SimSMoE: Toward Efficient Training Mixture of Experts via Solving Representational Collapse

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Abstract

Sparse mixture of experts (SMoE) have emerged as an effective approach for scaling large language models while keeping a constant computational cost. Regardless of several notable successes of SMoE, effective training such architecture remains elusive due to the representation collapse problem, which in turn harms model performance and causes parameter redundancy. In this work, we present Similarity-based Sparse Mixture of Experts (SimSMoE), a novel similarity of neural network algorithm, that guarantees a solution to address the representation collapse issue between experts given a fixed FLOPs budget. We conduct extensive empirical evaluations on three large language models for both Pre-training and Fine-tuning tasks to illustrate the efficacy, robustness, and scalability of our method. The results demonstrate that SimSMoE significantly enhances existing routing policy and outperforms other SMoE routing methods in performance for the tasks. Our implementation is publicly available at https://github.com/giangdip2410/SimSMoE.

1 Introduction

Large Language Models (LLMs) have achieved significant breakthroughs across multiple fields, including natural language processing (NLP) tasks (Brown et al., 2020; Zhang et al., 2022; Touvron et al., 2023) and visual representation learning (Jia et al., 2021; Zhu et al., 2023). In the era of large language models (LLMs), Sparse mixture of experts (SMoE)(Shazeer et al., 2017; Zoph et al., 2022; Xue et al., 2024; Jiang et al., 2024) offers a scalable way to enhance efficiency by activating only a few specialized experts, reducing computation while maintaining strong performance. Compared to dense models, SMoE accelerates inference by activating only a subset of experts instead of the entire pool at once (Artetxe et al., 2022; Krajewski et al., 2024)

Despite the fact that SMoE has demonstrated its capabilities across various tasks (Riquelme et al., 2021; Mustafa et al., 2022; Gupta et al., 2022), training efficiency remains a challenge due to the issue of representation collapse, wherein either only a few experts receive routed tokens or all experts converge to learn similar representation. This issue was initially identified and theoretically proven by XMoE (Chi et al., 2022), followed by consequent works by SMoE-Dropout (Chen et al., 2023a); HyperRouter (Do et al., 2023). To address the limitation, several publications have focused on router policy improvement. Examples include proposals for better routing policies, such as those by Zhou et al.(Zhou et al., 2022a), StableMoE(Dai et al., 2022), XMoE (Chi et al., 2022), as well as optimal routing policies like the one suggested by CompeteSMoE (Pham et al., 2024). These solutions employ indirect approaches that concentrate on token allocation, expecting that enhanced allocation will resolve the collapse among experts. However, the existing methods suffer from several limitations. For example, while XMoE (Chi et al., 2022) and StableMoE (Dai et al., 2022) show promising results, they do not guarantee to solve the representation collapse issue. Additionally, CompeteSMoE (Pham et al., 2024) faces inefficiency problems arising from the requirement to activate all experts.

This paper proposes a novel training framework, named SimSMoE, which directly addresses the collapse issue by emphasizing similar representations among experts. More specifically, we introduce a quantitative method to illustrate the collapse issue between experts using the centered kernel alignment (CKA) metric (Kornblith et al., 2019a). Our effective training strategy comprises three stages: (1) Selecting potential collapsed experts; (2) Identifying collapsed experts; (3) Solving the representation collapse issue. SimSMoE can be applied

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to any routing algorithms, as it directly improves expert representations. Moreover, our method guarantees superior SMoE training strategies compared to the existing methods by quantifying the similarity between expert representations and minimizing similarity among experts by the CKA (Kornblith et al., 2019a) loss function. We then evaluate the proposed method by conducting pre-training of Large Language Models (LLMs) on several advanced SMoE architectures, such as GLaM (Du et al., 2022), Brainformer (Zhou et al., 2024), or Mistral (Jiang et al., 2024), followed by fine-tuning on downstream tasks.

