the hyperparameter settings of the experiments in Table 7, including the parameters involved in the decoding process, the adaptive draft-exiting mechanism, and the random sampling. For the adaptive draft-exiting mechanism, we set the initial threshold $\gamma = 0.6$, $\epsilon = 0.01$, $\beta_1 = 0.5$, $\beta_2 = 0.9$, and α is slightly tuned for the data and model, as detailed in Table 7. For sampling-based inference, we by default use $top\_p = 0.85$ for text summarization tasks, and 0.95 for code generation tasks.

In addition, the key experimental environments on the A100-40GB are CUDA 11.6, PyTorch 1.13.1, and Transformer 4.33.1; For the A100-80GB, the environment is CUDA 11.8, PyTorch 2.0.1, and Transformer 4.33.1. We use an A100-40GB to conduct experiments for LLaMA-2-13B, LLaMA-2-13B-Chat, and CodeLLaMA-13B. We use two A100-80GB with HuggingFace's accelerate[6] to conduct experiments for LLaMA-2-70B.

We randomly select 8 instances from the train set and use them to evaluate the inference time per token for Bayesian optimization. This randomness not only ensures the generalizability of our approach but also mitigates any potential bias that could be introduced by the data selection process. The offline Bayesian optimization time for 1000 iterations is about 2.5 hours for LLaMA-2-13B, LLaMA-2-13B-Chat, and CodeLLaMA-13B, and about 6 hours for LLaMA-2-70B.

C Effect of Skip Strategy

Here, we explore the effect of various skip strategies on the performance of generated draft models. We evaluate the CNN/DM on LLaMA-2-13B. Initially, we determine the number of skipped layers using Bayesian optimization, as illustrated in Figure 6(a). We find that the attention layer skips 24 layers, while the MLP layer skips 12 layers. We proceed to apply four strategies, each involving an equal number of layer skips: skipping the initial layers ("First"), middle layers ("Mid."), final layers

[6] https://github.com/huggingface/accelerate (Apache-2.0 License)

Data	Model	Decoding		Adaptive Draft-Exiting					Random Sampling	
		T	K	α	ϵ	β_1	β_2	γ_0	top_p	temperature
CNN/DM	LLaMA-2-13B	512	12	0.90	0.01	0.50	0.90	0.60	0.85	0.20
CNN/DM	LLaMA-2-13B-Chat	512	12	0.85	0.01	0.50	0.90	0.60	0.85	0.20
CNN/DM	LLaMA-2-70B	512	12	0.85	0.01	0.50	0.90	0.60	0.85	0.20
XSum	LLaMA-2-13B	512	12	0.85	0.01	0.50	0.90	0.60	0.85	0.20
XSum	LLaMA-2-13B-Chat	512	12	0.70	0.01	0.50	0.90	0.60	0.85	0.20
XSum	LLaMA-2-70B	512	12	0.85	0.01	0.50	0.90	0.60	0.85	0.20
HumanEval	CodeLLaMA-13B	512	12	0.90	0.01	0.50	0.90	0.60	0.95	0.60
GSM8K	CodeLLaMA-13B	512	12	0.90	0.01	0.50	0.90	0.60	0.95	0.60
GSM8K	CodeLLaMA-13B-Instruct	512	12	0.80	0.01	0.50	0.90	0.60	0.95	0.60
MT-bench	LLaMA-2-13B-Chat	512	12	0.85	0.01	0.50	0.90	0.60	0.85	0.20

Table 7: Hyperparameter settings. γ_0 represents the default initial value of γ.

Strategy	First	Mid.	Last	Rand.	BO
ROUGE-2	**0.108**	**0.108**	0.107	0.107	**0.108**
AR	0.091	0.393	0.508	0.592	**0.919**
Speedup	0.696×	0.887×	0.951×	1.01×	**1.57**×

Table 8: The effects of different skip strategies on the performance of CNN/DM on LLaMA-2-13B.

#Iteration	200	400	600	800	1000
ROUGE-2	**0.108**	0.107	**0.108**	**0.108**	**0.108**
AR	0.903	**0.938**	0.920	0.919	0.919
Speedup	1.35×	1.52×	**1.58**×	1.57×	1.57×

Table 9: The effect of the number of iterations of Bayesian optimization.

