Once Read is Enough: Finetuning-free Language Models with Cluster-guided Sparse Experts for Long-tail Domain Knowledge

Anonymous Author(s) Affiliation Address email

Abstract

 Language models (LMs) only pretrained on a general and massive corpus usu- ally cannot attain satisfying performance on domain-specific downstream tasks, and hence, finetuning pretrained LMs is a common and indispensable practice. However, domain finetuning can be costly and time-consuming, hindering LMs' deployment in real-world applications. In this work, we consider the incapability to memorize domain-specific knowledge embedded in the general corpus with rare occurrences and "long-tail" distributions as the leading cause for pretrained LMs' inferior downstream performance. Analysis of Neural Tangent Kernels (NTKs) reveals that those long-tail data are commonly overlooked in the model's gradient updates and, consequently, are not effectively memorized, leading to poor domain- specific downstream performance. Based on the intuition that data with similar semantic meaning are closer in the embedding space, we devise a Cluster-guided Sparse Expert (CSE) layer to actively learn long-tail domain knowledge typically neglected in previous pretrained LMs. During pretraining, a CSE layer efficiently cluster domain knowledge together and assign long-tail knowledge to designate extra experts. CSE is also a lightweight structure that only needs to be incorporated in several deep layers. With our training strategy, we found that during pretrain- ing, data of long-tail knowledge gradually formulate isolated, "outlier" clusters in an LM's representation spaces, especially in deeper layers. Our experimental results show that only pretraining CSE-based LMs is enough to achieve superior performance than regularly pretrained-finetuned LMs on various downstream tasks, implying the prospects of finetuning-free language models.

1 Introduction

 In natural language processing, it is a prevalent paradigm to pretrain language models (LMs) on a large-scale unlabeled corpus covering a plethora of knowledge, and those pretrained LMs have exhibited impressive performance in language tasks in the general domain [\[40\]](#page-11-0). When it comes to downstream tasks requiring specialized domain knowledge, e.g., legal search or medical question answering [\[24,](#page-10-0) [7\]](#page-9-0), those models usually fail to expertise in such knowledge and cannot acquire desirable performance. As such, finetuning on domain-specific datasets is deemed essential to fulfill pretrained LMs' potential in various downstream tasks [\[22,](#page-10-1) [14,](#page-9-1) [41,](#page-11-1) [36\]](#page-11-2). However, finetuning an LM could require domain expertise from humans, for instance, the involvement of a doctor for healthcare tasks [\[31\]](#page-11-3), which can be costly and laborious. The associated catastrophic forgetting issue [\[27\]](#page-10-2) could further complicate the finetuning process.

 In this work, we re-visit the pretraining-finetuning paradigm and raise the following question: *is finetuning indispensable to LMs*? Notably, the domain-specific knowledge necessary for various

Submitted to 38th Conference on Neural Information Processing Systems (NeurIPS 2024). Do not distribute.

Figure 1: a) The top 20 subreddits with the highest amount of data in the Reddit Comments Dataset, where a typical long-tail distribution can be observed. b) Language Models struggle to memorize long-tail domain knowledge during pre-training. The less frequently a sentence appears in the training corpus, the higher its perplexity, indicating that it is not effectively memorized.

 downstream tasks is usually embedded in the pretraining corpus of extensive information sources. Those pieces of domain-specific information may only appear a few times in the massive corpus, significantly less frequently than other ubiquitous and general knowledge, and there can be numerous pieces of such rare information, a distribution usually defined as "long-tail". In Fig [1\(a\),](#page-1-0) we plot the frequency of the top-20 subreddits count on Reddit Comments Dataset [\[2\]](#page-9-2), and a typical long- tail distribution can be observed. Previous works have verified that LMs are not good learners of long-tail knowledge in the pretraining dataset with Question-Answering as the downstream task[\[21\]](#page-10-3). Our experiments, as shown in Figure [1\(b\),](#page-1-1) further illustrate that pretrained LMs do not adequately retain domain-specific knowledge in long-tail sequences which is evidenced by a surge in perplexity corresponding to decreased frequency score. This could result in inferior performance on downstream tasks. Finetuning improves LMs' domain performance by providing a second lesson, which could be avoided if the first (pretraining) is appropriately delivered. To unveil the hidden mechanisms under LM's incapability to learn long-tail domain-specific knowl- edge, we investigate the behaviors of a GPT on the Wikipedia dataset. We examine LMs' learning capabilities on long-tail data by analyzing the Neural Tangent Kernels (NTKs) of long-tail data and all data. Recent research [\[5,](#page-9-3) [39\]](#page-11-4) has indicated that the updating of deep networks can be governed by the gradient direction corresponding to the principle eigenvector of an NTK matrix, which reflects the most common gradient-descending direction across the entire input space. Following those works, we consider an NTK's principle eigenvector (PE) gradient direction as a primary indicator of an LM's overall gradient-updating direction over a data space. Our analysis has revealed that the PE gradient direction of long-tail data, indicating the gradient-descending direction from long-tail knowledge, is

 generally diverged from that of overall data, which rules the overall updating of network parameters. The observation that long-tail data cannot substantially impact LMs' parametric updates under regular pretraining settings explains pretrained LMs' incompetence on domain-specific knowledge of rare occurrences, necessitating an effective solution.

 To this end, we propose the Cluster-guided Sparse Expert (CSE) layer, an effective, efficient, and easy-to-implement approach to improve LMs' long-tail knowledge awareness. In a CSE layer, with intuition such that data with similar semantic meaning are closer in the embedding space, we perform efficient clustering on the embeddings to group data from different domains, and additional experts will be assigned to explicitly and appropriately memorize the information within those clusters. Models trained with CSE show pronounced cluster structure in the embedding space, where long-tail data forms small, outlier clusters. We empirically demonstrate that converting several deep layers into CSE ones can be enough to achieve satisfying results, such as the last two layers of GPT[\[29\]](#page-10-4) or BERT[\[10\]](#page-9-4), and the incurred computational costs are comparatively small and arguably acceptable. We have verified that pretrained CSE-based LMs have outperformed regularly pretrained-finetuned LMs on downstream tasks from various domains, which implies that domain finetuning may not be essential if long-tail knowledge can be sufficiently learned.

