LM-Infinite: Zero-Shot Extreme Length Generalization for Large Language Models

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Abstract

Today's large language models (LLMs) typically train on short text segments (e.g., <4K tokens) due to the quadratic complexity of their Transformer architectures. As a result, their performance suffers drastically on inputs longer than those encountered during training, substantially limiting their applications in real-world tasks involving long contexts such as encoding scientific articles, code repositories, or long dialogues. Through both theoretical analysis and empirical investigation, this work identifies three major factors contributing to this length generalization failure. Our theoretical analysis reveals that commonly used techniques like using a sliding-window attention pattern or relative positional encodings are inadequate to address them. Answering these challenges, we propose LM-Infinite, a simple and effective method for enhancing LLMs' capabilities of handling long contexts. LM-Infinite is highly flexible and can be used with most modern LLMs off-the-shelf. Without any parameter updates, it allows LLMs pre-trained with 2K or 4K-long segments to generalize to up to 200M length inputs while retaining perplexity. It also improves performance on downstream tasks such as Passkey Retrieval and Qasper in the zero-shot setting. LM-Infinite brings substantial efficiency improvements: it achieves $2.7 \times$ decoding speed up and $7.5 \times$ memory saving over the original model. Our code will be publicly available upon publication.

1 Introduction

Large language models (LLMs) have recently advanced the state-of-the-art across various natural language processing tasks. They typically train on text segments of fewer than 4K tokens (Touvron et al., 2023b; Team, 2023), primarily due to the computational overhead quadratic in the input lengths of their Transformer architectures. As a result, they face challenges in generalization to inputs that are excessively longer than what they are trained on and suffer substantial deterioration in their performance (Tworkowski et al., 2023; Chen et al., 2023a). This limits their applicability in tasks that require long-range contexts, such as encoding scientific articles, source code repository generation, or long-context dialogues.

Extensive efforts have been devoted to addressing this length generalization challenge. Relative positional encodings such as RoPE (Su et al., 2021) and Alibi (Press et al., 2021) have been widely adopted by state-of-the-art LLMs, which calculate attention based on inter-token distance instead of absolute positions, hoping to avoid model failures due to unseen absolute position embeddings. Moreover, although applying a sliding-window attention pattern on the Transformer architecture can reduce the memory overhead (Beltagy et al., 2020; Ding et al., 2023; Zaheer et al., 2020), they are not directly applicable to pre-trained models for length generalization without further training. Through both theoretical analysis and empirical investigation, §3 pinpoints three primary factors underlying the length generalization failures: (1) the challenge of handling unseen distances among tokens, (2) the difficulty of attending to unseen numbers of tokens, and (3) implicitly encoded absolute positional information in initial tokens. These challenges can make LLMs' computational features, such as attention logits and hidden vectors, deviate from the training distribution, leading to failures of length generalization. Existing techniques fall short of addressing these underlying issues.

Answering these challenges, we propose LM-Infinite, a simple and effective method to enhance Transformer LLMs' capabilities for modeling long contexts*without parameter updates*. LM-Infinite consists of two major components designed to alleviate the three factors above. (1) a Λ -shaped attention mask and (2) a ceiling on attention dis-

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tances. The former forces the model to attend to only the beginning of the sequence and the most recent tokens within a pre-defined window, ignoring the rest. The latter component caps the relative distance values to the maximum the model has seen during training. It can also optionally re-introduce top-k tokens in the middle to achieve better performance in some downstream tasks. LM-Infinite is highly flexible and applies to any off-the-shelf LLMs that use relative positional encoding and does *not* require any finetuning.

Our experiments thoroughly evaluate LM-Infinite on a variety of tasks and LLMs. On ArXiv (academic papers) and OpenWebText2 (Reddit posts) LM-Infinite facilitates zero-shot generalization for a wide range of LLMs to texts up to 200M tokens, retaining the language modeling perplexity and generation quality. Without any parameter updates, LM-Infinite improves scores compared with the original model and truncation baselines on downstream tasks including Passkey Retrieval (Mohtashami and Jaggi, 2023) and Qasper (Dasigi et al., 2021), which are two established benchmarks for long-context evaluation. We observe a 37.2% gain on Passkey Retrieval and a 1.2% gain on Qasper in the zero-shot setting. LM-Infinite also brings substantial efficiency improvements: it achieves $2.7 \times$ decoding speed up and $7.5 \times$ GPU memory saving over the original LLMs.

2 Background and Related Work

2.1 Relative Positional Encodings

The traditional absolute positional encodings provide the absolute position information, usually with the help of a sequence of vectors called *position* embeddings (Vaswani et al., 2017; Kenton and Toutanova, 2019; Ke et al., 2020). They, however, have trouble when the model encounters unseen positions in inputs longer than the training length. Relative positional encodings aim to address the limitations of previous-generation positional encoding methods and consider the relative distances between tokens instead of the absolute positions. Examples include a learned attention logit bias in T5 (Raffel et al., 2020), Transformer-XL (Dai et al., 2019), Skyformer (Chen et al., 2021), Sketching (Chen et al., 2022) and Sandwich (Chi et al., 2023), a fixed linear attention decay (Press et al., 2021), and rotating query and key sequences based on distances such as RoPE (Su et al., 2021; Li et al., 2023), CAPE (Likhomanenko et al., 2021) and

XPos (Sun et al., 2022; Ding et al., 2023). Despite some promising empirical evidence, length generalization failures are still widely observed when directly applied to large language models (Kaiokendev, 2023). In what follows, we briefly discuss two widely used relative positional encoding methods. They lay out the necessary context for our onward discussion and experiments.

Rotary Position Embedding (RoPE; Su et al., 2021) It rotates the key and query vectors based on positions before computing the inner product. Specifically, each vector **x** (either key or query) is split into pairs of elements $\{(x_0, x_1), (x_2, x_3), \dots\}$, with each pair interpreted as a 2-dimensional vector. RoPE then rotates the vector (x_a, x_{a+1}) of token *i* with angle $\theta_{a,i} =$ $i\omega_a$, where ω_a is the rotating speed associated with dimension pair (a, a + 1). After rotation, the 2-D vector becomes $\begin{pmatrix} \cos i\omega_a & -\sin i\omega_a \\ \sin i\omega_a & \cos i\omega_a \end{pmatrix} \begin{pmatrix} x_i \\ x_{i+1} \end{pmatrix}$. They show that the inner product between rotated query \mathbf{q}_i and rotated key \mathbf{k}_j is solely determined by $\mathbf{q}_i, \mathbf{k}_j$, and their relative distance i - j. We always have $i \geq j$ due to the causal attention mask.