#Token	0	20M	40M	60M	75M
ROUGE-2	**0.106**	**0.106**	**0.106**	**0.106**	**0.106**
AR	0.695	0.902	0.901	0.900	0.893
Speedup	1.15×	1.91×	1.94×	**1.96**×	1.85×

Table 10: The effect of the number of tokens on aggressive skip performance.

K	10	12	14	16	18
ROUGE-2	0.107	**0.108**	**0.108**	**0.108**	0.107
AR	**0.924**	0.919	0.916	0.913	0.911
Speedup	1.57×	1.57×	**1.58**×	**1.58**×	**1.58**×

Table 11: The effect of the max draft token under the adaptive draft-exiting mechanism.

("Last"), and randomly sampling layers ("Rand."). The layer skip distribution is visualized in Figure 7.

Table 8 reveals that the fixed strategies of layer skip (first, middle, last) or random skip yield minimal acceleration compared to Bayesian optimization (BO) results. These suboptimal strategies, not optimized for average inference time, result in a draft model with subpar performance (manifested as very low AR), inefficient resource utilization in the drafting phase, and ultimately, a lack of speedup. Furthermore, a slightly enhanced speedup is observed when skipping the last layers, likely due to the more severe redundancy in the model's final portion.

D Number of Iterations of BO

Subsequently, we explore the influence of the iteration number of Bayesian optimization on the performance of our decoding scheme and report the results in Table 9. The layer skip distribution corresponding to different iteration numbers is depicted in Figure 8.

When applied to the LLaMA-2-13B for the CNN/DM task, we observe that while a higher number of iterations can yield increased acceleration, even a relatively modest number of iterations (e.g., 200) effectively reduces inference time, achieving a speedup of 1.35×. Notably, the performance metrics for the 800 and 1000 iterations exhibit consistency due to the same layers being skipped, as shown in Figure 8.

E Aggressive Skip

In pursuit of higher inference acceleration for users with ample resources, we explore a more aggressive skip strategy to obtain the draft model. To mitigate the performance degradation associated with the aggressive skip, we further train the draft model using 50,000 instances from the Pile dataset (Gao et al., 2020), truncating the length of each to 512 tokens, which total up to 25 million tokens. We repeat this training for 3 epochs, resulting in a cumulative utilization of 75 million tokens.

The implementation of the aggressive skip involves skipping the top-K layers based on Bayesian optimization probabilities. For instance, in the case of LLaMA-2-13B, as illustrated in Figure 9, we opt to skip 75% of the attention layers (30 layers) and 32.5% of the MLP layers (13 layers).

Table 10 reveals that when we employ a more aggressive skip without further training (#token is 0), there is a noticeable decrease in the draft model's quality, with an average acceptance rate of only 0.695. This leads to a significantly reduced speedup of merely 1.15×. Nevertheless, by dedicating a portion of the corpus to training, we notably enhance the draft model's quality, increasing the AR to 0.900, in line with the target acceptance rate of 0.90. This enhancement enables a further improvement in speedup from 1.57× (shown in Table 1) to 1.96× (trained for 60M tokens), as more layers are skipped[7]. After training on 75 million tokens, the reason for the reduced acceleration is that we believe the model has a certain degree of overfitting. It is essential to highlight that the aggressive skip strategy necessitates both an extended training process and the additional storage of trained draft models. However, this trade-off is deemed acceptable for users with rich resources.

F Effect of Max # of Draft Tokens

Ideally, increasing the maximum number of draft tokens K while maintaining a high acceptance rate should lead to further improvements in inference acceleration. To explore this, we test the CNN/DM task using LLaMA-2-13B, varying the max draft token K, and present the results in Table 11. It is noteworthy that as K increases, the speedup remains relatively stable. This observation is primarily attributed to the fact that most tokens do not benefit from excessively large K and tend to exit early. In summary, our inference approach shows *insensitivity* to K thanks to the adaptive draft-exiting mechanism. Moreover, setting a relatively large value for K (our default is 12) allows this mechanism to perform optimally.

