Improving Referring Ability for Biomedical Language Models

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Abstract

Existing auto-regressive large language models (LLMs) are primarily trained using documents from general domains. In the biomedical domain, continual pre-training is a prevalent method for domain adaptation to inject professional knowledge into powerful LLMs that have been pre-trained in general domains. Previous studies typically conduct standard pre-training by randomly packing multiple documents into a long pre-training sequence. Recently, some existing works suggest that enhancing the relatedness of documents within the same pre-training sequence may be advantageous. However, these studies primarily focus on general domains, which cannot be readily applied in the biomedical domain where the distinction of fine-grained topics is harder. Is it possible to further improve the pre-training for biomedical language models (LMs) using exactly the same corpus? In this paper, we explore an improved approach to continual pre-training, which is a prevalent method for domain adaptation, by utilizing information from the citation network in this challenging scenario. Empirical studies demonstrate that our proposed LinkLM data improves both the intra-sample and inter-sample referring abilities of auto-regressive LMs in the biomedical domain, encouraging more profound consideration of task-specific pre-training sequence design for continual pre-training.[1]

1 Introduction

Pre-trained language models (PLMs) benefit from large-scale, readily accessible, unsupervised texts. Particularly in the biomedical domain, numerous studies conducted pre-training on academic papers and abstracts to enhance representations and professional knowledge (Gu et al., 2021; Beltagy et al., 2019; Bolton et al., 2024). Most of them

PubMedQA
Abstract:
To examine patterns of knowledge and attitudes among adults aged>65 years unvaccinated for influenza. […]
Question:
Do patterns of knowledge and attitudes exist among unvaccinated seniors?
Answer: *yes*

MedMCQA
Question:
In a 6-month-old child, thick curd like white patch appears on the buccal mucosa. On rubbing it leaves an erythematous patch. Most likely diagnosis is:
A. Tuberculosis
B. Lichen planus
C. Lupus erythematous
D. Candidiasis
Answer: *Candidiasis*

Figure 1: Examples of PubMedQA and MedMCQA datasets. PubMedQA requires intra-sample referring ability, whereas MedMCQA mainly measures acquired knowledge from the LM itself or needs to refer to few-shot examples (inter-sample referring).

are encoder-based language models (Ho et al., 2024). With the development of auto-regressive language models (LMs), numerous studies have demonstrated their superior generalization ability and performance compared to encoder-based PLMs when the models are sufficiently large (Brown et al., 2020; Ouyang et al., 2022; Taylor et al., 2022). They can not only understand instructions or background information provided in the context, which can be considered as the *intra-sample referring ability* (as shown in Figure 1), but also adapt to new tasks by referring several provided demonstrations, which can be regarded as the *inter-sample referring ability*. Moreover, with the advent of remarkable open-sourced large language models (LLMs), such as the Llama family (Touvron et al., 2023a,b), researchers turn to explore the possibility of conducting continual pre-training to develop

[1]Our codes are publicly available in https://github.com/Coldog2333/BioLinkLM.

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LLMs tailored for specific-domains (Chen et al., 2023; Huang et al., 2023; Wu et al., 2024).

Several pre-training methods have been proposed for encoder-based models, including masked language modeling, next sentence prediction (Devlin et al., 2019), document relation prediction (Yasunaga et al., 2022), translation language modeling (CONNEAU and Lample, 2019). These methods have effectively helped in learning specific knowledge and significantly promoted the development of encoder-based LMs. However, to the best of our knowledge, most auto-regressive LMs adhere to a conventional method for preparing input sequences for pre-training or continual pre-training, which involves first shuffling the corpora, followed by the random packing (concatenation) of documents until the concatenated sequence reaches the prescribed maximum input length (Radford et al., 2019; Brown et al., 2020; Touvron et al., 2023a; Chen et al., 2023).

Recently, some studies demonstrate that the standard pre-training method for auto-regressive LMs can be further improved by designing appropriate pre-training sequences (Levine et al., 2021; Gu et al., 2023; Shi et al., 2023; Zhao et al., 2024), such as incorporating relevant texts into the preceding context. LinkBERT (Yasunaga et al., 2022) constructs three types of segment pairs based on a citation network to classify whether they are continuous, linked, or random, motivating models to capture the citing relationship between two text segments. Considering its success, we consider whether this methodology can be extended to auto-regressive LMs, helping them learn to capture relationships between multiple text segments and improving their referring ability. Therefore, in this paper, we explore the linking information from the citation network to construct sequences for training an auto-regressive LM, which we call it as LinkLM. Specifically, we design the pre-training sequences by organizing the documents based on their citing relationships. When optimizing the language modeling objective, auto-regressive LMs can learn to refer to possible information from the previous context. As illustrated in Figure 2, when predicting the tokens in the abstract D_1^1 (<PMID 37893869>), models can access information from its citing papers, learning from the findings about other detection tools (e.g., ENFEN Battery in D_2^1) and different aspects (e.g., neurobiology in D_2^2). Furthermore, by referring D_2^1, D_3^1, and D_4^1, we can understand Attention Deficit Hyperactivity Disorder (ADHD) with a series of related works along the science history. Therefore, training with LinkLM data encourages LMs to refer to necessary information from the previous context, and therefore enhances models' referring ability, which can be used in tasks such as open-book question answering (Mihaylov et al., 2018; Jin et al., 2019) and the In-Context Learning (ICL) setting (Dong et al., 2022).