AliBi (Press et al., 2021) It offsets all attention logits between tokens i, j by a linear term -m(i - j) and become $\mathbf{q}_i^{\mathsf{T}} \mathbf{k}_j - m(i - j)$. To this end, the MPT-7B codes implement an offset matrix as an additive term in attention logits.

2.2 Efforts Towards Length Generalization

In light of generalization failures observed in LLMs, one straightforward solution is to finetune LLMs on longer text sequences (Chen et al., 2023a; Tworkowski et al., 2023; Tao et al., 2023; Kiyono et al., 2021; Anil et al., 2022). These approaches do not address the underlying causes of length generalization failures and require massive training resources. Other solutions propose to grant LLMs access to longer contexts without really reading them in full (Zhou et al., 2023; Bueno et al., 2022; Mohtashami and Jaggi, 2023; Yang et al., 2023). Augmenting LLMs with retrieval-based memories (Wu et al., 2021; Guu et al., 2020; Borgeaud et al., 2022; Khandelwal et al., 2019; Kaiser et al., 2016; Yogatama et al., 2021) also make LLMs applicable to a large database. These designs, however, usually need finetuning and are not directly compatible with the existing LLMs. Our work, in contrast, facilitates zero-shot length generalization. Another similar work (Ratner et al., 2023) increases con-



Figure 1: We identify three factors underlying the length generalization failure in LLMs in §3. (a) Factor 1: Unseen distances between tokens cause attention logits to explode. (b) Factor 2: An unseen number of tokens can cause attention entropy to increase beyond the training range as the length increases. (c) Factor 3: Starting few tokens occupy a distinct feature region and should not be discarded. The two blue regions at the upper center and lower right correspond to the initial tokens that are highly concentrated but also very far from later tokens. The lower-left region contains the thousands of overlapping dots corresponding to the later tokens.

text length with attention patterns without further training. However, it is limited to the in-context learning setting.

3 Why do Transformer LLMs Fail to Generalize to Long Contexts?

Through a series of theoretical and experimental investigations, this section aims to identify the potential causes underlying current LLMs' failure in length generalization. Our discussion assumes Transformer-based LLMs that use relative positional encodings, as this design is widely adopted in today's LLMs (Touvron et al., 2023b; Team, 2023). We use Llama-2 (Touvron et al., 2023b), which is pre-trained with 4K-length segments, for investigation. On sequences longer than the training length, we will show that the unseen inter-token distances, the increasing number of attended tokens, and the implicitly encoded position information of the starting tokens can all make certain computational features out of the training distribution. As deep models can be sensitive to input distribution shifts, these factors need to be handled for LLMs to generalize to unseen lengths.

Factor 1: challenges in handling unseen distances among tokens With relative positional encoding, the impact of positions on the attention weight between two tokens depends solely on their relative distance. As the sequence length grows exceedingly long, some distance values will surpass those seen during training. We make the following informal theoretical claim: **Theorem 1.** (Informal) For an attention mechanism using relative positional encoding, the attention logits must explode to infinities to differentiate previously unseen distances apart as the sequence length increases.

The formal theorem and its proof can be found in Appendix C. We also empirically verify this on Llama-2 on the ArXiv dataset truncated down to 8K length. We extract the attention logits of all attention heads and their maximum attention logits on different sequence lengths in Figure 1(a). It shows the average and variance among attention heads. We see that the attention logits increase to substantially larger values when the sequence length exceeds the training length of 4K. To mitigate this issue, we conjecture that it may help to cap the relative distance values to the maximum that the model has seen during training (i.e., a distance ceiling). However, as we will see from the proposition below, addressing logit explosion leads to another challenge.

Factor 2: attending to unseen numbers of tokens On longer sequences, tokens at later positions must distribute attention weights across a larger context. We then make the following claim that, if attention logits are bounded but the number of tokens to attend to is not limited, it can cause the attention entropy to increase beyond the training range:

Proposition 1. *If the attention logits are bounded, as the sequence becomes longer, the attention entropy grows to infinity.*

A formal statement as well as the proof can be



Figure 2: (a) LM-Infinite is a plug-and-play solution for various LLMs, consisting of a Λ -shaped mask and a distance ceiling during attention. For clarity, this figure shows a toy scenario where $L_{\text{pre-train}}$ and n_{starting} are both 2. (b) We also provide a conceptual model for understanding how relative position encoding works.

found in Appendix D. This conclusion is further empirically verified by plotting the attention entropy against context lengths in Figure 1(b). The curve shows an ever-increasing attention entropy. This trend, although increasing logarithmically, is still harming the LLMs' performance, as we will illustrate in the ablation study in §5.2 and Figure 5. This suggests that we should bound the attention context size to ensure that the attention entropy stays in seen ranges during pre-training and avoid degenerated outputs. A simple windowed attention, where each token only attends to the nearest tokens within a distance, might handle factors 1 and 2. This is similar to the block-diagonal attention mask used in XPos (Sun et al., 2022) and Longformer (Beltagy et al., 2020). However, as we will show in the next paragraph, this introduces another factor that can also fail LLMs.

Factor 3: starting tokens occupy a distinct feature space Perhaps counter-intuitively:

Observation 1. Even without explicit absolute positional embeddings, attention outputs of the first few tokens can occupy a distinct representational space compared to other positions. Therefore, when passed to later layers, these starting tokens have distinct value vectors from their lower-layer outputs.

This follows from Theorem 1 in Kazemnejad et al. (2023), which proves that the absolute positions can be implicitly encoded in the outputs of tokens of a single attention layer, even *without* positional encodings. In their construction, the starting tokens'

signals are the strongest and easiest to distinguish from other tokens. As relative positional encoding is strictly more expressive than no positional encoding setting in Kazemnejad et al. (2023) (e.g., by letting all distances have the same attention function), the same conclusion applies to relative positional encoding as well.