G Adaptation

We here adopt skipping intermediate layers as a simple yet effective strategy to expedite the drafting stage. While other acceleration techniques such as quantization and structured pruning exist, they fail to offer speed-up proportional to their compression ratio. Meanwhile, they require a separate copy of the altered model parameters, thereby increasing memory overhead. This contradicts the key requirement of no extra memory. Consequently, we adopt layer skipping in our approach. However, our scheme can be integrated with quantization (Dettmers et al., 2022) and sparsification (Sun et al., 2023) to further reduce resource consumption. In this section, we explore the combination of self-speculative decoding with quantization and sparsification techniques to adapt to users with limited computing resources. We conduct experiments on the CNN/DM task using LLaMA-2-13B, and the layer skip distribution corresponding to the draft model is shown in Figure 10.

[7]This finding aligns with the recent Sheared-LLaMA (Xia et al., 2023), which shows the effectiveness of pruning followed by further training on a small amount of data.

Quantization	bf16	fp8	fp4	nf4
ROUGE-2 ↑	0.107	0.105	0.101	**0.114**
AR ↑	0.910	0.911	**0.913**	0.910
VRAM (GB) ↓	37.2	27.5	**19.6**	19.7
Latency (ms) ↓	**32.4**	113	152	126
Speedup ↑	1.53×	**1.61**×	1.36×	1.35×

Table 12: Performance of self-speculative decoding combined with different quantization schemes of LLM.int8().

Sparsification	dense	unstructured	4:8	2:4
ROUGE-2 ↑	0.107	0.114	**0.115**	0.110
AR ↑	0.910	**0.918**	0.912	0.911
VRAM (GB) ↓	37.2	**35.9**	**35.9**	**35.9**
Latency (ms) ↓	32.4	30.4	**29.2**	30.9
Speedup ↑	**1.57**×	1.50×	1.47×	1.48×

Table 13: Performance of self-speculative decoding combined with different sparsification schemes of wanda.

G.1 Quantization

First, we integrate our inference approach with the quantization technique, LLM.int8()[8] (Dettmers et al., 2022). We evaluate the performance of three quantization schemes: fp8 (8-bit floating-point), fp4 (4-bit floating-point), and nf4 (4-bit normalized float), in comparison to the default bf16 (16-bit brain float point). The results are presented in Table 12. In all quantization settings, we skip the 'lm head' layer of the model and do not employ double quantization to save an additional 0.4 bits.

Table 12 illustrates that all three quantization schemes effectively reduce the video memory demand during inference. Notably, the fp4 quantization results in up to a nearly two-fold reduction in memory demand to just 19.6 GB. While there may be an increase in the average inference latency per token due to the dequantization process, this approach makes LLM suitable for scenarios with

[8]https://github.com/TimDettmers/bitsandbytes (MIT License)

Data	Model	Method	Perfor.	Speedup
GSM8K	CodeLLaMA-13B	Autoreg.	0.104	1.000×
GSM8K	CodeLLaMA-13B	Self-Spec.	0.101	1.351×
GSM8K	CodeLLaMA-13B-Ins.	Autoreg.	0.223	1.000×
GSM8K	CodeLLaMA-13B-Ins.	Self-Spec.	0.213	1.263×
MT-bench	LLaMA-2-13B-Chat	Autoreg.	6.940	1.000×
MT-bench	LLaMA-2-13B-Chat	Self-Spec.	6.930	1.269×

Table 14: Evaluation on solving math problem and open-domain chitchat tasks. We use greedy decoding for the accuracy of GSM8K. We use random sampling for the average score at task-level of the MT-bench with various temperatures of 0.7 for 'writing' and 'roleplay', 0.1 for 'stem' and 'humanities', and greedy decoding for the rest of the tasks, according to (Zheng et al., 2023).

limited device memory.

G.2 Sparsification

Subsequently, we assess the performance of self-speculative decoding combined with sparsification techniques, specifically wanda[9] (Sun et al., 2023), which includes unstructured sparsity and structured N:M sparsity (4:8 and 2:4) with the sparsity ratio of 0.5. The N:M sparsity constraint specifies that no more than N out of every M contiguous weights can be non-zero.