Our contributions are summarized as follows:

- We have presented that datasets show a long-tail distribution, with domain specific data in the long-tail, and revealed that long-tail data cannot substantially affect LMs' training, which is a leading cause of LMs' incompetence on learning rare, domain-specific knowledge.
- We have devised a Cluster-guided Sparse Expert (CSE) architecture to better pretrain LMs to memorize the long-tail domain knowledge. With such a training strategy, LMs can effectively capture long-tail domain data in the representation space as outlier clusters, thereby enhancing their ability to handle less frequent contexts efficiently.

 • Promising performance on downstream tasks has verified the effectiveness of the proposed method, indicating that finetuning may not be indispensable to LMs.

2 Analysis of Long-Tail Domain Data

84 In this section, we first elucidate the challenges associated with learning from long-tail data through gradient analysis. We then explore the embedding space using the Cluster-guided Sparse Expert (CSE) layer, which effectively captures the structural nuances of long-tail data. Furthermore, we examine the dynamics of these clustering structures, offering insights into how the learning processes of long-tail clusters adapt and evolve across various training stages and model layers.

2.1 Challenges in Learning Long-Tail Domain Data

 This subsection explores the significant challenges posed by long-tail domain data within language models (LMs). The primary issue stems from the divergence in gradient directions between long-tail data and the general gradient-updating trajectory of these models, which critically hampers effective learning.

94 2.1.1 Preliminaries and Definitions

 Informed by seminal works [\[12,](#page-9-5) [19\]](#page-10-5), we utilize Neural Tangent Kernels (NTKs) to scrutinize the gradient behavior of neural networks under a gradient descent training regime. The NTK, represented 97 as $\Theta(\mathcal{X}, \mathcal{X})$, is defined as the outer product of the gradients of network outputs relative to its 98 parameters $\Theta(\mathcal{X}, \mathcal{X}) = J_{\theta}(\mathcal{X}) J_{\theta}(\mathcal{X})^{\top}$, where $J_{\theta} = \nabla_{\theta} f(\mathcal{X}; \theta)$ denotes the Jacobian matrix of the 99 function f at the data points \mathcal{X} .

 To determine the predominant gradient-descending direction across the input space, which is influ- enced by the gradient direction associated with the principal eigenvector of the NTK matrix, we first perform an eigenvalue decomposition of the NTK matrix. Recognized as a positive semi-definite real 103 symmetric matrix, the NTK decomposes into $\Theta = \mathbf{U}\mathbf{\Lambda}\mathbf{U}^{\top} = \sum_{i=1}^{n} \lambda_i \mathbf{u}_i \mathbf{u}_i^{\top}$. Here, *n* represents 104 the total number of training instances. The principal eigenvector \mathbf{u}_{max} is identified as the vector corresponding to the maximum eigenvalue. Then the primary gradient direction for a given input set \mathcal{X} is $\mathbf{g}_{\theta}(\mathcal{X}) = \mathbf{u}_{max}J_{\theta}(\mathcal{X})$. Building upon above preliminaries, we introduce the metric of Gradient Consistency (GC) to evaluate the alignment between gradient directions for specific data subsets and the overall dataset.

109 **Definition 1** (Gradient Consistency (GC)). Let \mathcal{X}' be a specific subset of the training set \mathcal{X} . The 110 gradient consistency of \mathcal{X}' is evaluated by computing the cosine similarity between the most prevalent 111 *gradient direction of* \mathcal{X}' and that of the entire dataset \mathcal{X} :

$$
GC_{\theta}(X') = \frac{\mathbf{g}_{\theta}(\mathcal{X}) \cdot \mathbf{g}_{\theta}(\mathcal{X}')}{\|\mathbf{g}_{\theta}(\mathcal{X})\| \|\mathbf{g}_{\theta}(\mathcal{X}')\|}.
$$
 (1)

 A higher GC value indicates that the model's optimization updates are well-aligned with the needs of the specific subset X' , suggesting focused and effective learning of this data. Conversely, a lower value indicates suboptimal learning of these data, pointing to potential areas for improvement in model training strategies.

2.1.2 Gradient Consistency (GC) Analysis

 We assess the sentences from Wikipedia on a standard GPT model using sentence frequency score to gauge how frequently each sentence appears in the corpus. This score is calculated by averaging the frequency of its constituent tokens. Figure [2\(a\)](#page-3-0) displays the relationship between GC and sentence frequency score. Additionally, the figure includes a histogram that details how many percentage of sentences across the whole dataset falling into each frequency bin.

 There is a significant correlation between gradient consistency and the frequency with which sentences appear in the corpus. Notably, for sentences less frequently encountered in the dataset, the model demonstrates substantial ineffectiveness in learning. As demonstrated, the GC value sharply declines from 0.8 to 0.4 as the sentence frequency score decreases from 0.3 to 0.2. Furthermore, the GC value continues to diminish as the sentence frequency score decreases further, indicating that the model's gradient descent direction struggles to align with the requirements of these rare sentences.

 Our analysis indicates that the optimization requirements for long-tail sentences are significantly overlooked under standard pretraining conditions, resulting in the unique characteristics of long-tail domain data not being effectively captured. This oversight substantially impairs the performance of LMs when learning domain-specific knowledge involving rare occurrences, underscoring the need

for a more effective solution.

Figure 2: a) The correlation between sentence frequency score and gradient consistency. A histogram is also included showing how many percentage of sentences across the whole dataset falling into each frequency bin. b) A sampled embedding space containing 4 long-tail clusters, taken from our CSE layers.

2.2 Embedding Space Analysis With Cluster-guided Sparse Expert (CSE) layer

 Prior research[\[2\]](#page-9-2) has shown that extensive domain-specific data reside within the long-tail distribution of a general pretraining corpus, as illustrated in Figure [1\(a\).](#page-1-0) These data, often semantically similar, are likely to cluster closely within the embedding space, facilitating potential aggregation for dedicated learning. However, our analysis in Section [2.1](#page-2-0) underscores significant challenges in learning from long-tail data. Specifically, the model's gradient updates frequently fail to align with the optimization needs of these data, leading to their underrepresentation in the embedding space. Such misalignment obscures the inherent group structures that these domain data form based on their semantic similarities, thereby impeding dedicated learning efforts.