As an empirical verification, we take the hidden states output by the second layer of Llama-2 and plot a Principal Component Analysis (PCA) projection into a 2-d plane in Figure 1(c). More figures for other layers can be found in §E. The dots correspond to the first 4096 tokens in 32 sequences, with blue ones corresponding to the initial tokens and red tokens being the tail ones. The two blue regions at the upper center and lower right correspond to the initial highly concentrated tokens (whose positions are around $0 \sim 25$) and are very far from later tokens. The lower-left region contains the remaining overlapping tokens in a sequence (zoomed in to another box). The plot shows that the vector representations of the initial tokens concentrate on regions in the feature space that are distinct from the remaining tokens. This fresh finding reveals a fundamental flaw of the sliding-window attention pattern, which restricts the attention to the most recent tokens within a predefined window size, a widely adopted baseline recently (Beltagy et al., 2020; Ding et al., 2023; Zaheer et al., 2020). As attention is essentially a weighted average over the value vectors, sliding-window attention discards the initial tokens, keeping the attention output from reaching the regions that value vectors of the initial

tokens occupy. This enforces the model to handle a different region during the computation, introducing additional generalization challenges. As a straightforward solution to this issue, **the initial tokens need to be kept in the attention computation.**

4 Our proposal: LM-Infinite

Inspired by the analyses and take-away messages in the previous section, we propose LM-Infinite to achieve zero-shot length generalization for LLMs. An overview of LM-Infinite is illustrated in Figure 2(a). This simple solution consists of two components: a Λ -shaped attention mask and a distance ceiling. Besides, re-introducing the middle top-ktokens is optional for enhanced downstream performance.

A-shaped attention mask It contains two attention spans: the *starting* one allows each token to attend to the first n_{starting} tokens if they come before the current one; the ending one allows each token to attend to most recent L_{pretrain} tokens. L_{pretrain} is the maximum length during training. Other tokens are ignored. In ablation studies in §A, we find that choosing $n_{\text{starting}} \in [5, 100]$ generally achieves equally good performance. Note that $n_{\text{starting}} = 0$ (i.e., attending only to the most recent tokens) substantially hurts the performance. This resolves Factors 2 and 3 in §3 by both limiting the number of tokens under attention and ensuring the starting few tokens are attended.

Distance ceiling LM-Infinite further bounds the "effective distance" to L_{pretrain} . This only affects the starting few tokens when attended by tokens at later positions. Specifically, in relative positional encoding, the original attention logit is $w(\mathbf{q}, \mathbf{k}, d)$, where d is the distance between two tokens. Now we modify it as $w(\mathbf{q}, \mathbf{k}, d')$ where $d' = \min(d, L_{\text{pretrain}})$. Figure 2(a) shows an illustrative example where the distance ceiling is $L_{\text{pretrain}} = 2$. This addresses Factor 1 in §3 by bounding the distance value in attention calculation.

Optionally attending to top-k **tokens in the middle** LM-Infinite can optionally attend to k tokens in the middle with the largest attention logits. This is particularly useful in downstream tasks where information in the middle tokens matters (§5.3). Here the k tokens are selected independently for each attention head in layers higher than h-th layer, and have an attention distance of $d = \frac{1}{2}L_{\text{pre-train}}$. These hyperparameters are selected based on a held-out Passkey Retrieval validation set, where we set k = 5 and h = 5, with more details in Appendix A. Our selection of k and h does not depend on task-specific tuning, and in our experiments, we apply this same set of hyperparameters in all other downstream tasks and achieve consistent improvements. These intermediate tokens do not hurt performance. Rather, in the evaluation of downstream tasks in §5.3, intermediate tokens are more useful and selectively attending to top-k tokens brings substantial performance improvements with little impact on the efficiency. For LLM generation and inference, however, we find the intermediate tokens unnecessary to attend to for LM-Infinite to achieve good perplexity or generation quality.

LM-Infinite's **A**-shaped mask is conceptually similar to the attention patterns derived from heuristics (Beltagy et al., 2020; Ding et al., 2023; Zaheer et al., 2020). However, we formally show in §3 Factor 3 that these previous approaches theoretically cannot generalize to unseen lengths but require parameter updates. This inherent limitation motivates the other two components in LM-Infinite to achieve zero-shot length generalization.

Implementation details LM-Infinite is applicable in all Transformer models with relative positional encoding. One only needs to replace the attention function in each Transformer layer with LM-Infinite without any parameter updates. The Λ -shaped attention mask is relatively straightforward to implement. In RoPE, attention logits in the ending attention span follow the original calculation. In the starting attention span (excluding its overlap with the ending span), we keep all k vectors unrotated and rotate all q vectors to a fixed distance L_{pretrain} . Then the logits in two spans can be composed. Augmenting AliBi with LM-Infinite is also straightforward. We simply clip the offset matrix with a minimum value of $-|mL_{\text{pretrain}}|$ and apply the Λ -shaped attention mask.

Discussion. In Figure 2(b), we show a conceptual model of how relative positional encoding functions. This conceptual model reflects the design choices of LM-Infinite. In this conceptual model, a long context can be roughly partitioned into 3 parts: The *starting tokens* encode strong absolute position information (Factor 3). As explained in §3, they are essential to attention to because their features occupy a distinct region in the feature space. As attention is essentially a weighted average over



Figure 3: LM-Infinite flattens the negative log-likelihood (NLL) curves of various LLMs on ArXiv dataset without any parameter updates. The trends are similar to MPT-7B-Storywriter, an explicitly fine-tuned LLM. Llama-2 outputs NaN values on long sequences so the curve is relatively shorter.

			ArXiv				OpenWebText2				
Model	L_{pretrain}	2K	4K	8K	16K	32K	2K	4K	8K	16K	
Long-context Tra	ining/Fine	etuning									
Sandwich	512	5.0	5.2	5.3	-	-	23.3	23.8	24.7	-	
XPos	1K	21.6	20.7	-	-	-	-	-	-	-	
LongLLaMA	8K	8.2	7.4	-	6.9	-	-	-	-	-	
MPT-7B-SW	65K	6.5	5.4	4.3	4.4	3.6	9.8	10.9	6.6	5.1	
Vanilla											
MPT-7B	4K	5.5	2.5×10^{2}	1.1×10^{3}	1.7×10^{3}	1.6×10^{3}	8.3	1.3×10^{2}	1.9×10^{2}	1.3×10^{2}	
LLaMA	2K	3.8	$1.0{ imes}10^4$	6.0×10^{4}	6.8×10^{4}	4.9×10^{4}	6.2	6.6×10^{3}	4.6×10^{5}	4.4×10^{4}	
GPT-J-6B	2K	3.9	1.3×10^{3}	1.0×10^{3}	1.6×10^{3}	2.8×10^{2}	8.8	7.5×10^{2}	1.3×10^{3}	1.8×10^{3}	
Llama-2	4K	3.4	3.8	8.5×10^{3}	NaN	NaN	6.2	5.8	6.5×10^{3}	NaN	
LM-Infinite											
MPT-7B	4K	5.7	6.8	5.8	6.0	4.6	8.5	12.2	8.5	8.9	
LLaMA	2K	4.4	4.5	3.7	4.2	1.0	6.3	6.1	9.5	7.0	
GPT-J-6B	2K	3.8	3.1	3.0	3.1	2.1	8.8	8.5	6.5	7.4	
Llama-2	4K	4.3	3.6	3.3	4.2	6.5	6.1	5.3	8.3	8.2	