Table 13 shows that while sparsification may not dramatically reduce VRAM requirements, it does result in a reduction in the average inference latency per token to varying degrees. However, the speedup is slightly down because the base model is also accelerated.

H Exploration of Diverse Tasks

We want to mention that our approach does not require model fine-tuning and its lossless characteristic is task-agnostic. However, we are open to evaluating the effectiveness of our approach on more diverse tasks. Here, we further explore the performance of our decoding scheme on solving math problems (Grade School Math 8K (Cobbe et al., 2021)) and open-domain chitchat (MT-bench (Zheng et al., 2023)). For GSM8K, we evaluate on base model CodeLLaMA-13B and CodeLLaMA-13B-Instruct and report the problem-solving accuracy of 1318 questions in the test set. For MT-bench, our base model is LLaMA-2-13B-Chat, and we use its program script to ask GPT-4 to give a score of 10 points for each round using their prompt templates and report the average score for a total of 160 answers for two turns of 80 questions.

[9] https://github.com/locuslab/wanda (MIT License)

Model	Method	HumanEval		Speedup
CodeLLaMA-13B	Autoreg.	pass@10	0.659	1.000×
CodeLLaMA-13B	Self-Spec.	pass@10	0.659	1.345×
CodeLLaMA-34B	Autoreg.	pass@10	0.671	1.000×
CodeLLaMA-34B	Self-Spec.	pass@10	0.695	1.330×

Table 15: Evaluation of code generation tasks with different model sizes. We use random sampling with a temperature of 0.6 for pass@10.

Grade School Math 8K (GSM8K): A dataset of 8.5K high-quality linguistically diverse grade school math word problems. The dataset was created to support the task of question answering on basic mathematical problems that require multi-step reasoning. Solutions primarily involve performing a sequence of elementary calculations using basic arithmetic operations (+-×÷) to reach the final answer. This task is generally used to test logic and math in language modeling.

MT-bench: A benchmark consisting of 80 high-quality multi-turn questions. MT-bench is designed to test multi-turn conversation and instruction-following ability, covering common use cases and focusing on challenging questions to differentiate models. The tasks identify 8 common categories of user prompts to guide its construction: writing, roleplay, extraction, reasoning, math, coding, knowledge I (STEM), and knowledge II (humanities/social science). For each category, The task manually designed 10 multi-turn questions.

Regarding using Bayesian optimization 1,000 iterations to generate a draft model, for GSM8K, we randomly sampled 4 samples from the training set as a development set; for MT-bench, we let GPT-3.5 generate 8 examples according to 8 topics to form an optimized use development set. Other relevant hyperparameters are shown in Table 7.

For GSM8K, we achieve a 1.35× acceleration without compromising task performance. Regarding MT-bench, spanning writing, roleplay, reasoning, math, coding, extraction, stem, and humanities, presents substantial task diversity, posing challenges for generating high-quality and diverse output from draft models. Nevertheless, we still achieve a speedup of about 1.27× with lossless task performance. These findings demonstrate the robustness and commendable performance of our approach across diverse tasks.

Model	CNN/DM	XSum
LLaMA-2-13B (ours)	0.106	0.124
LLaMA-2-13B-Chat (ours)	0.144	0.109
LLaMA-2-70B (ours)	0.130	0.118
OPT (66B)	0.136	0.126
Davinci (175B)	0.127	0.126
Palmyra X (43B)	0.049	0.149
GPT-NeoX (20B)	0.123	0.102
Luminous Base (13B)	0.110	0.105
BLOOM (176B)	0.080	0.030
YaLM (100B)	0.017	0.021

Table 16: Our model with self-speculative decoding vs. Mainstream LLMs with autoregressive.

Model	Method	ROUGE			Speedup
		1	2	L	
CNN/DM	Autoreg.	0.263	0.106	0.181	1.000×
CNN/DM	Self-Spec.	0.266	0.108	0.183	1.429×
XSum	Autoreg.	0.327	0.124	0.260	1.000×
XSum	Self-Spec.	0.328	0.125	0.261	1.377×

Table 17: Evaluation on text generation tasks with various metrics and greedy decoding.