 To address the issues outlined above and to facilitate a more effective examination of long-tail domain data in the embedding space, we propose the Cluster-guided Sparse Expert (CSE) layer. This layer groups proximate long-tail data points into clusters and directs them to specialized experts for dedicated learning. As demonstrated in Figure [3\(a\),](#page-4-0) the GC value of long-tail data initially increases at the beginning of the training stage but rapidly declines thereafter, indicating that the model's inability to capture the learning dynamics of long-tail data begins early in the training process. Our CSE layer capitalizes on the clustering structure at the point where the GC value peaks, subsequently taking effect to channel domain-specific clusters into dedicated learning pathways. Further details about this approach are provided in Section [3.](#page-5-0)

 The clustering results from the CSE-based LM, shown in Figure [2\(b\),](#page-3-1) reveal four smaller clusters alongside a predominant one. Detailed analysis shows high domain coherence within the smaller clusters, each comprising sentences closely related to specific domains. The average sentence frequency score of these domain clusters falls into the long-tail of the sentence frequency distribution, as shown in Figure [2\(a\).](#page-3-0) In contrast, the predominant cluster, colored in purple, contains a diverse mix of more common data and exhibits a higher average sentence frequency compared to the smaller clusters. Further analysis of sentences with frequency scores below 0.2 shows their random distribution across clusters, suggesting these extremely infrequent sentences may serve as noise in the learning process.

 This analysis demonstrates that our proposed CSE-based architecture effectively groups long-tail data from the same domains for dedicated learning, fostering a domain-specific clustering structure within the embedding space. The long-tail domain clusters, distinct from clusters containing common data, show a higher degree of compactness and are clearly separated, highlighting the unique features embodied by these clusters.

2.3 Dynamic of Long-Tail Domain Clusters

 In this subsection, we explore the learning dynamics of long-tail domain data by tracking how clusters evolve across different training stages and model layers. We utilize K-Means clustering [\[20\]](#page-10-6) and employ the elbow method to determine the optimal number of clusters.

 Long-tail clusters can be seen early in the training stage. As shown in Figure [3\(b\)](#page-4-1) and Figure [3\(c\),](#page-4-2) the number of clusters quickly peaks early in the training stage, accompanied by a peak in inter-cluster distances. This indicates that our CSE-based architecture effectively promotes the formation of a clustering structure early on.

 The swift emergence of these clusters signifies substantial model adaptation to global features at the start of training, allowing for effective differentiation between clusters. As training progresses, inter-cluster distances gradually decrease, suggesting a stabilization in the learning dynamics and a

potential shift in focus toward refining intra-cluster nuances.

Figure 3: a) Evolution of the Gradient Consistency (GC) of long-tail data over the former 8000 training steps. GC scores beyond this range are omitted, as they consistently remain below 0.2. b) Evolution of number of clusters over training steps. c) Evolution of inter-cluster distances over training steps.

177 Long-tail clusters become more pronounced with increasing network depth. Figures [3\(b\)](#page-4-1) and [3\(c\)](#page-4-2) demonstrate that the number of clusters is consistently higher in the deeper layers compared to the lower layers, with inter-cluster distances escalating significantly in the last two layers and reaching their maximum in the final layer. This pattern indicates that clusters become increasingly distinct and better separated as they progress through the network's layers.

 The enhanced separation of clusters in deeper layers can be attributed to the hierarchical feature extraction inherent in deep neural networks. As data moves through successive layers, the network abstracts and compiles more complex features, transitioning from general to more specific attributes. This hierarchical processing allows the final layers to capture and enhance subtle distinctions between different data groups, leading to more defined and isolated clusters. This process not only underscores

Figure 4: a) Overview of the Cluster-guided Sparse Expert (CSE) layer. b) The cluster number fluctuation is mainly caused by the big common cluster. These four figures arranged sequentially from top to bottom, were sampled at every 10,000 steps throughout the process from the FFN of the 10-th layer in a GPT model.

¹⁸⁷ the capability of deep layers to refine and emphasize key features but also illustrates the network's ¹⁸⁸ efficiency in encoding progressively finer-grained information as layer depth increases.

¹⁸⁹ 3 Clsuter-guided Sparse Expert (CSE)

 To avoid the troublesome and costly domain finetuning, we design a novel strategy, named Clsuter- guided Sparse Expert (CSE), to help the model capture the long-tail domain knowledge during pretraining. Since long-tail domain data show poor gradient consistency with overall data, we employ a sparse expert architecture within the Transformer model to assign data to different parameters, thereby avoiding the gradient conflict in each parameter group. This strategy can be applied on either attention or FFN. To dispatch data, with a straightforward and generally accepted intuition such that data with similar semantic meaning are closer in the embedding space, we design a very simple, efficient but effective online clustering algorithm operating concurrently with the language model pretraining, separate embeddings into different clusters, and use the outcome of this algorithm to instruct the dispatching of embeddings. The proposed algorithm is outlined in Algorithm [1.](#page-5-1)

 Dimension Reduction In high- dimensional vector clustering, computational efficiency poses a significant challenge due to the $\widetilde{O(d^2)}$ complexity of computing 205 vector distance where d denotes the dimensionality. So, we em- ploy the same way of dimension reduction as is discussed in Sec- tion [2](#page-2-1) before applying cluster- ing on the embeddings, using a Gaussian random initialized matrix to project embeddings to a low-dimensional space[\[23\]](#page-10-7). This process, grounded in the Johnson-Lindenstrauss Lemma, effectively preserves the pairwise distances between embeddings

Algorithm 1 Cluster-guided Sparse Expert

Require: w : Warm-up step count

Require: N: Initialization data count

- **Require:** M: Gaussian random matrix $\in \mathbb{R}^{d \times d'}$ for reducing dimension
- **Require:** S: Incoming embedding stream

Require: α : center update factor

- 1: Wait w steps till the warm-up end.
- 2: Sample N data and run a clustering algorithm. Initialize cluster structure with the outcome by recording the cluster center c_i and radius r_i for each cluster.
- 3: for v in S do
- $4:$ $v' = Mv$
- 5: $i = \arg \min_{j=1}^C ||v' c_j||/r_j$

6: Dispatch v to parameter group i

7: $c_i = \alpha c_i + (1 - \alpha)v'$

```
8: end for
```

```
218 while reducing their dimension-
```
²¹⁹ ality, thereby enhancing the efficiency of our clustering algorithm.