The main contributions of this paper are: (1) *demonstrating the representation collapse problem in SMoEs using CKA, which has not been previously explored*; (2) *proposing the CKA loss function to address this collapse*; (3) *conducting extensive experiments on LLM pre-training and fine-tuning on downstream tasks*; and (4) *providing an in-depth analysis of common token feeding and the representation collapse metric, showing that SimSMoE improves performance over existing methods.*

2 Background

2.1 Sparse Mixture of Experts

Inspired by conditional computation (Srivastava et al., 2013; Bengio et al., 2013) that activates only some relevant weights of a model on a per-token basis, the Sparse Mixture of Experts (SMoE) model (Shazeer et al., 2017), as an example of conditional computation, with each layer consists N experts and a trainable router which selects the most appropriate k experts to process each input sample. In this paper, we apply SMoE for Transformer-based architectures(Chi et al., 2022; Dai et al., 2022; Do et al., 2023) by replacing the feed-forward neural network layer in Transformers(Vaswani et al., 2023) with the Mixture-of-Experts layer, drawing inspiration from (Du et al., 2022; Zhou et al., 2024; Jiang et al., 2024). Each Mixture-of-Experts layer consists of a set of multi-layer perceptrons (MLPs), each with two layers and a ReLu non-linearity function(Agarap, 2019). Denoting the output of the multi-head attentions (MHA) as x, the output of SMoE with N experts is a weighted sum of each expert's computation $E_i(x)$ by the router function $G(x)$:

$$f_{\text{SMoE}}(\boldsymbol{x}) = \sum_{i=1}^{N} G(\boldsymbol{x})_i \cdot E_i(\boldsymbol{x}) \qquad (1)$$

Where $G(x)$ is computed by TOP_k function as equation (2) that determines the contribution of each expert to the SMoE output.

$$G(\mathbf{x}) = \text{TOP}_k(\text{softmax}(\mathbf{W}\mathbf{x} + b)) \qquad (2)$$

In this research, we primarily focus on top-2 routing ($K = 2$), as studies(Zhou et al., 2022b; Zoph et al., 2022; Sukhbaatar et al., 2024; Pham et al., 2024) have demonstrated its superior balance between training efficiency and testing performance.

2.2 Challenge of effective Sparse Mixture of Experts Training

Recent studies (Chi et al., 2022; Do et al., 2023) emphasize the challenge of representation collapse during SMoE training, illustrating that the Jacobian matrix of experts output with respect to input $x \in R^d$ is a linear combination of the expert embeddings ($e \in R^N$). Thus, the phenomenon arises due to $d >> N$ in practice.

As the existing solutions (Chi et al., 2022; Dai et al., 2022; Do et al., 2023; Pham et al., 2024) assume that the collapse problem is a result of ineffective router algorithms, their efforts are directed towards proposing better router mechanisms. Despite these efforts, training SMoE remains unstable and prone to redundant parameters. Thus, a reliable strategy is needed to enhance expert representation and prevent collapse. With this objective in mind, we introduce SimSMoE, presenting two main contributions: (i) Illustrating the collapse problem by a quantitative approach; and (ii) Addressing the issue among experts by CKA loss function (Kornblith et al., 2019a).

3 Methodology

We present Similarity Sparse Mixture of Experts (SimSMoE), which utilizes the strengths of existing routing algorithms (Dai et al., 2022; Chi et al., 2022; Jiang et al., 2024), directly tackling the representation collapse by minimizing the similarity among expert representations.