I Exploration of Other Model Sizes

The model size may also have an impact on speedup, thus additional results on CodeLLaMa-34B can further validate the effectiveness of the proposed approach. As shown in Table 15, we observed that the speedup of CodeLLaMa-34B compared to CodeLLaMa-13B is not significant. We attribute this to the inherent low redundancy in CodeLLaMa-34B. To verify this, we further calculated the proportion of skipped layers in both models. We found that CodeLLaMa-34B skips 45.8% of the layers, while CodeLLaMa-13B skips 42.5%, indicating no significant difference in the skipped layer proportions. In contrast, for the more noticeably accelerated transition from LLaMa-2-13B to LLaMa-2-70B, there is a 10% increase in the proportion of skipped layers. Additionally, according to the analysis in Table 5 of the original paper, for the attention layer, which incurs higher time costs, there is a 5% decrease from CodeLLaMa-13B to CodeLLaMa-34B. Therefore, we believe that the limited inherent redundancy in CodeLLaMa-34B leads to an insignificant improvement in acceleration.

J Exploration of Output Quality

J.1 Quantitative Analysis

LLMs Comparison. Considering this non-fine-tuned, one-shot setting, our score is indeed quite competitive. We attach in Table 16 the performance of other mainstream large language models on CNN/DM and XSum as a reference (data from HELM leaderboard (Liang et al., 2022)).

Diverse Metrics. Our experimental setup mainly follows the work of DeepMind (Chen et al., 2023). For summarization tasks, ROUGE-2 is a widely recognized evaluation metric, as adopted by (Chen et al., 2023; Liang et al., 2022), in addition to ROUGE-1 and ROUGE-L. However, we want to emphasize that we have not disregarded the importance of other metrics such as ROUGE-1 and ROUGE-L. Indeed, we have maintained records of these results as part of our comprehensive analysis, and we will attach them in the appendix in the revision. The results are presented below. And we can see that our conclusions remain consistent – we have been successful in achieving a significant acceleration in task performance without compromising the quality of the outputs. We believe this reaffirms the robustness and efficacy of our approach.

J.2 Qualitative Analysis

We present more qualitative evidence to supplement the quantitative ROUGE-2 score. Please note, however, that our approach is inherently lossless and the performance evaluation is conducted on the original model without any fine-tuning. The task performance of our self-speculative decoding is therefore reliant on the inherent capabilities of the base model utilizing autoregressive decoding. Specifically, using the same base model, in the greedy setting, generation results from self-speculative decoding are **identical** to those of autoregressive decoding; In the sampling setting, the results generated are from the same distribution as those for autoregressive decoding. These properties of speculative decoding have been mathematically proven in previous work (Leviathan et al., 2023). Finally, to address concerns, we present a case study on LLaMA-2-13B, detailed in the Table 18.

K Discussion of Pre-defined Anchor

Here, we discuss why we do not use a predefined speedup ratio, but a predefined acceptance rate (target acceptance rate) in the adaptive draft exit mechanism. The pre-defined acceptance rate is related to the quality while the pre-defined speedup ratio is related to the efficiency. It seems that these two anchors do not conflict and correspond to differ-

ent application scenarios. The predefined speedup ratio is an interesting idea, but using a predefined speedup as an anchor seems difficult to apply to real-world testing. In the self-speculative decoding process, adapting the exit threshold based on the current acceleration ratio and predefined speedup ratio involves significant computational overhead.

To elaborate, for each instance, we would need first to employ autoregressive decoding to obtain its generation time and then execute self-speculative decoding to calculate the current acceleration ratio. This sequential process would substantially reduce the generation speed. In contrast, the adaptive exit mechanism based on the acceptance rate doesn't entail such dependencies. The current acceptance rate can be directly obtained after completing a draft and verification process.

Moreover, compared to the predefined speedup ratio, which can be any number greater than 1, the target acceptance rate is a value ranging from 0 to 1 (usually greater than 0.7). This range is straightforward to determine for different tasks and models.

L Algorithm with Sampling

We first demonstrate self-speculative sampling with greedy sampling by integrating the adaptive draft-exiting mechanism in Algorithm 3.