Though the success of constructing appropriate pre-training sequences has been revealed by some previous works (Gu et al., 2023; Shi et al., 2023; Zhao et al., 2024), they primarily focus on general domains where the distinction of topics is less challenging than that in the biomedical domain. Additionally, they only trained their models from scratch. However, after pre-training with large-scale, randomly concatenated documents, LMs may tend to avoid breaking document boundaries (i.e., $[EOS]$ token) to refer to adjacent concatenated documents. Whether the conclusion still holds under the continual pre-training scenario is not clear. Since continual pre-training is a prevalent practice for developing biomedical LLMs, we focus on this setting in our experiments.

In summary, our contributions are threefold:

- We propose a novel algorithm for pre-training sequence design exploiting citation information from a citation network to improve referring ability for biomedical language models.
- Our empirical studies fill the gaps in previous research, demonstrating that constructing appropriate pre-training sequences is also promising under the continual pre-training setting. And it improves both intra-sample and inter-sample referring ability of auto-regressive language models.
- Our experiments on one-shot evaluation with retrieved demonstrations show that our method can further boost performance in this scenario, emphasizing the potential of designing task-specific pre-training sequences.

2 Related Work

2.1 Domain Adaptation

Among domain-specific LMs, there are three dominant architectures: encoder-only, encoder-decoder, and decoder-only Transformer (Ho et al., 2024). For encoder-only models, BioLinkBERT

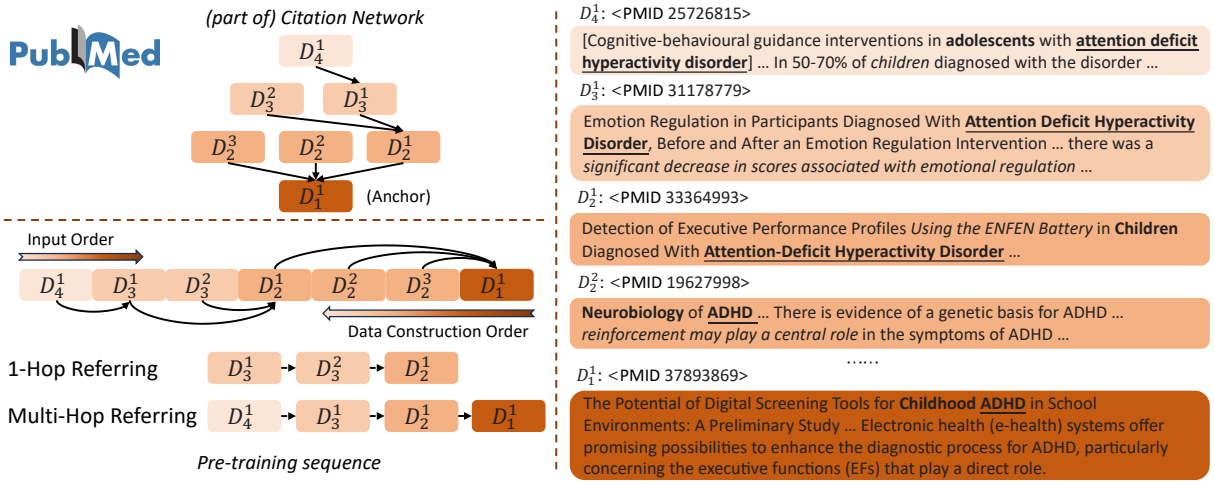


Figure 2: Example of LinkLM data construction. The detailed process is described in Algorithm 1. In this example, the pre-training sequence contains a series of works discussing Attention Deficit Hyperactivity Disorder (ADHD). Training with LinkLM data, models can not only learn to predict an anchor abstract by referring to its citing references, but also benefit from the multi-hop references, which are not linked directly.

(Yasunaga et al., 2022) introduced a pre-training objective, document relation prediction (DRP), to identify whether a pair of segments is contiguous, linked, or random. For encoder-decoder models, BioT5 (Pei et al., 2023) constructed various tasks by incorporating molecule and protein representations into pure texts, learning the relation between biochemistry representations and their surrounding contexts. For decoder-only models, Galactica (Taylor et al., 2022) and Meditron (Chen et al., 2023) carefully processed input texts by inserting the title of the cited paper when the input texts contain citation annotations. This series of work shows that careful design of pre-training input sequences can indeed improve LMs beyond the standard pre-training. However, most of them require fine-grained annotations, which are expensive to collect. Although BioLinkBERT exploited the citation network, it remains unclear whether it is still available and how it can be applied to auto-regressive LMs.