Initialization We commence by training a baseline dense model devoid of any expert structure. Our findings in Section [2](#page-2-1) illuminate an initial rise in gradient consistency between long-tail domain data and the general dataset at the onset of training, subsequently followed by a downturn. Consequently, we adopt a warm-up stage, letting the model learn the common features of long-tail and non-long- tail data. In our experiments, this process typically accounts for no more than 1% of the overall 225 training. We then sample N instances from the dataset and use its clustering result to initialize the cluster structure. We utilized DBSCAN [\[30\]](#page-10-8) in our experiments, a clustering algorithm that does not explicitly require the number of clusters. For every identified cluster, we document its centroid and define its radius as the average distance of all constituent data points from this central point

 After this warm-up period, we fix the number of clusters and copy the module into cluster number copies. The module selection is introduced in the next paragraph. In our experiments, we noticed that the variations in the number of clusters were primarily driven by the splitting and merging of larger clusters, as illustrated in Figure [4\(b\);](#page-5-2) the smaller, long-tail clusters, however, remained largely unchanged. Consequently, adopting the initial clustering configuration directly, without further adjustments during training, was found to have no detrimental effect on model performance or the distribution of data handling. This approach capitalizes on the stability of the long-tail clusters and the dynamics of the larger ones, ensuring efficient data processing without compromising accuracy.

237 Select Layer Our motivation for performing clustering is rooted in the premise that semantically similar data tends to be closer. However, it is important to note that models learn the semantics of data progressively through layers; as we delve deeper into the model layers, the semantic information becomes increasingly rich, which may in turn amplify distinctions between data points. To quantify this variation, we apply our strategy only on layers with larger inter-cluster distance. Since the last 2 layers show a significant increase in inter-cluster distance, we apply our strategy in the last 2 layers, which is also the empirical best practice observed in existing moe-related works.[\[11,](#page-9-6) [26\]](#page-10-9)

244 Dispatch Embeddings For each coming embedding, we decide the index of the expert it is dispatched 245 to with $i = \arg \min_{j=1}^n ||v' - c_j||/r_j$, where c_j denotes the center of cluster j, and r_j denotes the 246 radius of cluster j. Note that the v' here is the sequence embedding rather than a token embedding and is defined as the mean of all token embeddings in the sequence[\[17\]](#page-10-10), and the dispatching also happens on the sequence level.

249 Update cluster center The model's parameter space undergoes gradual updates throughout training, causing a slow drift in the embedding space as the parameters evolve. To tackle this, we incorporate a dynamic mechanism to update the cluster centers concurrently with the assignment of clusters. For 252 a given cluster mc_i , let its center at time t be denoted as c_i^t . When a new embedding v arrives and 253 is assigned to mc_i , we update c_i^t with: $c_i^{t+1} = \alpha \cdot c_i^t + (1 - \alpha) \cdot v'$, where, $\alpha \in [0, 1]$ is a center 254 update factor that determines the influence of the new embedding v' on the existing center c_i^t . This adaptive updating scheme ensures that cluster centers remain representative of the current state of the embedding space, even as it evolves through the training process.

4 Related Works

 Long-Tail Prior research addressing the issue of long-tail learning has predominantly been con- ducted within the domain of computer vision. The objective is to accurately recognize and classify rare or infrequently occurring classes in a given dataset together with frequently occurring classes [\[43\]](#page-11-5). There are several approaches to address the problem, including re-weighting [\[8\]](#page-9-7), logit adjustment [\[4,](#page-9-8) [44\]](#page-12-0), robust distributional matching [\[18,](#page-10-11) [35\]](#page-11-6), and knowledge transfer [\[38,](#page-11-7) [34\]](#page-11-8). [\[37\]](#page-11-9) declare that as the number of samples increases, the diminishing phenomenon suggests that there is a decreasing marginal benefit for a model to extract additional information from the data due to the presence of information overlap. Research in natural language processing has identified significant limitations in language models' capacity to learn long-tail knowledge [\[28,](#page-10-12) [3\]](#page-9-9). Furthermore, [\[45\]](#page-12-1) suggests that attempting to address this issue during the finetuning stage is often too late.

 Domain-Specific Finetuning Domain-specific finetuning, also known as domain-specific pretrain- ing, is highly advantageous to assist language models in requiring specialized domain knowledge. In one approach, contextualized embeddings are adapted to text from the target domain using masked language modeling, as detailed by Han and Eisenstein [\[16\]](#page-10-13). The concept of multi-phase pretraining involves secondary-stage unsupervised pretraining, exemplified by broad-coverage domain-specific

 BERT variants like BioBERT [\[25\]](#page-10-14). Research by Gururangan et al. [\[15\]](#page-9-10) extends this by proposing domain-adaptive pretraining (DAPT) from a broader corpus and task-specific pretraining (TAPT) which uses unlabeled data increasingly aligned with the task distribution. These studies underscore the importance of domain-relevant data for pretraining in both high and low-resource scenarios [\[16,](#page-10-13) [15\]](#page-9-10).

5 Experiments

 This section presents the experimental results of our model and other methods. In the experiments, our model only undergoes a pretrained phase, reading domain-specific data once. Other methods are pretrained on the same dataset and then finetuned on domain-specific datasets. Subsequently, all models are used as embedding models with all parameters frozen to generate embeddings for downstream tasks.

 Dataset and Evaluation We employ Wikipedia [\[13\]](#page-9-11) as our pretraining dataset, which is also widely accepted in other works [\[25,](#page-10-14) [10\]](#page-9-4). We adopt some legal and medical domain-specific downstream tasks to show the effectiveness of our model. To ensure that the pretraining data do contain domain knowledge required by the downstream tasks, we mixed a relatively small amount (less than 8%) of legal-domain-specific data [\[1\]](#page-9-12) and medical-domain-specific data [\[9\]](#page-9-13) into the pretraining data to simulate a long-tail distribution. The datasets selected are listed in Table [3](#page-13-0) in Appendix [A.](#page-13-1) Concurrently, we report the test perplexity of each model after the pretraining phase, serving as evidence of model convergence. Task performances are reported by accuracy.