In addition to the greedy version of self-speculative decoding that we have presented in the main paper, we also explore a variant that incorporates random sampling, that also incorporated a complete adaptive draft-exiting mechanism, as shown in Algorithm 4. This approach introduces an element of randomness into the selection of tokens for speculative decoding, as opposed to the deterministic nature of the greedy version. In our setup, random sampling is affected by two parameters: temperature and top_p. Higher values of temperature or top_p lead to greater token diversity, while lower values make token selection more deterministic. This variant could potentially lead to diverse decoding paths and outcomes, which may be beneficial in certain scenarios, such as code generation.

Algorithm 3 Self-Speculative Decoding (Greedy)

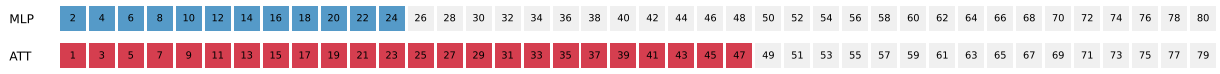
LLM $p(x|\boldsymbol{z}^*, x_1, ..., x_t)$ where $x_1, ..., x_t$ is the prompt, $\boldsymbol{z}^*$ is a vector that represents the specific layers to bypass; target sequence length T; max draft tokens to generate K. We denote the original LLM as $p(x|\vec{0}, x_1, ..., x_t)$, where $\vec{0}$ is a zero vector, indicating all layers are used in inference. We denote the acceptance rate (AR) at e-th drafting stage as AR_e.
$i \leftarrow t$
while $i < T$ **do**
  for $j \leftarrow i, ..., i + K$ **do** ▷ Drafting Stage
    $x_{j+1} \leftarrow \arg\max p(x|\boldsymbol{z}^*, x_1, ..., x_j)$
    if $\max p(x|\boldsymbol{z}^*, x_1, ..., x_j) < \gamma$ **then** ▷ Draft Exit
      Break
  for $i \leftarrow i, ..., j$ **do** ▷ Verification Stage
    if $x_{i+1} \neq \arg\max p(x|\vec{0}, x_1, ..., x_i)$ **then**
      $x_{i+1} \leftarrow \arg\max p(x|\vec{0}, x_1, ..., x_i)$
      Break
  $i \leftarrow i + 1$
  If all draft tokens are accepted, generate next token $x_{i+1} \leftarrow \arg\max p(x|\vec{0}, x_1, ..., x_i)$ and $i \leftarrow i + 1$
  $AR \leftarrow \beta_1 AR + (1 - \beta_1) AR_e$ ▷ γ Update
  if $AR \leq \alpha$ **then**
    $\gamma + \epsilon$
  else
    $\gamma - \epsilon$
  $\gamma \leftarrow \beta_2 \gamma + (1 - \beta_2)\tilde{\gamma}$
return $x_1, ..., x_T$

Data	Temp.	Article/Document	Summary/Highlight		
			Reference	Autoregressive	Self-Speculative
CNN/DM	0.0	An Arkansas woman became a little richer this week after finding a large diamond at Crater of Diamonds State Park. Susie Clark, of Evening Shade, found the 3.69-carat white diamond in a 37.5-acre search field on Thursday, her last day of a trip to the park with her husband. Clark,	Susie Clark, of Evening Shade, Arkansas, found the diamond on Thursday at Crater of Diamonds State Park . The 3.69-carat gem is teardrop-shaped about the size of a pinto bean . Park interpreter said it's the largest of the 122 diamonds found this year .	woman who found a 3.69-carat white diamond at Crater of Diamonds State Park in Arkansas has named the gem a 'hallelujah diamond' because she spotted the gem shortly after praying that she would find something .	woman who found a 3.69-carat white diamond at Crater of Diamonds State Park in Arkansas has named the gem a 'hallelujah diamond' because she spotted the gem shortly after praying that she would find something .
CNN/DM	0.2	who first visited the park 33 years ago with her mother and grandmother, prayed to God, asking, 'Are you doing to bless me and let me find a diamond today?' as she searched the field. Susie Clark, of Evening Shade, Arkansas, found a 3.69-carat white ...	Susie Clark, of Evening Shade, Arkansas, found the diamond on Thursday at Crater of Diamonds State Park . The 3.69-carat gem is teardrop-shaped about the size of a pinto bean . Park interpreter said it's the largest of the 122 diamonds found this year .	woman who found a 3.69-carat diamond at Crater of Diamonds State Park in Arkansas has named the gem a 'hallelujah diamond' because she spotted the gem shortly after praying that she would find something .	woman who found a 3.69-carat white diamond at Crater of Diamonds State Park in Arkansas has named the gem a 'hallelujah diamond' because she spotted the gem shortly after praying that she would find something .
XSum	0.0	The flight provider operates a "bug bounty" scheme that rewards hackers for privately disclosing security flaws rather than sharing them	US airline United has rewarded two hackers who spotted security holes in its website with a million free flight miles each.	Airlines has given out its first rewards to hackers who reported security flaws in its website.	Airlines has given out its first rewards to hackers who reported security flaws in its website.
XSum	0.2	online. It has given the maximum reward of a million flight miles, worth dozens of trips, to two people. One security expert said the ...	US airline United has rewarded two hackers who spotted security holes in its website with a million free flight miles each.	airline has given out two million flight miles to hackers who found security flaws in its website.	airline has given the maximum reward of a million flight miles, worth dozens of trips, to two people.