3.1 SimSMoE

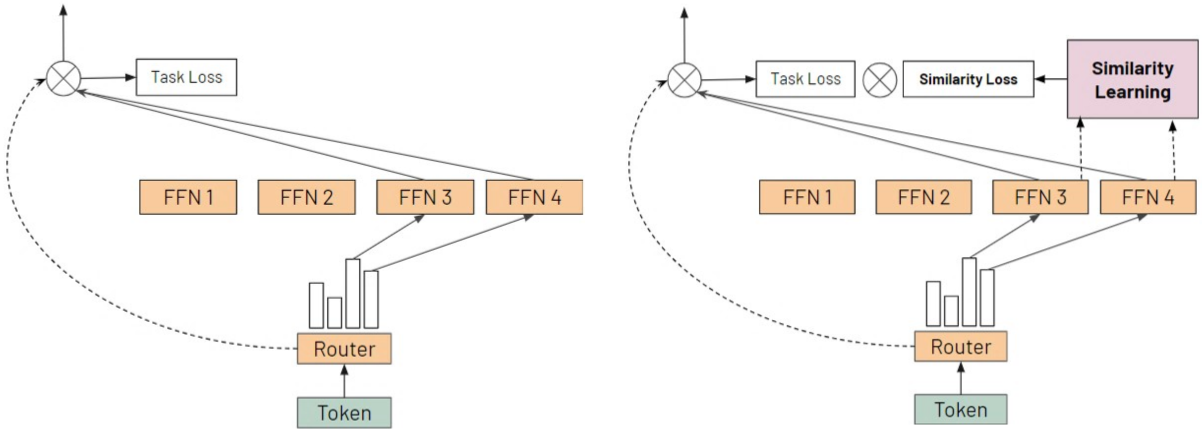
Similarity Reduction. In order to alleviate the representation collapse issue mentioned in Section 2.2, we introduce the Similarity Learning module in Figure 2 that helps to minimize the Similarity of Experts Representations. As shown in Figure 1b, the Similarity Learning module uses the outputs of experts as input and employs the Similarity Loss described in Section 3.2 to diversify the experts' representations. The key innovation of Similarity Learning consists of two main parts: (i) quantifying the collapse issue; (ii) diversifying experts' representations using the Similarity Loss described in Section 3.2. For more detail, the Similarity Learning is illustrated as Algorithm 1. Consequently, the similarity-based SMoE training procedure can be summarized in the following four steps: (1) Calculate the number of shared tokens per expert pair from router $G(x)$, and update the total number of input tokens per expert; (2) Calculate the similarity of selective experts; (3) Update the total loss if the similarity exceeds the similarity threshold; (4) Optimize the total loss in the same manner as training SMoE.

An Effective and Reliable Algorithm. One of the biggest challenges for minimizing the similarity among experts is the vast number of possible expert combinations. Given N experts, there are $\binom{N}{2} = \frac{N!}{2!\cdot(N-2)!} = \frac{(N-1)\cdot N}{2}$ expert pairs. To verify the collapse issue of all expert pairs, it is necessary to loop over each pair, calculating their hidden representations and comparing them. This process is equivalent to activating N experts. Due to its contradiction with the conditional computation philosophy of SMoE, proposing an effective algorithm to implement the Similarity Learning is necessary. Section 4.5 demonstrates that a higher frequency of common tokens leads to the severity of the collapse. Hence, the training algorithm of SimSMoE introduces two hyperparameters: $f*$, which represents the frequency for checking the collapse issue in the representation, and T^*, a threshold for identifying the collapse issue as Algorithm 1. Indeed, $f*$ controls computational resources, while T^* controls the quality of the collapse identification method. Given T as a similarity index between two experts, if $T \geq T^*$, it solves the collapse problem. On the other hand, if $T < T^*$, the algorithm focuses on optimizing the task loss during the SMoE training process. Thus, if we denote p as the performance of SimSMoE and p^* as performance of SMoE, we have $p \geq p^*$. In addition, both $f*$ and T^* are tuned during the training processes.

The input for the Similarity Learning module comes from a pair of experts. Thus, the most effective way to implement the module is by using the expert outputs from the SMoE training process. The module is workable for top-1 routing, however, it requires activating one additional expert in each iteration. The Similarity Learning module works best for top-k routing ($k \geq 2$), as it fully utilizes the output from pairs of experts to minimize the similarity among them. Additionally, SimSMoE can be applied to any routing algorithm such as StableMoE (Dai et al., 2022) or XMoE (Chi et al., 2022) to enhance model performance by addressing the representation collapse problem.