292 Baselines Since our strategy is not restricted to a specific model structure, we adopt both BERT [\[10\]](#page-9-4) and GPT [\[29\]](#page-10-4) as the base models and compare all the strategies on these base models respectively. We also compare with a Switch-MoE [\[11\]](#page-9-6) version of them to show the effectiveness of our routing strategy. More Detailed implementation setting is listed in Appendix [A.](#page-13-1)

5.1 Main Result

 Table [1](#page-7-0) and Table [2](#page-8-0) shows the performance of all models/strategies under our experiment setting with a trainable linear classifier for downstream tasks. */med means a model finetuned on medical- domain-specific data, and */legal means a model finetuned on legal-domain-specific data. We tested Clsuter-guided Sparse Expert on Attention and FFN respectively, denoted as MoA and MoF.

 Our method outperforms other models/strategies on almost all tasks, with an average improvement of around 3%, showing an ability to learn long-tail data from the pretraining dataset. Our method can be applied to either the Attention module or the FFN module, and both way will yield a better result compared with the finetuned baselines, showing a potential for eliminating the need for domain finetuning. While in certain scenarios, domain finetuning remains indispensable due to the privacy concerns associated with proprietary data, we argue that when pretraining datasets encompass domains similar to the proprietary one, our approach can still facilitate an enhanced domain finetuning performance. It is also notable that domain finetuning leads to overfitting and even catastrophic forgetting, resulting in a decrease in performance on tasks from non-related domains. More details are shown in Appendix [A.](#page-13-1)

Models	Pretrain ppl	Overruling	Casehold	GAD	EUADR	SST ₂	average
BERT/med	37.00 37.00	86.67 86.67	50.51	67.09 66.83	84.23 84.79	66.86 65.14	71.07 ± 0.22 70.87 ± 0.23
BERT/legal MoE/med	31.00	85.00	50.93 50.49	64.52	83.10	64.79	69.58 ± 0.20
MoE/lgeal	31.00	85.83	50.30	64.32	84.79	63.88	69.82 ± 0.19
Ours/MoA Ours/MoF	28.25 34.64	86.62 89.10	50.94 50.82	72.90 71.65	90.09 91.23	66.60 67.98	73.43 ± 0.18 74.16 ± 0.20

Table 1: Results of strategies applied on BERT

Models	Pretrain ppl	Overruling	Casehold	GAD	EUADR	SST ₂	average
GPT/med	55.59	88.33	49.82	71.56	84.23	73.90	73.57 ± 0.17
GPT/legal	55.59	89.17	50.58	71.69	81.69	74.50	73.53 ± 0.23
MoE/med	40.69	91.25	50.11	72.77	83.38	72.03	73.91 ± 0.12
MoE/legal	40.69	91.60	49.68	72.66	83.38	71.97	73.86 ± 0.23
Ours/MoA	42.99	91.68	50.70	71.75	85.91	74.61	74.93 ± 0.08
Ours/MoF	43.38	93.33	51.26	73.30	85.63	76.00	75.90 ± 0.19

Table 2: Results of strategies applied on GPT

5.2 Analysis

Expert analysis We analyze our model's embedding space to determine if our method dispatches embeddings correctly. We sample data and perform a forward inference pass through the model, visualizing the dispatching path of our model. As is shown in Figure [5,](#page-8-1) our distribution strategy correctly and effectively dispatches data from different long-tail clusters to different experts. We further visualize the NTK in each expert of our model, and it can be observed that by dispatching long-tail data separately, the NTK in each expert becomes more consistent. Whereas in a baseline model, its NTK matrix shows a poor consistency of the batch data, since long-tail and non-long-tail data are not separated.

Figure 5: a) The embedding space and routing result of our model. b) The NTK in each expert in our model. c) The NTK in baseline. b) and c) are sampled from the FFN in the 10th layer.

320 Overhead Analysis For our method, the warm-up phase incurs no additional computation. At the end of the warm-up, The clustering algorithms are bounded by their worst-case time complexity $O(N^2d')$, thus their impact on the total FLOPs compared to the whole pretraining is negligible when posed against the extensive computations involved in the model's forward-backward passes. 324 Our dispatching strategy introduces $O(Cd'^2)$ for comparing distance with each cluster, which is also negligible. For baseline methods, since they all undergo a finetuning stage, they introduce an additional 5% computation compared to the pretraining stage under our experimental settings.

6 Conclusion

 In this paper, we seek to elucidate why language models require domain finetuning despite the presence of domain knowledge in their pretraining data. Our investigation uncovers that Sentences with lower frequency scores show diminished gradient consistency, resulting in increased test perplex- ity. This misalignment, particularly pronounced in low-frequency sentences, culminates in elevated test perplexity, suggesting a deficiency in effectively leveraging domain-specific information. To address this challenge, we introduce Cluster-guided Sparse Experts (CSE), grouping diverse long-tail domain data and dispatching them to different experts to enhance gradient consistency within each expert, thereby enabling the model to incorporate long-tail domain knowledge during pretraining. Experiments suggest that our approach has the potential to supplant the need for a dedicated domain finetuning stage. Through this approach, long-tail domain instances promote the formation of small, outlier clusters in the representation space, exhibiting a characteristic signature across varying stages of training and architectural depths.