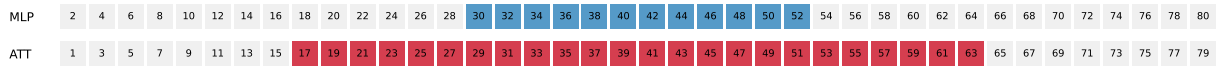
Table 18: Case study of CNN/DM and XSum on LLaMA-2-13B.

Algorithm 4 Self-Speculative Decoding

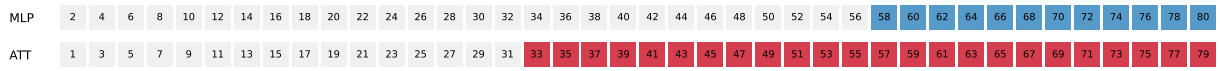
LLM $p(x|\boldsymbol{z}^*, x_1, ..., x_t)$ where $x_1, ..., x_t$ is the prompt, $\boldsymbol{z}^*$ is a vector that represents the specific layers to bypass; target sequence length T; max draft tokens to generate K. We denote the original LLM as $p(x|\vec{0}, x_1, ..., x_t)$, where $\vec{0}$ is a zero vector, indicating all layers are used in inference. We denote the acceptance rate (AR) at e-th drafting stage as AR_e.
$i \leftarrow t$
while $i < T$ **do**
  for $j \leftarrow i, ..., i + K$ **do** ▷ Drafting Stage
    $x_{j+1} \leftarrow$ sample $p(x|\boldsymbol{z}^*, x_1, ..., x_j)$
    if $\max p(x|\boldsymbol{z}^*, x_1, ..., x_j) < \gamma$ **then** ▷ Draft Exiting
      Break
  for $i \leftarrow i, ..., j$ **do** ▷ Verification Stage
    $r \leftarrow$ sample from a uniform distribution $U[0, 1]$
    if $r \geq \min(1, \frac{p(x|\vec{0}, x_1, ..., x_i)}{p(x|\boldsymbol{z}^*, x_1, ..., x_i)})$ **then**
      $x_{i+1} \leftarrow$ sample from $\frac{\max(0, p(x|\vec{0}, x_1, ..., x_i) - p(x|\boldsymbol{z}^*, x_1, ..., x_i))}{\sum_x \max(0, p(x|\vec{0}, x_1, ..., x_i) - p(x|\boldsymbol{z}^*, x_1, ..., x_i))}$
      Break
  $i \leftarrow i + 1$
  If all draft tokens are accepted, generate next token $x_{i+1} \leftarrow$ sample $p(x|\vec{0}, x_1, ..., x_i)$ and $i \leftarrow i + 1$
  $AR \leftarrow \beta_1 AR + (1 - \beta_1) AR_e$ ▷ γ Updating
  if $AR \leq \alpha$ **then**
    $\gamma + \epsilon$
  else
    $\gamma - \epsilon$
  $\gamma \leftarrow \beta_2 \gamma + (1 - \beta_2)\tilde{\gamma}$
return $x_1, ..., x_T$



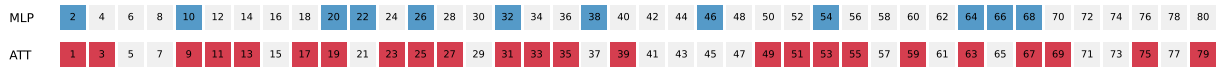
(a) First: Skip the first 24 layers of attention and 10 layers of MLP.