2.2 Pre-training Sequence Design

Recently, in the general domain, some researchers have shown that even without fine-grained annotations, we can still construct meaningful and useful input sequences for pre-training. Levine et al. (2021) proved that by pre-pending semantically related texts measured by RoBERTa (Liu et al., 2019) sentence embeddings, sentence representations and open-domain question-answering abilities of auto-regressive LMs can be improved. Zhou et al. (2022) constructed hyperlink-induced question-passage pairs based on the hyperlink networks to enhance dense passage retriever (DPR). Gu et al. (2023) trained a task-specific classifier to identify the intrinsic tasks within the pre-training texts and clustered those whose intrinsic tasks are the same into the same context, improving the in-context learning ability of LMs. Shi et al. (2023) retrieved similar texts using Contriever (Izacard et al., 2022) and concatenated them one by one to form long input sequences. Zhao et al. (2024) showed that packing documents from a single source could be more effective than packing documents sampled randomly from the entire pre-training corpora. In the scientific domain, SPECTER (Cohan et al., 2020) constructed contrastive pre-training samples to enhance the document-level representations. However, it introduced extra classifiers during pre-training and may not be applicable for auto-regressive LMs.

In this paper, we explore a more challenging case, where all documents discuss a similar topic. Even the *standard* way can provide pre-training sequences with relevant context (belonging to the biomedical-related topics). Therefore, this leads to a research question: Is it possible to further improve the pre-training for biomedical language models using exactly the same corpus?

Additionally, existing studies primarily explore training models from scratch (Gu et al., 2023; Shi et al., 2023; Zhao et al., 2024). However, it is unclear whether this conclusion still holds in continual pre-training, which is a prevalent method

in domain adaptation. Levine et al. (2021) integrated similar texts selected via K-Nearest Neighbor (KNN) into the context after several steps of warming up, which could be considered as an attempt at continual pre-training. However, the LMs they used were relatively small, containing only 345M parameters. In this paper, we focus on this continual pre-training setting to improve the referring ability of biomedical language models.

3 Preliminary Experiment

All references of a given paper can serve as background information, but their importance towards the given paper is different. Therefore, it is necessary to rank them based on their significance. A natural solution is using retrievers. As one of our preliminary experiments, we realize that retrievers are not as reliable as we expect in identifying the most appropriate reference for a given abstract. Before using the retriever to select references that provide sufficient background information for the following anchor abstract, we should first understand *how well a retriever can find out the reference that provides the most information for predicting a given abstract*. We know the information that a reference provides can be measured by

$$I(ref; anchor) = P(anchor) - P(anchor|ref) \quad (1)$$

where $P(anchor)$ is the perplexity of an anchor abstract, and $P(anchor|ref)$ is the perplexity of the anchor abstract when the reference is provided in the context. For each reference, $P(anchor)$ is constant, so we can measure the information and rank references directly by $P(anchor|ref)$.

To the best of our knowledge, Meditron (Chen et al., 2023) is currently the best open-sourced biomedical LM because it is continually pre-trained with biomedical texts on the top of the powerful LLM, Llama-2 (Touvron et al., 2023b), so that it can provide a relatively accurate measurement for conditional perplexity. Therefore, we use Meditron-7B to compute the ranking of references as the ground truth. Subsequently, we use some popular models including the Contriever[2] to rank the references of a given abstract. We selected 1,000 anchor abstracts for this analysis. Results are summarized in Table 1. Kendall's Tau measures the correspondence between two rankings, while HitN@Top5 represents the proportion that one of the top-N predictions exists in top-5 references ranked by Meditron-7B.

Model	Params	Kendall's Tau	Hit1@Top5	Hit3@Top5
GPT-2	0.1B	0.087	43.4%	69.0%
GPT-2 medium	0.3B	0.665	69.5%	88.5%
GPT-2 large	0.6B	0.664	70.3%	88.3%
BioMedLM	2.7B	0.590	66.0%	86.8%
Llama-2-7B	7B	0.882	89.7%	98.5%
Contriever	0.1B	0.098	48.6%	71.4%
Meditron-7B	7B	1.000	100%	100%

Table 1: Ranking performance of models. HitN@Top5 represents the proportion that one of the top-N predictions exists in top-5 references ranked by Meditron-7B.

Considering Kendall's Tau and HitN@Top5, we realize that Contriever cannot accurately provide the most appropriate reference for the given abstract, despite its widespread usage in information retrieval. Specifically, only 48.6% of the top-1 retrieved reference falls in the top-5 references ranked by Meditron-7B. And the proportion of the cases where at least one of the top-3 retrieved references falls in the top-5 references ranked by Meditron-7B is 71.4%. Compared to GPT-2 (Radford et al., 2019) which has a similar number of parameters, Contriever does not show a superior performance. However, we should point out that the dense passage retriever (DPR) is more computationally efficient than auto-regressive LMs because it decouples the encoding of a pair of texts. Nevertheless, it is still a good choice in the field of information retrieval. Therefore, as a trade-off, using DPR necessitates retrieving multiple references simultaneously to ensure that the selected references can provide sufficient information to predict the following anchor abstract.

4 Methodology

In the scenario of pre-training biomedical LMs, we usually collect abstracts or full papers as the pre-training corpus. The key of our methodology is to construct a long input sequence containing relevant information in the context. Scientific researchers typically cite pertinent papers to support their conclusions and these citing papers are often previous stages of their research. Based on this, we construct the pre-training input sequence with the help of the citation network, which is easy to obtain in the biomedical domain. Algorithm 1 shows the procedure of our methodology.