Table 1: Perplexity on ArXiv and OpenWebText2 test split. LLMs with LM-Infinite achieve the highest perplexity on 7 out of 9 columns while requiring no parameter updates. L_{pretrain} indicates the lengths of the text segments that the models are trained on.

 v_i vectors, without the starting few tokens, the attention output can not reach regions that v_i vectors of the initial tokens occupy. The *rear tokens* provides primarily their relative positions to the final tokens. Their importance probably arises from the "recency bias" (Peysakhovich and Lerer, 2023) learned by LLMs during pre-training. The *middle tokens* encode less position-sensitive information. As analyzed in Factor 2, including too many intermediate tokens does more harm than good to length generalization.

5 Evaluation

We evaluate LM-Infinite with LLaMA-7B (Touvron et al., 2023a), Llama-2-7b (Touvron et al., 2023b), MPT-7B (Team, 2023), and GPT-J-

6B (Wang and Komatsuzaki, 2021). LLaMA-7B and GPT-J-6B are pre-trained with 2K lengths and the other models are pre-trained with 4K lengths. LLaMA, Llama-2, and GPT-J use RoPE encoding, and MPT-7B uses Alibi encoding. MPT-7B-Storywriter (fine-tuned on long sequences) is used as one of the baselines.

5.1 Language Modeling with Extremely Long Context

We use ArXiv and OpenWebText2 corpora from the Pile dataset (Gao et al., 2020), which contain preprint papers from ArXiv and Reddit submissions, respectively. We evaluate with negative loglikelihood (NLL) and perplexity (exponential of NLL). Figure 3 plots the NLL curves on the ArXiv



Figure 4: LM-Infinite generalizes Llama-2 to an extreme length of 200M. The dashed line is the NLL at 8K length of the vanilla Llama-2 model.

dataset. Here, we break down the models' perplexity performance by positions so that the curve shows the NLL that the model achieves around that specific position, averaged across all evaluated sequences. Llama-2 outputs NaN probabilities on sequences that are slightly longer than 10K, thereby its shorter curve. All vanilla models run out of memory at \sim 32K lengths.¹ The baselines' NLL quickly blows up when the tested sequences are longer than what they train on. With LM-Infinite, all models can generalize to sequences that are substantially longer than the lengths they are trained on, retaining the NLL performance. This validates our length failure factor analyses in §1. The longer ends of curves have larger variances because of fewer documents of those lengths. In Figure 4, we further evaluate LM-Infinite + Llama-2 on a sequence of 200M tokens, which is constructed by sampling with replacement from the ArXiv dataset and concatenating all data. LM-Infinite shows the ability to remain stably low log-perplexity level over extreme lengths.

Table 1 summarizes the perplexity performance at a few milestone lengths (2K, 4K, 8K, 16K, and 32K) on ArXiv and OpenWebText2, which shows a similar trend. OpenWebText2 has very few data instances over a length of 32K, so we omit the column. With LM-Infinite, all models can generalize to unseen lengths, and LM-Infinite achieves best perplexity in 7 out of 9 cases. On LLaMA + LM-Infinite, the perplexity decreases as length increases and position becomes larger. Surprisingly, *without*



Figure 5: Ablation study on LLaMA in §5.2. x-axis is token position and y-axis is negative log-likelihood (NLL). The vanilla model (vanilla), using a windowed attention (window), using only a Λ -shaped attention mask (Λ), and only the ceiling the distance value (ceiling) all more or less suffer from perplexity explosion. Only LM-Infinite can retrain the performance while generalizing to unseen lengths.

any parameter update, LM-Infinite outperforms many strong baselines that are trained on substantially longer text segments. As a direct comparison, MPT-7B+LM-Infinite achieves only slightly worse performance than its fine-tuned counterpart, MPT-7B-Storywriter. This confirms that LM-Infinite is a promising alternative to resource-consuming finetuning.

5.2 Ablation Study

Figure 5 provides an ablation study with the LLaMA model on the ArXiv dataset about why both components in LM-Infinite are essential for maintaining LLM functionality over the length of 8K. We compare LM-Infinite with its variants to show the efficacy of the design and also to validate the factors in §3. Among all curves, only LM-Infinite has relatively stable log-perplexity, meaning that components in LM-Infinite are all essential for successful length generalization. The vanilla LLM model (the "vanilla" curve) fails immediately with exploding NLL. If we only apply Λ -shaped mask (the " Λ " curve) and do not bound inter-token distance (Factor 1), the NLL still explodes immediately after pre-training lengths. The "ceiling" curve only applies the distance ceiling technique but not the Λ -shaped mask to limit the number of attended tokens. The performance still degenerates (evidenced by an ever-increasing NLL). This confirms that the existence of Factor 2, too many to-

¹We run on a single A100 GPU with 80GB GPU memory.

		Passkey Retrieval									
Model	6K	8K	10K	12K	16K	average	-				
Original	0.0	0.0	0.0	0.0	0.0	0.0	1.2				
Truncated	66.0	55.3	38.8	32.8	27.3	44.0	30.1				
LM-Infinite	70.3	90.8	86.5	79.3	79.1	81.2	31.3				

Table 2: Downstream evaluation on Passkey Retrieval and Qasper. LM-Infinite enables Llama-2 to consistently outperform both the original model and the baseline that truncates inputs to 4K. The truncation baseline drops excessive tokens altogether when the context is longer than the model's pretraining length, keeping only the most recent ones, which happens before the forward pass starts without changing the attention mechanism.