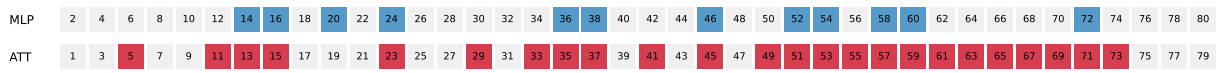
(b) Middle: Skip the middle 24 layers of attention and 10 layers of MLP.



(c) Last: Skip the last 24 layers of attention and 10 layers of MLP.

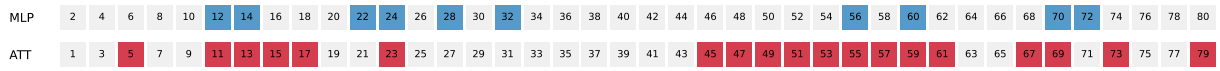


(d) Random: Skip the 24 layers of attention and 10 layers of MLP randomly.

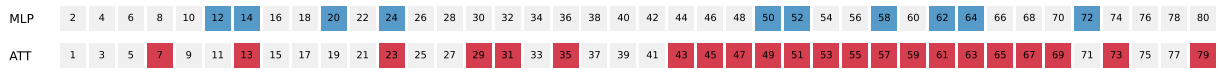


(e) BO: Skip the 24 layers of attention and 10 layers of MLP by Bayesian Optimization.

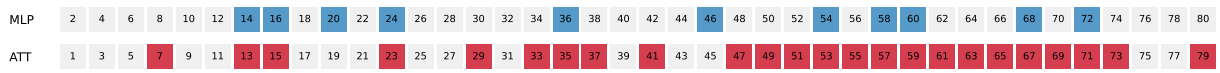
Figure 7: Visualization of layer skip distributions in LLaMA-2-13B using different strategies.



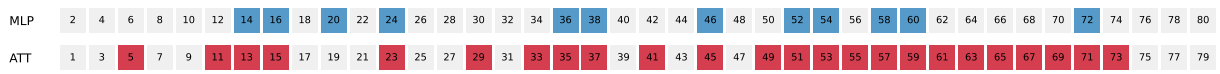
(a) 200 Iterations



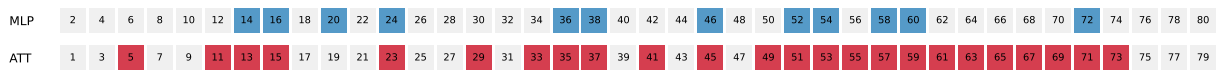
(b) 400 Iterations



(c) 600 Iterations



(d) 800 Iterations



(e) 1000 Iterations

Figure 8: Visualization of LLaMA-2-13B layer skip distribution for different BO iteration numbers.

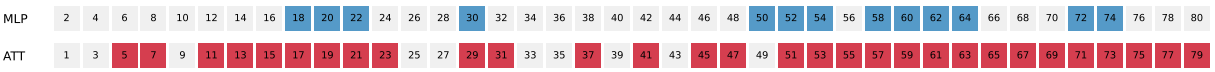


Figure 9: Visualize aggressive skip of 75% attention layers and 32.5% MLP layers of LLaMA-2-13B.

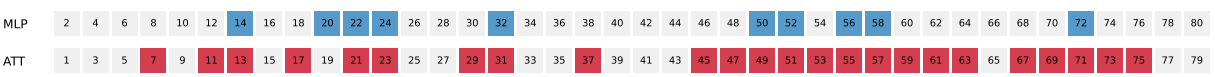


Figure 10: Visualization of layer skip distribution in LLaMA-2-13B for quantization and sparsification.