To develop biomedical LMs, we use one of the most commonly used data sources, PubMed Ab-

[2]We use `facebook/contriever-msmarco` checkpoint (supervised version) from Hugging Face.

Algorithm 1 LinkLM Sequence Construction

Require: $\mathcal{G} = (\mathcal{D}, \mathcal{L})$: Citation network
Require: $\mathcal{R}(d)$: Return the citing references
Require: $Retriever$
$P \leftarrow [], Q \leftarrow []$
while $|\mathcal{D}| > 0$ **do**
  Randomly select d_i from $\mathcal{D}$
  $Q.append(d_i)$
  $\mathcal{D}.remove(d_i)$
  while $\mathcal{R}(d_i) \cap \mathcal{D} \neq \emptyset$ **do**
    $K \leftarrow Poisson(3)$
    $\bar{\mathcal{D}} \leftarrow TopK(\mathcal{R}(d_i) \cap \mathcal{D}, Retriever, K)$
    $d_j \leftarrow \arg\max_{d \in \bar{\mathcal{D}}} indegree(d)$
    $Q.extend(\bar{\mathcal{D}} \backslash d_j)$
    $Q.append(d_j)$
    $\mathcal{D}.remove(\bar{\mathcal{D}})$
    $d_i \leftarrow d_j$
  end while
  $P.append(Q[:: -1])$
  $Q \leftarrow []$
end while
Shuffle P
return P: List of abstracts

stract[3]. After pre-processing the raw data, we extract both textual and citing information, forming a citation network $\mathcal{G}$. We begin with a randomly selected abstract as the anchor (e.g., D_1^1 in Figure 2). Unlike previous works (Shi et al., 2023; Zhao et al., 2024), we select multiple relevant references at the same time to increase the hit rate of selected references. This approach addresses the limitations of retrievers, which do not always retrieve the most relevant reference from the given candidates, as discussed in Section 3. To increase the diversity of our LinkLM data, we randomly sample the number of selected references, K, following a Poisson distribution. According to Table 1, setting $\lambda = 3$ allows a relatively high proportion (71.4%) of cases where retrieved references can provide enough information for the anchor abstract, whereas when λ is larger, it will increase the risk of introducing less relevant references in the context. Therefore, we adopt a Poisson distribution with an expected value of three. With the help of a given retriever, we select the top-K relevant references (e.g., D_2^1, D_2^2, and D_2^3 in Figure 2) from all references. To increase the possibility of constructing longer sequences, we select the reference with the largest in-degree among these K selected references. Assuming that D_2^1 has the largest in-degree, we continue the construction with D_2^1 until none of the references have any citing papers (e.g., D_4^1 in Figure 2 has no citing papers). The rest of the relevant references are ordered randomly in the queue Q. After the construction, we reverse the constructed sequence so that the later documents are supported by the earlier ones.

At the beginning of the data construction, we easily obtain multi-hop long sequences. However, since we delete nodes once they are visited to prevent duplication of pre-training samples, the original citation graph becomes sparse gradually. Many sequences will be composed by a single document at the end of the process. Therefore, after constructing all sequences, we perform sequence-wise shuffling so that the sequences comprising a single document will be distributed uniformly alongside other longer sequences. In this way, each batch contains linked long sequences, making full use of the constructed LinkLM data.

5 Experiments

5.1 Datasets

In the continual pre-training stage, we download the raw data from the PubMed 2024 Annual baseline[4] updated until December 14, 2023. We use PubMed parser (Achakulvisut et al., 2020) to extract necessary information including the title, abstract, and citations. We exclude isolated data points that are not cited by any paper and their citations are missing. We also exclude data points without any title or abstract. After preprocessing, we obtain approximately 25 million samples as the source for pre-training.

For evaluation, we use four widely used biomedical multi-choice question-answering (MCQA) datasets, as listed below.

- **MedMCQA** (Pal et al., 2022) is a large-scale MCQA dataset collected from the AIIMS & NEET PG entrance exam, containing more than 194k QA pairs. In the default evaluation setting, LMs can only access the question and four candidate options. Therefore, it is usually used to assess the biomedical knowledge memorized by models. Since the testing set does not provide the ground-truth answers, we use its validation set for evaluation.

[3] https://ftp.ncbi.nlm.nih.gov/pubmed/baseline/

[4] https://ftp.ncbi.nlm.nih.gov/pubmed/baseline/

	Train	Evaluation	#Choice	#Token/Sample Aver	#Token/Sample Max	w/ Context
MedMCQA	182,822	4,183	4	61.5	573	✗
MMLU-Medical	45	1,871	4	124.1	1,192	✗
USMLE-QA	10,178	1,273	4	251.8	1,152	✗
PubMedQA	211,269	1,000	3	437.1	1,909	✓

Table 2: Statistics of four biomedical MCQA datasets. Different from the other three MCQA datasets, an extra abstract is provided for each question in the PubMedQA dataset.

- **MMLU-medical** is a subset derived from MMLU (Hendrycks et al., 2020), containing 57 tasks across various fields. We select the QA pairs if they belong to one of the following topics: *high school biology, college biology, college medicine, professional medicine, medical genetics, virology, clinical knowledge, nutrition, and anatomy*. MMLU-medical is also a four-choice MCQA task and it is mainly designed to measure knowledge acquired during pre-training. We adhere to the official setting using development set for few-shot learning.