		B	BLEU					ROU	GE		
Model	L_{pretrain}	2K	4K	8K	16K	32K	2K	4K	8K	16K	32K
ArXiv											
MPT-7B	4K	0.0	0.2	0.0	0.0	0.4	5.6	3.6	5.9	1.7	1.4
MPT-7B-SW	65K	16.6	21.5	15.2	18.9	14.8	26.5	30.1	26.6	27.4	27.0
MPT-7B + LM-Infinite	65K	16.1	20.2	12.6	13.9	19.7	23.8	24.9	24.1	29.0	26.6
Llama-2	4K	26.6	0.0	0.0	0.0	0.0	31.4	0.2	0.0	0.0	0.0
Llama-2 + LM-Infinite	4K	26.9	23.6	23.9	24.8	18.4	31.8	30.9	28.8	29.2	20.4
OpenWebText2											
MPT-7B	4K	0.9	0.9	1.0	1.0	-	7.5	6.6	6.4	6.8	-
MPT-7B-SW	65K	8.4	6.1	7.5	8.4	-	21.0	19.3	18.5	22.0	-
MPT-7B + LM-Infinite	4K	5.0	4.1	5.1	2.8	-	16.6	15.4	16.2	16.0	-
Llama-2	4K	8.8	0.0	0.0	0.0	-	22.4	0.2	0.0	0.0	-
Llama-2 + LM-Infinite	4K	9.0	7.2	9.7	9.6	-	21.9	21.2	19.6	19.6	-

Table 3: Text generation quality on ArXiv and OpenWebText2. LM-Infinite consistently generalizes the generation quality to extreme lengths, achieving performance that is comparable to or better than the fine-tuned LLM, MPT-7B-Storywriter. Some 0 BLEU scores are caused by the poor generation quality from the vanilla LLMs as they generate mostly nonsensical texts.

kens, is still harming the LLMs' performance. The "window" curve shows a baseline with the slidingwindow attention pattern, which only attends to the most recent tokens in a sliding window without altering the input text. It produces the second worst NLL values, which indicates a significant performance and fluency degradation. This confirms our theoretical analysis of factor 3. Due to its visibly much worse performance, we exclude it from other evaluations.

Another similar baseline to "window" is the truncation baseline, which drops excessive tokens altogether when the context is longer than the model's pre-training length, keeping only the most recent ones. This truncation process happens before the forward pass starts and essentially removes the truncated text from the input to the model without changing the attention mechanism. We compared this baseline in two places in the paper. In §5.3 and Table 2, LM-infinite outperforms this baseline on downstream tasks. In Section 5.4 and Figure 6, LM- infinite achieves a better trade-off between computation complexity and generation quality than this baseline.

5.3 Downstream Evaluation

As LLMs are often deployed for downstream tasks, we evaluate how LM-Infinite performs on two long-input tasks under the zero-shot setting: Passkey Retrieval (Mohtashami and Jaggi, 2023) and Qapser (Dasigi et al., 2021). Passkey Retrieval buries a passkey at a random position in a long distraction text and, in the end, asks what the passkey is. Qasper is a question-answering dataset on scientific papers with a total of 1.5K testing questionanswer pairs. We evaluate Llama-2-7b-chat, as its instruction tuning enables good task-solving ability (Bai et al., 2023), with middle top-5 tokens enabled on higher than 5-th layer (see §4 for definition and Appendix A for hyperparameter selection). Results are listed in Table 2. LM-Infinite consistently outperforms the baselines on both tasks, with



Figure 6: LM-Infinite achieves a better trade-off between computation complexity with generation quality than simple truncation.

a 37.2 percentage gain on Passkey Retrieval and a 1.2 percentage gain on the Qasper task. Passkey retrieval locates useful information uniformly in a sequence, so the performance of the truncated baseline largely depends on whether the remaining part covers the passkey. On Qasper, the top-*k* attention is necessary for achieving good performance, which indicates that similarly important information in the middle needs to be attended to. This suggests that it can improve downstream task performance on long inputs without fine-tuning while the vanilla model immediately fails.

5.4 Generation Quality

We further evaluate LM-Infinite's generation quality on ArXiv and OpenWebText2 test sets, with BLEU (Papineni et al., 2002) and ROUGE (Lin, 2004) (ROUGE-L). We let the LLMs generate 100 tokens after each milestone length and use the following 100 tokens in original texts as references. As the generation is time-consuming, we sample 100 long sequences for evaluation for each dataset. The results are summarized in Table 3. The trend is similar to that in the last section: without parameter updates, LM-Infinite successfully allows LLMs to retain their generation quality while generating sequences longer than training, comparable to the fine-tuned baselines such as MPT-7B-SW. The generation results from the vanilla LLMs are poor and contain mostly nonsensical texts, resulting in many close-to-zero scores. For some BLEU scores, it yields zero {2,3,4}-gram overlaps with the reference texts. As BLEU is weighted geometric mean over $\{1,2,3,4\}$ -gram precisions, the

final BLEU scores for those columns are 0. Appendix Table 8 presents some generation output examples that can provide a good picture of the generation quality. We also evaluate the efficiency in Appendix G: with 32K-long sequences, LM-Infinite achieves $2.7 \times$ decoding speedup and $7.5 \times$ GPU memory saving.

A few example generations are shown in Appendix H. We also compare LM-Infinite with a simple truncation-based baseline by repeatedly truncating excessive contexts. However, as the generation length increases, frequent truncations and re-encoding of new contexts are required. The larger the truncation window is, the more context is kept, but the larger the computational overhead. We let the models generate 10k tokens on ArXiv. In Figure 6, it is clear that LM-Infinite achieves a substantially better quality-efficiency tradeoff. With similar computation, LM-Infinite outperforms the baseline by about 5 BLEU. To achieve a similar BLEU, LM-Infinite incurs only <25% computational overhead than the truncation baseline.