References

- 341 [1] Caselaw access project. <https://case.law/>, 2024.
- [2] Reddit comments dataset. [https://clickhouse.com/docs/en/getting-started/](https://clickhouse.com/docs/en/getting-started/example-datasets/reddit-comments) [example-datasets/reddit-comments](https://clickhouse.com/docs/en/getting-started/example-datasets/reddit-comments), 2024 .
- [3] Mallen A., Asai A., Zhong V, Das R., Khashabi D., and Hajishirzi H. When not to trust language models: Investigating effect. *in Proceedings of the 61st Annual Meeting of the Association for Computational Linguistics (Volume 1: Long Papers)*, 2023.
- [4] Krishna Menon Aditya, Jayasumana Sadeep, Singh Rawat Ankit, Jain Himanshu, Veit Andreas, and Kumar. Sanjiv. Long-tail learning via logit adjustment. *arXiv preprint arXiv:2007.07314*, 2020.
- [5] Benjamin Bowman and Guido Montúfar. Spectral bias outside the training set for deep networks in the kernel regime. *ArXiv*, abs/2206.02927, 2022. URL [https://api.semanticscholar.](https://api.semanticscholar.org/CorpusID:249431476) [org/CorpusID:249431476](https://api.semanticscholar.org/CorpusID:249431476).
- [6] Àlex Bravo, Janet Piñero, Núria Queralt-Rosinach, Michael Rautschka, and Laura I Furlong. Extraction of relations between genes and diseases from text and large-scale data analysis: implications for translational research. *BMC Bioinformatics*, 16(1), February 2015. doi: 10.1186/s12859-015-0472-9. URL <https://doi.org/10.1186/s12859-015-0472-9>.
- [7] Ilias Chalkidis, Manos Fergadiotis, Prodromos Malakasiotis, Nikolaos Aletras, and Ion An- droutsopoulos. Legal-bert: "preparing the muppets for court'". *ArXiv*, abs/2010.02559, 2020. URL <https://api.semanticscholar.org/CorpusID:222141043>.
- [8] Huang Chen, Li Yining, Change Loy Chen, and Tang Xiaoou. Learning deep representation for imbalanced classification. *In Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition*, 2016.
- [9] Arman Cohan, Franck Dernoncourt, Doo Soon Kim, Trung Bui, Seokhwan Kim, Walter Chang, and Nazli Goharian. A discourse-aware attention model for abstractive summarization of long documents. In *Proceedings of the 2018 Conference of the North American Chapter of the Association for Computational Linguistics: Human Language Technologies, Volume 2 (Short Papers)*, pp. 615–621, New Orleans, Louisiana, June 2018. Association for Computational Linguistics. doi: 10.18653/v1/N18-2097. URL <https://aclanthology.org/N18-2097>.
- [10] Jacob Devlin, Ming-Wei Chang, Kenton Lee, and Kristina Toutanova. Bert: Pre-training of deep bidirectional transformers for language understanding. *arXiv preprint arXiv:1810.04805*, 2018.
- [11] W. Fedus, B. Zoph, , and N. Shazeer. Switch transformers: Scaling to trillion parameter models with simple and efficient sparsity. *Journal of Machine Learning Research*, 2022.
- [12] Stanislav Fort, Gintare Karolina Dziugaite, Mansheej Paul, Sepideh Kharaghani, Daniel M. Roy, and Surya Ganguli. Deep learning versus kernel learning: an empirical study of loss landscape geometry and the time evolution of the neural tangent kernel. In Hugo Larochelle, Marc'Aurelio Ranzato, Raia Hadsell, Maria-Florina Balcan, and Hsuan- Tien Lin (eds.), *Advances in Neural Information Processing Systems 33: Annual Con- ference on Neural Information Processing Systems 2020, NeurIPS 2020, December 6- 12, 2020, virtual*, 2020. URL [https://proceedings.neurips.cc/paper/2020/hash/](https://proceedings.neurips.cc/paper/2020/hash/405075699f065e43581f27d67bb68478-Abstract.html) [405075699f065e43581f27d67bb68478-Abstract.html](https://proceedings.neurips.cc/paper/2020/hash/405075699f065e43581f27d67bb68478-Abstract.html).
- [13] Wikimedia Foundation. Wikimedia downloads. URL <https://dumps.wikimedia.org>.

 [14] Zhen Guo and Yining Hua. Continuous training and fine-tuning for domain-specific language models in medical question answering. *ArXiv*, abs/2311.00204, 2023. URL [https://api.](https://api.semanticscholar.org/CorpusID:264832958) [semanticscholar.org/CorpusID:264832958](https://api.semanticscholar.org/CorpusID:264832958).

 [15] Suchin Gururangan, Ana Marasovic, Swabha Swayamdipta, Kyle Lo, Iz Beltagy, Doug Downey, ´ and Noah A. Smith. Don't stop pretraining: Adapt language models to domains and tasks. *ArXiv*, abs/2004.10964, 2020. URL [https://api.semanticscholar.org/CorpusID:](https://api.semanticscholar.org/CorpusID:216080466) [216080466](https://api.semanticscholar.org/CorpusID:216080466).

- [16] Xiaochuang Han and Jacob Eisenstein. Unsupervised domain adaptation of contextualized embeddings for sequence labeling. In *Conference on Empirical Methods in Natural Language Processing*, 2019. URL <https://api.semanticscholar.org/CorpusID:202541481>.
- [17] Junjie Huang, Duyu Tang, Wanjun Zhong, Shuai Lu, Linjun Shou, Ming Gong, Daxin Jiang, and Nan Duan. Whiteningbert: An easy unsupervised sentence embedding approach. *arXiv preprint arXiv:2104.01767*, 2021.
- [18] Zheng Huangjie, Chen Xu, Yao Jiangchao, Yang Hongxia, Li Chunyuan, Zhang Ya, Zhang Hao, Tsang Ivor, Zhou Jingren, and Zhou. Mingyuan. Contrastive attraction and contrastive repulsion for representation learning. *Transactions on Machine Learning Research*, 2023.
- [19] Arthur Jacot, Clément Hongler, and Franck Gabriel. Neural tangent kernel: Conver- gence and generalization in neural networks. In Samy Bengio, Hanna M. Wallach, Hugo Larochelle, Kristen Grauman, Nicolò Cesa-Bianchi, and Roman Garnett (eds.), *Advances in Neural Information Processing Systems 31: Annual Conference on Neural Informa- tion Processing Systems 2018, NeurIPS 2018, December 3-8, 2018, Montréal, Canada*, pp. 8580–8589, 2018. URL [https://proceedings.neurips.cc/paper/2018/hash/](https://proceedings.neurips.cc/paper/2018/hash/5a4be1fa34e62bb8a6ec6b91d2462f5a-Abstract.html) [5a4be1fa34e62bb8a6ec6b91d2462f5a-Abstract.html](https://proceedings.neurips.cc/paper/2018/hash/5a4be1fa34e62bb8a6ec6b91d2462f5a-Abstract.html).
- [20] Anil K. Jain. Data clustering: 50 years beyond k-means. *Pattern Recognit. Lett.*, 31:651–666, 2008. URL <https://api.semanticscholar.org/CorpusID:11152703>.