- **USMLE-QA** (Zhang et al., 2018) is an MCQA task based on United States Medical License Exams (USMLE), which requires a certain piece of knowledge or an answer based on a patient's condition description. We use the English four-choice version subset for evaluation.

- **PubMedQA** (Jin et al., 2019) is a three-choice MCQA task (yes/no/maybe). For each question, a related abstract from PubMed is provided, making it suitable for evaluating the intra-sample referring ability of LMs.

Table 2 summarizes their statistics. We compute the probability of generating each option and select the one with the lowest perplexity as the final prediction. We report model accuracy and calculate micro-average accuracy since different datasets have different numbers of testing samples.

5.2 Experimental Settings

Due to the limitation of our computation resources, we chose TinyLlama-1.1B[5] as our experimental subject, which was pre-trained sufficiently using 3T tokens (Zhang et al., 2024). After tokenization, we obtained approximately 8B tokens for continual pre-training. We followed most of the original hyperparameters of pre-training TinyLlama with a context length of 2048 tokens. Further details are provided in Appendix C.1. In the following comparisons, 'Vanilla' denotes the original TinyLlama. 'Standard' and 'LinkLM' represent the continually pre-trained TinyLlama with randomly packed documents and LinkLM data, respectively.

[5]We used `TinyLlama/TinyLlama-1.1B-intermediate-step-1431k-3T` checkpoint from Hugging Face.

5.3 Intra-Sample Referring Ability

As discussed in Section 5.1, among these four medical MCQA tasks, PubMedQA requires LMs to answer questions by referring to the given related abstract. Therefore, we perform a zero-shot evaluation on PubMedQA to evaluate the intra-sample referring ability of LMs. We observe fluctuations across different checkpoints. To better visualize their differences, we smooth the average accuracy with windows of size three. Figure 3 illustrates the zero-shot performance on PubMedQA. We find that after training approximately 3B tokens, the LM pre-trained with LinkLM data consistently and significantly outperforms standard pre-training, indicating the effectiveness of our proposed method. Additionally, Table 3 shows the quantitative performances of four biomedical MCQA datasets. Compared to the vanilla TinyLlama, continual pre-training enriches the biomedical knowledge of LMs, leading to a 10.3% relative improvement (from 29.59 to 32.63) from vanilla TinyLlama to continual pre-trained TinyLlama. However, with our designed LinkLM data, though it can also achieve a 9.4% relative improvement compared to the vanilla TinyLlama, performances on some datasets (e.g., MedMCQA, MMLU-Medical, etc.) slightly drop compared to standard pre-training. This observation indicates that while using LinkLM data encourages LMs to refer to previous contexts, it may also weaken memorization during pre-training.

5.4 Inter-sample Referring Ability

Auto-regressive biomedical LMs are usually employed under the in-context learning scenario,

Accuracy (%)		MedMCQA	MMLU-Medical	USMLE-QA	PubMedQA	Average (Micro)
Vanilla	(0 shot)	25.34	24.91	26.47	60.10	29.59
Standard	(0 shot)	29.55	25.98	28.83	62.80	32.63
LinkLM	(0 shot)	28.97	25.44	27.26	**66.00**	32.36
Vanilla	(3 shot, Random)	22.96±0.52	26.03±0.32	25.56±0.37	64.80±1.40	29.05
Standard	(3 shot, Random)	25.78±0.61	26.53±0.94	26.34±1.20	63.73±0.53	30.59
LinkLM	(3 shot, Random)	27.13±0.28	25.24±1.26	27.36±0.84	65.67±0.87	31.37
Vanilla	(1 shot, KNN)	30.10	**26.94**	26.55	62.30	32.69
Standard	(1 shot, KNN)	36.96	25.98	30.32	64.20	36.75
LinkLM	(1 shot, KNN)	**38.47**	25.01	**30.48**	64.10	**37.30**

Table 3: Quantitative performances of the vanilla TinyLlama and final checkpoints that are continually pre-trained in the standard way or with our LinkLM data on four biomedical MCQA datasets. The best and second-best performances are highlighted in bold and underlined, respectively. For standard few-shot evaluation, we run multiple times with three different random seeds to reduce the variant of the results.

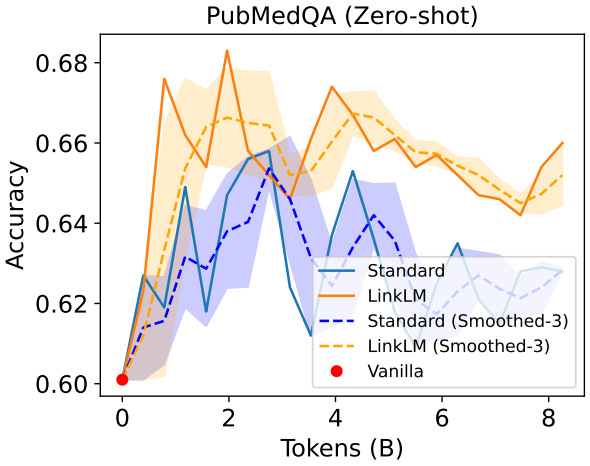
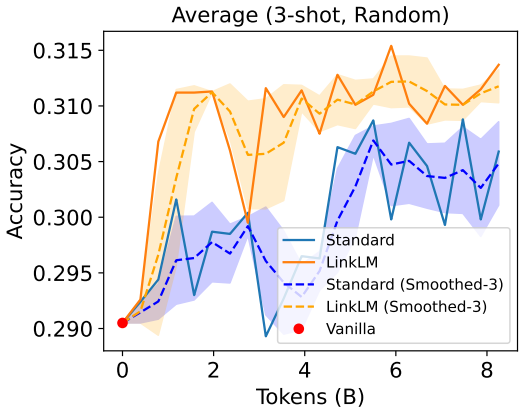