6 Conclusions and Future Work

This work proposes a zero-shot length generalization method for various off-the-shelf LLMs without parameter updates. Through theoretical analysis and empirical investigation, this work identifies three major factors contributing to this length generalization failure. Our theoretical analysis further reveals why truncating the attention window and relative positional encodings are inadequate to address them. Our solution, LM-Infinite, is a simple and effective method for enhancing LLMs' capabilities of handling long contexts. It allows LLMs pre-trained with 2K or 4K-long segments to generalize to up to 200M length inputs while retaining perplexity. It also improves performance on downstream tasks such as Passkey Retrieval and Qasper in the zero-shot setting. It brings substantial efficiency improvements: a $2.7 \times$ decoding speed up and a $7.5 \times$ memory saving over the original model. LM-Infinite's computational efficiency and ease of use allow researchers without enormous computational resources to use LLMs on long sequences. Future work can investigate if these techniques allow for more efficient and effective LLM pre-training and fine-tuning. Another direction is to apply LM-Infinite to applications such as long reasoning, long-dialogue, retrieval-augmented generation, or long literature generation.

Limitations

This work evaluates a wide range of open-domain LLMs. However, without access to the source code of proprietary LLMs such as ChatGPT, the proposed method could not be evaluated on them. Furthermore, due to limited computational resources and time, the proposed method has not been evaluated on texts with even larger lengths, such as 1G. The model is designed on relative positional encoding Transformer models, which is the mainstream backbone for most modern LLMs. The question of how LM-Infinite can enable more efficient fine-tuning or pre-training can also be explored in future work.

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A Implementation Details

In this section, we introduce some implementation details of LM-Infinite as well as the hyperparameter selection.

A.1 Computational resources

All experiments are run on single A100 GPUs with 80GB GPU memory each. The 200M length generalization runs for 20 hours. The downstream tasks take $3\sim7$ hours to evaluate each. Our work does not involve any training or fine-tuning. All models are loaded with Huggingface² code repository. Rouge and BLEU scores are loaded from evaluate³ package. Datasets and models are used with permission from their licenses.

A.2 The size of starting attention span

We vary the value of n_{starting} and find LM-Infinite to be tolerant with it taking a wide range of values without sacrificing the NLL values. Speicifically, we evaluate it on sequences of 16k length in the ArXiv validation set and calculate the average NLL.

			n _{starting}	g		
0	1	2	10	100	1000	2000
6.43	1.03	1.03	1.02	1.02	1.81	4.96

Table 4: Effect on LM-Infinite's NLL by varying n_{starting} .

A.3 Reintroducing Top-k Middle Tokens

This optional technique involves optionally attending to k tokens in the middle with the largest attention logits. Here, the k tokens are selected independently for each attention head and only apply to layers higher than h-th layer. These tokens have an attention distance of $d = \frac{1}{2}L_{\text{pre-train}}$. We select these hyper-parameters based on a held-out validation set of Passkey Retrieval. On Llama-2, we use k = 5 and h = 5. As an ablation study, we vary each hyper-parameter and observe its effects on Passkey Retrieval accuracy.

On the Qasper dataset, for both vanilla models and LM-Infinite, we use 6K sub-sequence of inputs as prompts and use a systematic prompt format described in Llama-2 paper (Touvron et al., 2023b).

			k			
1	3	5	10	20	50	200
0.69	0.81	0.81	0.79	0.8	0.79	0.73
-	Ta	able 5: E	ffect of	varying	; <i>k</i> .	_
		atten	tion dis	tance		
	512	1024	2048	3072	4096)
-	0.78	0.79	0.81	0.68	0.63	

Table 6: Effect of attention distance of the middle tokens.

B Additional Related Work

After our preprint, there have been papers that cite our work and investigate zero-shot or few-shot length generalization of LLMs. As many absolute or relative position encoding methods are based on periodic functions, (Qu, 2023; Ding et al., 2024; Liu et al., 2023; Jiang et al., 2023) propose to apply LLMs (fine-tuned or not) on decreased period frequencies (which is equivalent to interpolating position indices) to adapt LLMs to longer sequences. Some other papers finetune LLMs with designed attention patterns (Oren et al., 2024; Zhang et al., 2024a) on long contexts, using neural tangent kernel (Peng et al., 2023), or with low-rank adaptation(LoRA) (Chen et al., 2023b). (Yang and Hua, 2024) instead proposes a wait-to-attend mechanism to extend length limits for memory-based Transformers. Other ways of key-value cache selection/eviction methods are investigated in (Ren and Zhu, 2024; Dong et al., 2024; Zhang et al., 2024d). Similarly, (Huang et al., 2023; Lee et al., 2024) tackles long context by learning to dynamically prune, select, or summarize contexts. Alternatively, context compression methods (Shao et al., 2024) propose to learn to compress long contexts into shorter embedding sequences. Some work proposes alternative position encodings (Song et al., 2023; Zhang et al., 2024c; Zhu et al., 2023) or landmark token embeddings (Luo et al., 2024) that enable extendable context limits. (Xiao et al., 2024) is a later concurrent work to ours with a similar approach to LLM length generalization. Unlike our work, they feed a sequence to an LLM token-bytoken which limits their extreme length generalization (4M v.s. 200M of ours), and more importantly, they do not show improvements on downstream tasks without pre-training an LLM from scratch.

²https://huggingface.cohttps://huggingface.co

³https://huggingface.co/docs/evaluate/index

			h			
0	4	5	6	8	16	24
0.81	0.94	0.94	0.91	0.46	0.45	0.46

Table 7: Effect of varying h.

Finally, there is a lot of new benchmarks (Qiu et al., 2024; Zhang et al., 2024b; Yuan et al., 2024; Wang et al., 2024; Lv et al., 2024; Bai et al., 2024) proposed to evaluate the long-context performance of LLMs.

C Formal Statement of Theorem 1

Let us denote the logit function with relative position encoding as $w(\mathbf{q}, \mathbf{k}, d) \in \mathbb{R}$. It maps the query \mathbf{q} , key \mathbf{k} , and their distance d, to an attention logit. The final attention weights are usually calculated by a softmax operation. For example, given n tokens with indices $(1, \dots, n)$, the attention by the last token on a preceding token at position i is:

$$\operatorname{Attn}(\operatorname{token}_n, \operatorname{token}_i) = \frac{e^{w(\mathbf{q}_n, \mathbf{k}_i, n-i)}}{\sum_{j=1}^n e^{w(\mathbf{q}_n, \mathbf{k}_j, n-j)}} \quad (1)$$

Then the formal theorem of Theorem 1 is as follows:

Theorem 2. (Formal) Let q and k be random vectors sampled from training distributions $\mathcal{D}_{\mathbf{q}}$ and $\mathcal{D}_{\mathbf{k}}$, respectively, where $\mathcal{D}_{\mathbf{q}}$ and $\mathcal{D}_{\mathbf{k}}$ are the trained distributions for q and k, respectively. We use the pseudo-dimension $\dim_P(\cdot)$ defined in (Pollard, 1990), which measures the representation capacity of a function family. Assume that the set of distancebased logit functions $\mathcal{H} = \{w(\cdot, \cdot, d) | d \in \mathbb{N}\}$ has bounded pseudo-dimension dim_P(\mathcal{H}) = r^4 . Let us also define the distinguish-ability of two distances d and d' under w as their expected squared dif*ference:* $\mu_w(d, d') = \mathbb{E}_{\mathbf{q} \sim \mathcal{D}_{\mathbf{q}}, \mathbf{k} \sim \mathcal{D}_{\mathbf{k}}}(w(\mathbf{q}, \mathbf{k}, d) - \mathbf{k})$ $w(\mathbf{q}, \mathbf{k}, d'))^2$. We assume that w is not limited to recognizing only a finite group of distances, otherwise, all distances longer than a threshold will become almost the same as shorter distances. Formally, for any n, there is a partition of [0..n] into $\alpha(n)$ groups so that, $\mu_w(d, d') \leq \epsilon$ for any d, d'from the same group. $\alpha(n) \in \mathbb{N}$ is non-decreasing and unbounded function. Then we have:

$$\sup_{\mathbf{q},\mathbf{k},d\leq n} |w(\mathbf{q},\mathbf{k},d)| \geq \left(\frac{\alpha(n)}{2}\right)^{\frac{1}{2r}} \frac{\epsilon}{4e}.$$

We first borrow a lemma from (Haussler, 2018), which we paste below. Note that a cover size $\mathcal{N}(\epsilon, \mathcal{H}, \mu)$ is defined as the minimum cardinal of a cover-set \mathcal{H}' so that any element of $h \in \mathcal{H}$ will be within ϵ distance to at least one element $h' \in \mathcal{H}'$.

Lemma 3. Let \mathcal{H} be a function family mapping from space X to range [0, B], and its pseudodimension dim_P(\mathcal{H}) = r. Then for any probabilistic measure P on X, and $\epsilon \in [0, B]$, we have that the ϵ cover of \mathcal{H} under metric $\mu(h_1, h_2) = \mathbb{E}_{x \sim P}(h_1(x) - h_2(x))^2$ is bounded by:

$$\mathcal{N}_P(\epsilon, \mathcal{H}, \mu) \le 2\left(\frac{2eB}{\epsilon}\ln\frac{2eB}{\epsilon}\right)^{\frac{1}{2}}$$

With this lemma, we can go on to prove Theorem 2 as follows.

Proof. We prove by contradiction. Assume that $\sup_{\mathbf{q},\mathbf{k},d\leq n} |w(\mathbf{q},\mathbf{k},d)| < a = \left(\frac{\alpha(n)}{2}\right)^{\frac{1}{2r}} \frac{\epsilon}{4e}.$ Without loss of generality, we can shift all the values to range [0,2a]. Then the function family $\mathcal{H} = \{w(\cdot,\cdot,d) | d \in \mathbb{N}\}$ will have cover size $\mathcal{N}_P(\epsilon,\mathcal{H},\mu) \leq 2 \left(\frac{4ea}{\epsilon} \ln \frac{4ea}{\epsilon}\right)^r < \alpha(n).$

However, this is smaller than the number of different distances and relative weight attentions \mathcal{H} , which means that at least 2 functions will be close to each other $(w(\cdot, \cdot, d), w(\cdot, \cdot, d'))^2 < \epsilon$. This constitutes a contradiction with the distinguishability condition.

D Formal Statement and Proof of Proposition 1

The formal statement of Proposition 1 is the following:

Proposition 2. (Attention Entropy Explosion) Let $w_1, w_2, \dots, w_n \in [-B, B]$ be a sequence of attention logits. Then the entropy of the attention distribution they span is asymptotically lower bounded by $\ln n$:

$$H\left(\left(\frac{e^{w_i}}{\sum_{j=1}^n e^{w_j}} \middle| 1 \le i \le n\right)\right) = \Omega(\ln n)$$

The entropy approaches $+\infty$ as n grows larger.

Proof. Note that entropy on a discrete distribution is defined as $Entropy(P) = -\sum_{i} p_i \ln p_i$. Then the attention entropy determined by attention logits

 $^{^{4}\}mbox{This}$ is true for most current techniques. See discussions in Appendix F

 $\{w_i | 1 \le i \le n\}$ is

Entropy(Attention)

$$= -\sum_{i} \frac{e^{w_i}}{\sum_{j} e^{w_j}} \ln \frac{e^{w_i}}{\sum_{j} e^{w_j}}$$
$$= -\sum_{i} \frac{e^{w_i}}{\sum_{j} e^{w_j}} \left(w_i - \ln \sum_{j} e^{w_j} \right)$$
$$= -\sum_{i} \frac{e^{w_i}}{\sum_{j} e^{w_j}} w_i + \ln \sum_{j} e^{w_j}$$
$$\ge -\max_{i} w_i + \ln(ne^{-B})$$
$$\ge \ln n - 2B$$
$$= \Omega(\ln n)$$

E More on Implicitly Encoded Positions

We also plot the token features of more layers with PCA projection to the 2D plane in Figure 7. We see that from layer 2 to higher layers, the initial few tokens occupy a distinct region with later tokens. Therefore, if these tokens are discarded by window attention during attention, the attention output, which is a weighted sum of v_i vectors, will reside in a different region. This can explain why windowed attention does not work and why the first few tokens need to be kept by our Λ -shaped attention.

F Pseudo-Dimension Assumption on Attention Logit Functions

In Theorem 2, we assumed that the family of distance-based logit functions $\mathcal{H} = \{w(\cdot, \cdot, d) | d \in \mathbb{N}\}$ has a finite pseud-dimension. In this section, we demonstrate that most current implementations of relative positional encodings do have a finite pseudo-dimension. Let us discuss a few examples in the following:

T5-Bias and Alibi It is easy to see that, the difference between any two logit functions is uniform: $w(\cdot, \cdot, d_1) - w(\cdot, \cdot, d_2) = bias(d_1) - bias(d_2)$ regardless of the input. Therefore this family cannot shatter any set larger than 2, so the pseudo-dimension is 1.