 [21] Nikhil Kandpal, Haikang Deng, Adam Roberts, Eric Wallace, and Colin Raffel. Large language models struggle to learn long-tail knowledge. In *International Conference on Machine Learning*, pp. 15696–15707. PMLR, 2023.

- [22] Zixuan Ke, Yijia Shao, Haowei Lin, Hu Xu, Lei Shu, and Bing Liu. Adapting a language model while preserving its general knowledge. *arXiv preprint arXiv:2301.08986*, 2023.
- [23] Kasper Green Larsen and Jelani Nelson. The johnson-lindenstrauss lemma is optimal for linear dimensionality reduction. *arXiv preprint arXiv:1411.2404*, 2014.
- [24] Jinhyuk Lee, Wonjin Yoon, Sungdong Kim, Donghyeon Kim, Sunkyu Kim, Chan Ho So, and Jaewoo Kang. Biobert: a pre-trained biomedical language representation model for biomedical text mining. *Bioinformatics*, 36:1234 – 1240, 2019. URL [https://api.semanticscholar.](https://api.semanticscholar.org/CorpusID:59291975) [org/CorpusID:59291975](https://api.semanticscholar.org/CorpusID:59291975).
- [25] Jinhyuk Lee, Wonjin Yoon, Sungdong Kim, Donghyeon Kim, Sunkyu Kim, Chan Ho So, and Jaewoo Kang. Biobert: a pre-trained biomedical language representation model for biomedical text mining. *Bioinformatics*, 36(4):1234–1240, 2020.
- [26] D. Lepikhin, H. Lee, Y. Xu, D. Chen, O. Firat, Y. Huang, M. Krikun, N. Shazeer, and Z. Chen. Gshard: Scaling giant models with conditional computation and automatic sharding. *In Interna-tional Conference on Learning Representations*, 2021.
- [27] Yun Luo, Zhen Yang, Fandong Meng, Yafu Li, Jie Zhou, and Yue Zhang. An empiri- cal study of catastrophic forgetting in large language models during continual fine-tuning. *ArXiv*, abs/2308.08747, 2023. URL [https://api.semanticscholar.org/CorpusID:](https://api.semanticscholar.org/CorpusID:261031244) [261031244](https://api.semanticscholar.org/CorpusID:261031244).
- [28] Kandpal N., Deng H., Roberts A., Wallace E., and Raffel C. Large language models struggle to learn long-tail knowledge. *In International Conference on Machine Learning*, 2023.
- [29] Alec Radford, Jeffrey Wu, Rewon Child, David Luan, Dario Amodei, Ilya Sutskever, et al. Language models are unsupervised multitask learners. *OpenAI blog*, 1(8):9, 2019.
- [30] Erich Schubert, Jörg Sander, Martin Ester, Hans-Peter Kriegel, and Xiaowei Xu. Dbscan revisited, revisited. *ACM Transactions on Database Systems (TODS)*, 42:1 – 21, 2017. URL <https://api.semanticscholar.org/CorpusID:5156876>.
- [31] K. Singhal, Shekoofeh Azizi, Tao Tu, Said Mahdavi, Jason Wei, Hyung Won Chung, Nathan Scales, Ajay Kumar Tanwani, Heather J. Cole-Lewis, Stephen J. Pfohl, P A Payne, Mar- tin G. Seneviratne, Paul Gamble, Chris Kelly, Nathaneal Scharli, Aakanksha Chowdhery, P. A. Mansfield, Blaise Agüera y Arcas, Dale R. Webster, Greg S. Corrado, Yossi Ma- tias, Katherine Hui-Ling Chou, Juraj Gottweis, Nenad Tomaev, Yun Liu, Alvin Rajko- mar, Joëlle K. Barral, Christopher Semturs, Alan Karthikesalingam, and Vivek Natarajan. Large language models encode clinical knowledge. *Nature*, 620:172 – 180, 2022. URL <https://api.semanticscholar.org/CorpusID:255124952>.
- [32] Richard Socher, Alex Perelygin, Jean Wu, Jason Chuang, Christopher D. Manning, Andrew Ng, and Christopher Potts. Recursive deep models for semantic compositionality over a sentiment treebank. In *Proceedings of the 2013 Conference on Empirical Methods in Natural Language Processing*, pp. 1631–1642, Seattle, Washington, USA, October 2013. Association for Computational Linguistics. URL <https://www.aclweb.org/anthology/D13-1170>.
- [33] Erik M. van Mulligen, Annie Fourrier-Reglat, David Gurwitz, Mariam Molokhia, Ainhoa Nieto, Gianluca Trifiro, Jan A. Kors, and Laura I. Furlong. The eu-adr corpus: Annotated drugs, diseases, targets, and their relationships. *Journal of Biomedical Informatics*, 45(5): 879–884, 2012. ISSN 1532-0464. doi: https://doi.org/10.1016/j.jbi.2012.04.004. URL [https:](https://www.sciencedirect.com/science/article/pii/S1532046412000573) [//www.sciencedirect.com/science/article/pii/S1532046412000573](https://www.sciencedirect.com/science/article/pii/S1532046412000573). Text Mining and Natural Language Processing in Pharmacogenomics.
- [34] Chen Xu, Chen Siheng, Yao Jiangchao, Zheng Huangjie, Zhang Ya, and W. Tsang. Ivor. Learning on attribute-missing graphs. *IEEE Transactions on Pattern Analysis and Machine Intelligence*, 2022.
- [35] Chen Xu, Pan Yuangang, Tsang Ivor, and Zhang. Ya. Learning node representations against perturbations. *Pattern Recognition, 145:109976*, 2024.
- [36] Haoran Yang, Yumeng Zhang, Jiaqi Xu, Hongyuan Lu, Pheng Ann Heng, and Wai Lam. Unveiling the generalization power of fine-tuned large language models. *ArXiv*, abs/2403.09162, 2024. URL <https://api.semanticscholar.org/CorpusID:268385476>.
- [37] Cui Yin, Jia Menglin, Lin Tsung-Yi, Song Yang, and Belongie. Serge. Class-balanced loss based on effective number of samples. *In Proceedings of the IEEE/CVF Conference on Computer Vision and Pattern Recognition*, 2019.
- [38] Wang Yu-Xiong, Ramanan Deva, and Hebert. Martial. Learning to model the tail. *Advances in Neural Information Processing Systems*, 2017.
- [39] Shi Yubin, Chen Yixuan, Dong Mingzhi, Yang Xiaochen, Li Dongsheng, Wang Yujiang, P. Dick Robert, Lv Qin, Zhao Yingying, Yang Fan, Lu Tun, Gu Ning, and Shang Li. Train faster, perform better: Modular adaptive training in over-parameterized models. In *Advances in Neural Information Processing Systems 36: Annual Conference on Neural Information Processing Systems 2023, NeurIPS 2023, New Orleans, LA, USA, December 10 - 16, 2023*, 2023.
- [40] Wayne Xin Zhao, Kun Zhou, Junyi Li, Tianyi Tang, Xiaolei Wang, Yupeng Hou, Yingqian Min, Beichen Zhang, Junjie Zhang, Zican Dong, Yifan Du, Chen Yang, Yushuo Chen, Z. Chen, Jinhao Jiang, Ruiyang Ren, Yifan Li, Xinyu Tang, Zikang Liu, Peiyu Liu, Jianyun Nie, and Ji rong Wen. A survey of large language models. *ArXiv*, abs/2303.18223, 2023. URL <https://api.semanticscholar.org/CorpusID:257900969>.
- [41] Jiawei Zheng, Hanghai Hong, Xiaoli Wang, Jingsong Su, Yonggui Liang, and Shikai Wu. Fine- tuning large language models for domain-specific machine translation. *ArXiv*, abs/2402.15061, 2024. URL <https://api.semanticscholar.org/CorpusID:267897581>.
- [42] Lucia Zheng, Neel Guha, Brandon R. Anderson, Peter Henderson, and Daniel E. Ho. When Does Pretraining Help? Assessing Self-Supervised Learning for Law and the CaseHOLD Dataset. *arXiv e-prints*, art. arXiv:2104.08671, April 2021. doi: 10.48550/arXiv.2104.08671.
- [43] Zhou Zhihan, Yao Jiangchao, Wang Yan-Feng, Han Bo, and Zhang Ya. Contrastive learning with boosted memorization. *In International Conference on Machine Learning*, 2022.
- [44] Zhou Zhihan, Yao Jiangchao, Hong Feng, Zhang Ya, Han Bo, and Wang. Yanfeng. Combating representation learning disparity with geometric harmonization. *In Thirty-seventh Conference*
- *on Neural Information Processing Systems*, 2023.
- [45] Zeyuan Allen Zhu and Yuanzhi Li. Physics of language models: Part 3.1, knowledge storage and extraction. *arXiv preprint arXiv:2309.14316*, 2023.