Figure 3: Comparison between different pre-training strategies on PubMedQA (Smoothing window size=3). The full and dotted lines represent the exact and smoothed values of performances, respectively. The colored area represents the standard deviation within a smoothing window.

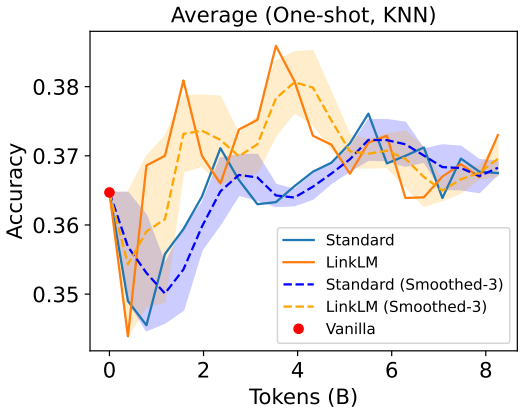
learning from the input-label mapping in previous demonstrations, which can be considered as the inter-sample referring ability. Therefore, we perform a few-shot evaluation on these four datasets, specifically conducting a three-shot evaluation. Figure 4a illustrates that pre-training with LinkLM data significantly outperforms the standard pre-training under few-shot evaluation. Remarkably, 90.48% of the checkpoints have better average accuracy across the four datasets than standard pre-training, which confirms again the effectiveness of LinkLM data under continual pre-training. However, compared to zero-shot performance, TinyLlama-1.1B does not consistently benefit from the provided demonstrations in standard few-shot settings, as evidenced by its performance on MedMCQA and USMLE-QA. The average performances even drop slightly for TinyLlama pre-trained in the standard way (about 6.3% relative degradation) and TinyLlama pre-trained with LinkLM data (about 3.1% relative degradation). We hypothesize that it is due to the quality of randomly sampled demonstrations that fail to provide useful information and may even disrupt LM predictions.

Inspired by KATE (Liu et al., 2022), which retrieves similar demonstrations to boost few-shot performance, we use Contriever to retrieve the top-K similar demonstrations from each training set. Contrary to the findings reported in Min et al. (2022), our results suggest that it is possible to retrieve helpful demonstrations from the training set, whose input-label mapping can benefit the prediction of the query. We perform a one-shot evaluation here since adding more retrieved demonstrations does not improve the performance in our case. Figure 4b shows the comparison between our method and standard pre-training. Under this experimental setting, we observe obvious improvements over standard few-shot evaluation, highlighting the importance of high-quality demonstrations in the ICL scenario. Although the LM trained with LinkLM data only slightly outperforms standard pre-training at the end of continual pre-training, there are 71.43% of checkpoints that have better average accuracy across four datasets than the standard pre-training. After pre-training for several steps, the LM pre-trained with LinkLM data can achieve good performance under this setting, indicating that LinkLM data can activate their potential on inter-sample referring ability when the demonstrations are closely related to the following query.

Table 3 demonstrates that using retrieved demon-



(a) Smoothed average accuracy across four biomedical MCQA tasks under three-shot evaluation (Window size=3)



(b) Smoothed average accuracy across four biomedical MCQA tasks under one-shot evaluation using retrieved demonstration (Window size=3)

Figure 4: Comparison between different pre-training strategies under few-shot evaluation. The full and dotted lines represent the exact and smoothed values of performances, respectively. The colored area represents the standard deviation within a smoothing window.

strations instead of using randomly sampled ones as in standard ICL can significantly boost few-shot performance. With appropriate demonstrations, LMs perform significantly better than those under the zero-shot setting. Compared to zero-shot performance, LMs continually pre-trained in the standard way and with our designed LinkLM data achieve 12.4% and 15.3% of relative improvement, respectively. We believe the reason is that in the standard ICL setting, the sampled demonstrations may not be strongly related to the current question, so they can only provide shallow information like task format (Min et al., 2022). Sometimes, they even distract the LMs. However, when using retrieved demonstrations, current questions can not only understand the task format but also learn from the input-label mapping and knowledge shown in the demonstrations. LMs trained with LinkLM data can further improve inter-sample referring ability during the continual pre-training stage, thus achieving larger improvement in few-shot evaluation.