Windowed Attention This operation is equivalent to limiting the family to a finite size $|\mathcal{H}| = d_{\max} + 1$, where d_{\max} is the size of the window. Therefore $\dim_P(\mathcal{H}) \leq d_{\max} + 1$. **NoPE** As there is no explicit positional encoding implemented, all distances are equivalent. The pseudo-dimension is 1.

RoPE, CAPE, and XPos For RoPE, the logit function $w(\mathbf{q}, \mathbf{k}, d)$ is the weighted sum of finite fixed sinusoidal functions $\{\sin(\omega_i d), \cos(\omega_i d)\}$. The size of this set is equivalent to the feature dimension number k. We know that $\dim_P(\mathcal{H}_1 + \mathcal{H}_1) \leq \dim_P(\mathcal{H}_1) + \dim_P(\mathcal{H}_2)$. Also, the scaling of a single function can only have a pseudodimension of 2. Therefore, the whole family has a bounded pseudo-dimension $\dim_P(\mathcal{H}) \leq 2k$. The analysis on CAPE and XPos is similar.

G Computational Efficiency Evaluation

To evaluate the computational efficiency of LM-Infinite, we run the Llama-2-7B model on 100 sequences of 32k length in the ArXiv dataset. The hardware is a single A100 GPU with 80GB GPU memory. As the memory is not enough to host the whole computation graph during decoding, we use DeepSpeed (Rasley et al., 2020) with Zero3 optimization. We also have to modify the computation code to further reduce GPU memory usage and prevent out-of-memory errors. With that in mind, the vanilla Llama-2-7B model encodes with an average speed of 48.19s per sequence, while LM-Infinite encodes with an average of 15.26s per sequence, a 3.16x speedup. The vanilla Llama-2-7B model decodes with 7.34s per token, while LM-Infinite decodes with 2.70s per token, a 2.72x speedup. We also evaluate the GPU memory usage on 32k-length inputs, the statistics of which are profiled with PyTorch Profiler. The vanilla model uses 33.2Gb memory per sequence, while LM-Infinite uses 4.41Gb per sequence, a $7.53 \times$ memory saving.

H Example Generation



Figure 7: In Llama, at second or higher layers, the initial few tokens encode a strong position signal and occupy a distinct feature region. Abandoning them might move the attention output vector out of the pre-training distribution.

Table 8: Example text generations on ArXiv and OpenWebText2 corpora after 8k context lengths.

	ArXiv Dataset
Context	Our proof of the Kottwitz formula imitates these arguments of Langlands and Rapoport of deriving the Kottwitz formula from their conjecture. As such, their theory of Galois gerbs is a major ingredient in this work. Another essential ingredient is a recent work of Kisin [@Kisin17] on the aforementioned conjecture of Langlands and Rapoport. Previously, Kottwitz [@Kottwitz92] proved the formula in PEL-type cases (of simple Lie type A or C) by a method which is based on the Honda-Tate theory. This method however cannot be applied in general Hodge-type situations, and indeed
Vanilla Llama-2	of this (of over-equary-her, and [(and, in thecister '- and an of the model to by. by, this, by the. It, and it, 7. –(of an equist (of the. to the [[[WNE (to. and for the (((de in the (for the andistile-c[de (for in an inc ort, ort (betness in >with (with, based (and (> such ((c of a or for the abstract as. of *. (up. W in the, of the or an. and of a.0 in (and of (over in such [near ($-of$ (([her (pro – [p for [with the of a: their in the in of '[alism in the, [(du of that of the (both [equ of the of [for ([of as of and of the of their of (($-for$ of the of the of the of the of the of his of the. of the of it (D with the d. and of of the of the of the of [of of a of a, [[for for a per of a of its of a (for of the and of the
LM-Infinite	Kottwitz [@Kottwitz84a] had formulated the conjecture, but at the time no idea had yet been established on how to prove it. This conjecture involves some algebraic statements of automorphic forms which have an algebraic nature, but are only valid for automorphic forms (which are not holomorphic automorphic forms [@Kaplansky1966]), whose (abstract) objects are Galois extensions of F and \overline{F} (which in general are not necessarily finite extensions), in other words a p-valued Hodge-type structure (in n- dimension). The Langlands-Rapoport conjecture is now established [@ScholzeShin13] whose formulation is in terms of (a more explicit class of) Hodge-type structures rather than these abstract Galois objects, and the automorphic side for p-adic L-functions are due to Kisin [@Kisin15].
	OpenWebText2
Context	This auto-structuration of a complete whole is defined as "auto-regulation". In the indi- vidual, the latter is established by biological rhythms, biological & mental regulations and mental operations. These can be theoretically formalized. Piaget refuses to accept that "real" dialectical tensions between physical objects are the true foundations of thought and cognition (its possibility, genesis & progressive development). Piaget never fills in what reality is. He maintains no ontological view on reality-as-such, considered to be the borderline of both the developing subject and its objective world, stage after stage. The cognitive is approached as a process, for rationality grows in developmental stages, each calling for a particular cognitive structure on the side of
Vanilla Llama-2	the in that, of it and and r' of the. of " of " of the pr of of of the of the of the [. of " - s (1 (of s of the " of quends of it & and of trail of the, the &, 1. – a and at-and and and the " for on the is, core by " (as (:: a (on its to " is a, (on, th is of all but". " in the, in the the the and in the for the., and of of the or of the :! of " A. of the of the, of the of the of [of the of the: of a th, and s of the of the the as of the, B of h. the —. the : a, and, in a: & (se and [((t, d of the and;, of the (,. (A. A. Pro: T. I " (b in the of the, of c) f" of, of the of the , of s of all ma of the [and of the of the of [of the of th
LM-Infinite	cognition. It develops gradually. For Piaget, the cognitive originates in experience as it is subjected to structure : i.e. as it is structured, ordered and transformed. In the first stage, the "sensorial stage", structures are formed and integrated based on perception. These structures are built by organic, biological and psychic transformations, which lead to experience. The "concrete operational stage" of intellectual development refers to a stage when the mind of the child starts to use the logic of the general rule and the rule of the general case. There is now a logical, conceptual and operational distinction of concepts. Reasoning is made explicit by applying logical operations, such as subtraction, addition and multiplication to the "mental" object as well as to the "perceived" world of reality. The child's logic can now make use of the logical operations, though for him (her) it is a conceptual understanding of abstract operational stage", logical operations are combined using logical or conceptual structures.