⁴⁹¹ Appendix

⁴⁹² A Experiments

⁴⁹³ Table [3](#page-13-0) shows the datasets used in our experiments. Table [4](#page-13-2) shows the hyperparameters used in our ⁴⁹⁴ implementations. We use a machine with 8 NVIDIA GeForce RTX 3090 GPUs with 24GB GPU ⁴⁹⁵ memory as our experiment platform. Pretraining costs about 24 hours.

Pretraining dataset	Description
Wikipedia ([13])	Wikipedia dataset containing cleaned articles of all languages. The datasets are built from the Wikipedia dump with one split per language. Each example contains the content of one full Wikipedia article with cleaning to strip markdown and unwanted sections.
legal(1])	In collaboration with Ravel Law, Harvard Law Library digi- tized over 40 million U.S. court decisions consisting of 6.7 million cases from the last 360 years into a dataset that is widely accessible to use.
PubMed([9])	PubMed comprises more than 36 million citations for biomedical literature from MEDLINE, life science journals, and online books.
Finetuning task	Description
Overruling ([42])	A law dataset corresponds to the task of determining when a sentence is overruling a prior decision.
$\text{Casehold}([42])$	Case Holdings On Legal Decisions, comprising over 53,000+ multiple choice questions to identify the relevant holding of a cited case.
GAD([6])	A relation extraction dataset, to decide if a gene is related to a specific disease.
EUADR([33])	Another relation extraction dataset, to decide if a gene is related to a specific disease.
SST2([32])	The Stanford Sentiment Treebank consists of sentences from movie reviews and human annotations of their sentiment.

Table 3: Datasets used for experiments

Hyperparameters	BERT-based	GPT-based
FFN modules	4	6
Attention modules	4	6
attention heads	8	12
our-strategy-based layers	2	2
transformer layers	12	12
Hidden dimension size	768	768
Droupt	0.1	0.1
Attention dropout	0.1	0.1
Sequence length	128	256
Batch size	100	64
Max steps	36k	300k
Learning rate decay	Cosine	Cosine
random seed used	14, 24	22,80

Table 4: Hyperparameters of Models

⁴⁹⁶ By monitoring the validation loss of the pretraining dataset(Figure [6\)](#page-14-0), we show the Catastrophic ⁴⁹⁷ Forgetting problem of the BERT model and its MOE method in the domain-specific finetuning phase.

⁴⁹⁸ Despite our attempts at various combinations of generic data and domain-specific data during domain

finetuning, the best outcome among these still resulted in a decline in model performance on domains

unrelated to its fine-tuning, indicating a limitation in the generalizability of the adapted model. As

 domain-specific finetuning proceeds, the validation loss of pretraining dataset has a significant rise and stays well above the convergence position of pretraining.

Figure 6: The validation loss of the pretraining dataset during the domain-specific finetuning phase.

B Limitations Discussions

 Although we use the method of mixing small-scale domain-specific datasets into pretraining data to simulate the long-tail distribution in those huge corpora, we cannot fully simulate the extremely rich

pretraining data used on LLMs due to the limited training resources.

NeurIPS Paper Checklist