Especially, on MedMCQA, LM trained with LinkLM data significantly outperforms LM trained in a standard way, no matter whether the demonstrations are randomly sampled or retrieved. By conducting a case study on MedMCQA, shown in Figure 5, we find that retrieved demonstrations from the training set are highly related to the following question and usually provide pertinent knowledge. Since TinyLlama pre-trained with LinkLM data can memorize knowledge and learn to refer to necessary information across different documents meanwhile during continual pre-training, it is also encouraged to refer to some information from previous contexts in downstream tasks after pre-training. There is an exception on MMLU-medical, where we find no significant improvement even when few-shot demonstrations are given. We attribute it to the insufficient number of candidate demonstrations since there are only 45 samples in the training set[6] as shown in Table 2, so that the randomly sampled or retrieved demonstrations could be less relevant to the testing sample, leading to no remarkable improvement over zero-shot evaluation.

One-shot example (with retrieved demonstration) for MedMCQA

```
Question: A 60 year old male presents with a creamy curd
like white patch on the tongue. The probable diagnosis is -
A. Candidiasis
B. Histoplasmosis
C. Lichen planus
D. Aspergillosis
Answer: Candidiasis

Question: In a 6-month-old child, thick curd like white
patch appears on the buccal mucosa. On rubbing it leaves an
erythematous patch. Most likely diagnosis is:
A. Tuberculosis
B. Lichen planus
C. Lupus erythematous
D. Candidiasis
Answer:
```

Prediction: *Candidiasis*

Figure 5: Example of one-shot ICL with the retrieved demonstration on the MedMCQA dataset

Note that in domain adaptation, we usually use

[6]More precisely, the 'training set' is the validation set of MMLU according to the official setting of the original paper.

documents in a single focused domain, and therefore even the *standard* approach concatenates documents with similar topics within the context, helping LMs to refer to necessary information across document boundaries (i.e., $[EOS]$ token). In our method, we explicitly arrange the related references in the context, improving the inter-sample referring ability further. From another aspect, our pre-training method narrows the gap between pre-training phases and ICL with retrieved demonstrations. Therefore, we can expect that the inter-sample referring ability will be improved further and more robust if we construct more LinkLM data for further training.

6 Conclusions

In this paper, we propose a pre-training sequence construction method for improving the referring ability of biomedical language models. Previous studies mostly focus on general domains and they train the LMs from scratch with designed pre-training sequences. In contrast, we explore this topic in a more challenging scenario, where the distinction of fine-grained topics is more difficult in the biomedical domain. Moreover, we explore it under the continual pre-training setting, since it is a prevalent method for developing domain-specific LMs now, filling the gap in this series of work. In this paper, we construct pre-training sequences by concatenating relevant references into the previous context using linking information from a citation network. Empirical studies show that compared to the standard pre-training (i.e., randomly packing documents), our method significantly improves the intra-sample referring ability and the inter-sample referring ability on biomedical MCQA tasks, which answers our research question: by carefully designing pre-training sequences, we can still improve the pre-training for biomedical language models by reordering the pre-training documents (using exactly the same corpus). Especially, pre-training using LinkLM data can further improve the performance when using retrieved demonstrations, revealing the future potential of our proposed methodology.

Limitations

Owing to limited computation resources, we only conducted experiments on a language model with 1.1B parameters (TinyLlama-1.1B) using up to 8B tokens, which may not be sufficient for biomedical LLM applications. Experiments on larger models with larger amounts of biomedical pre-training data are needed in the future. However, according to the current trend shown in our experiments, after training with more LinkLM data, the improvement compared to the standard pre-training would be larger.

Another limitation is that our methodology requires a citation network, restricting its applicability to other scientific domains where it is not easy to build the citation network. To address this, we believe that training a classifier for link prediction may be a possible solution. Besides, in other domains, the citation network can also be replaced by hyperlink networks or paragraph structures of long documents. However, due to the constraints of this paper's length, we will not explore this direction in depth.

Besides, full papers from PubMed Central[7] are also commonly used for pre-training biomedical LMs. However, most of the full papers exceed the maximum input length of existing foundation LMs. Although these full papers are also linked to the citation network, how to construct LinkLM data for them remains a challenge. Future efforts will consider separating full papers into several paragraphs and constructing better pre-training sequences to improve the referring ability of biomedical LLMs.

Ethics Statement

Though using LinkLM data can improve the referring ability for biomedical language models, particularly in retrieval-augmented tasks (e.g., PubMedQA) and in-context learning scenarios, some potential issues for biomedical LMs may also apply to our case, such as generating inappropriate clinical suggestions accompanied by hallucinations. We strongly recommend conducting a thorough assessment and careful alignment (e.g., employing RLHF (Ouyang et al., 2022)) before deployment to the real world.

The involved pre-trained language model, TinyLlama, is licensed under Apache License 2.0[8]. We adhere strictly to this license during our experiments. Regarding the involved dataset, PubMed Abstract, we collected the raw data following instructions on the official website[9], ensuring not to violate their terms.

[7] https://www.ncbi.nlm.nih.gov/pmc
[8] http://www.apache.org/licenses/LICENSE-2.0
[9] https://pubmed.ncbi.nlm.nih.gov/download/

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A Perplexity Evaluation

In addition to evaluating on downstream tasks, we also tracked the loss on the evaluation set. We sampled 10,000 abstracts from the excluded isolated data points to serve as the evaluation set for perplexity evaluation. As shown in Table 4, no significant difference was observed between the standard pre-training and pre-training with our LinkLM data, which is consistent with the findings of Liu et al. (2023) stating that LMs with similar pre-training losses may perform differently on downstream tasks.

Strategy	Eval Loss	Eval PPL
Standard	1.871	6.49
LinkLM	1.874	6.51

Table 4: Loss and perplexity on evaluation set.

B Evaluation in Other Tasks

In addition to evaluating our method on question-answering tasks, we also conducted evaluation in other tasks, including clinical natural language inference (NLI) and clinical fact verification tasks to further verify the effectiveness of our method. These two tasks require models to understand the relationship between two given sentences or documents so that they can be used to evaluate the referring ability of LMs. We used the mediqa-RQE dataset (Ben Abacha et al., 2019) as a representative dataset in NLI task, and the HealthVer dataset (Sarrouti et al., 2021) as a representative dataset in clinical fact verification task. Table 5 shows that no matter under zero-shot or few-shot settings, the LM continually pre-trained with our LinkLM data can perform better than that continually pre-trained in a standard way. Therefore, we can also conclude again the effectiveness of our proposed LinkLM method.

Accuracy (%)	mediqa-RQE	HealthVer
Standard (0 shot)	47.39	39.42
LinkLM (0 shot)	**49.13**	**41.20**
Standard (3 shot, Random)	51.45	35.03
LinkLM (3 shot, Random)	**52.75**	**35.51**

Table 5: Quantitative performances of the final checkpoints that are continually pre-trained in the standard way or with our LinkLM data on the mediqa-RQE and HealthVer datasets. The best performances are highlighted in bold. For standard few-shot evaluation, we run multiple times with three different random seeds to reduce the variant of the results.

C Experimental Details

C.1 Implementation Details

We chose TinyLlama-1.1B[10] as our experimental subject, which had been pre-trained sufficiently using 3T tokens (Zhang et al., 2024). After tokenization, we obtain approximately 8B tokens for continual pre-training. We follow most of the original hyperparameters for pre-training TinyLlama, using a context length of 2048 tokens. The global batch size we use is 0.5M tokens. According to the conclusions from Goyal et al. (2017), we use a smaller learning rate of 1e-4.

We used PyTorch (Paszke et al., 2019) and transformers library (Wolf et al., 2020) for implementation. Pre-trained checkpoints were downloaded from Hugging Face[11]. We also adopted Deepspeed Zero3 (Rajbhandari et al., 2020), flash-attention (Dao et al., 2022; Dao, 2024), and checkpointing techniques to speed up training. All experiments were conducted on 8 NVIDIA A100 (40GB) GPUs. Continual pre-training TinyLlama-1.1B with approximately 8B tokens cost approximately 24 hours on these 8 NVIDIA A100 GPUs.

C.2 Prompt Engineering

In our zero-shot and few-shot evaluation, we used the prompts following Gao et al. (2023) to complete the multi-choice question-answering tasks as shown in Table 6. And Table 7 shows an example for MedMCQA under the few-shot evaluation (#Shot=3). With the help of a retriever, we can retrieve relevant demonstrations from the training set to assist the prediction of the following queries, as shown in Figure 5, where we also find that the retrieved demonstrations actually provide not only the task format but also relevant knowledge, and therefore benefits the in-context learning.

[10] We used `TinyLlama/TinyLlama-1.1B-intermediate-step-1431k-3T` checkpoint from Hugging Face.

[11] `https://huggingface.co/models`

Prompt template for MedMCQA, USMLE-QA, and MMLU-Medical

```
Question: {question}
A. {option_a}
B. {option_b}
C. {option_c}
D. {option_d}
Answer:
```

Prompt template for PubMedQA

```
Abstract: {context}
Question: {question}
Answer:
```

Table 6: Prompt templates for MCQA tasks.

Three-shot example for MedMCQA

```
Question: Claw sign on x-ray is seen in?
A. Ischemic colitis
B. Intussusception
C. Sigmoid volvulus
D. Crohn's disease
Answer: Intussusception

Question: All of the following are microsomal enzyme inhibitors except
A. Glucocoicoids
B. Cimetidine
C. Ciprofloxacin
D. INH
Answer: Glucocoicoids

Question: A young female presents with a history of dyspnoea on exertion. On
examination, she has wide, fixed split S2 with ejection systolic murmur (III/VI)
in left second intercostal space. Her ECG shows left axis deviation. The most
probable diagnosis is -
A. Total anomalous pulmonary venous drainge.
B. Tricuspid atresia.
C. Ostium primum atrial septal defect.
D. Ventricular septal defect with pulmonary arterial hypertension.
Answer: Ostium primum atrial septal defect.

Question: Which of the following is not true for myelinated nerve fibers:
A. Impulse through myelinated fibers is slower than non-myelinated fibers
B. Membrane currents are generated at nodes of Ranvier
C. Saltatory conduction of impulses is seen
D. Local anesthesia is effective only when the nerve is not covered by myelin
sheath
Answer:
```

Table 7: An example of three-shot in-context learning for MedMCQA.