3.2 Similarity of Neural Network Representations

Inspired by the Similarity Index (Kornblith et al., 2019a), the Similarity Learning module addresses the representation collapse problems from two perspectives. First, the module directly measures a similarity score among experts and helps to identify which experts fail in diversity representation. Then, the Similarity Learning reduces the collapse issue by optimizing the Similarity Loss. Second, the Similarity Learning focuses on solving the collapse at the hidden representations of experts. This allows the method to leverage the advantages of routing techniques such as SMoE with the Balancing Loss (Fedus et al., 2022); X-MoE(Chi et al., 2022) StableMoE (Dai et al., 2022). We propose using similarity index based on centered kernel alignment (CKA) (Kornblith et al., 2019a) reliably identifies correspondences between representations in neural networks and an MLP with one hidden layer as a projection head (Figure 2) that maps representations to the space where the similarity loss is applied. Empirically, when scaling the model to larger hidden dimensions, we observe that the projection space can be increased, but one of the good choices is around N, with N is number of experts. Kornblith et al. (2019) (Kornblith et al., 2019a) introduces two versions of CKA: Linear CKA (LCKA) which focuses on linear kernel: $K_{\text{lin}} = (x_i \cdot x_j)_{i,j}$; and RBF CKA (RCKA) which applies Gaussian RBF kernel: $K_{G(\sigma)} = \left(e^{\frac{-\left|x_i - x_j\right|^2}{2\sigma^2}}\right)_{i,j}$. LCKA and RCKA give similar results in practice (Kornblith et al., 2019a). For RCKA, selecting bandwidth σ determines the extent to which the similarity of small distances is emphasized over large distances. When training the Similarity Learning Layer as Figure 2, we empirically observe that a larger σ performs more stably, so we recommend choosing σ in the range of $[0.8, 0.9]$.



(a) Sparse Mixture-of-Experts (SMoE) Architecture

(b) SimSMoE Architecture (Ours)

Figure 1: Illustration of the proposed SimSMoE architecture and a SMoE architecture. (a) A SMoE architecture selectively activates experts based on dot-product token-expert routing scores, directing the selected token to the chosen experts. (b) A SimSMoE architecture mitigates the issue of representation collapse by reducing the similarity among the selected experts.

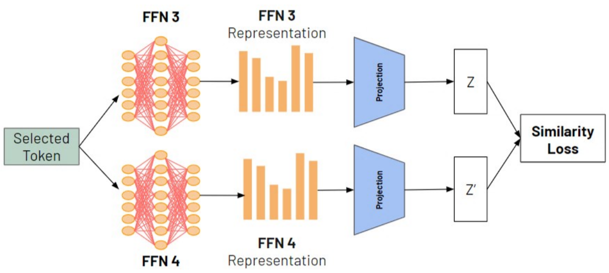


Figure 2: A Similarity Learning Layer (ours) to minimize the similarity among experts.

$$\mathrm{CKA}(K, L) = \frac{\mathrm{tr}(KHLH)}{\sqrt{\mathrm{tr}(KHKH)\,\mathrm{tr}(\mathrm{L\,H\,L\,H})}} \tag{3}$$

where $\|\|_F$ is the Frobenius norm and tr is the trace function. For RBF CKA, K and L are kernel matrices constructed by evaluating the RBF kernel, and H is the centering matrix $H_n = I_n - \frac{1}{n}\mathbf{1}\mathbf{1}^{\mathrm{T}}$.

3.3 Training Objective

The training objective is jointly minimizing the loss of the target task, an auxiliary balancing loss (Fedus et al., 2022; Chi et al., 2022) ($\mathcal{L}^{\text{balancing}}$) and a similarity loss ($\mathcal{L}^{\text{similarity}}$). Given K_i, L_j as the hidden representations of the i-th expert and the j-th expert respectively, the similarity loss is calculated based on the equation (3) as follows:

$$\mathcal{L}^{\text{similarity}} = CKA(K_i, L_j)$$

The overall training objective is to minimize:

$$\mathcal{L} = \mathcal{L}_{\text{task}} + \alpha \cdot \mathcal{L}^{\text{balancing}} + \beta \cdot \mathcal{L}^{\text{similarity}}$$

where α, β are coefficients for the balancing loss and the similarity loss respectively. The term $\mathcal{L}_{\text{task}}$ is defined by the specific task that Large Language Models (LLMs) are learning. For instance, we employ the masked language modeling loss for pre-training and fine-tuning on downstream tasks.

4 Experiment

We evaluate SimSMoE on both the mask language modeling task and downstream tasks and compare the performance of the algorithm to other state-of-the-art routing methods for SMoE training. We also present a detailed analysis of the impact of our method in addressing the representation collapse.

4.1 Experimental Settings

NLP tasks. We investigate two common tasks in pre-training and fine-tuning of LLMs. Firstly, we perform character-level language modeling on the enwik8 (Mahoney, 2011) or text8 datasets (Mahoney, 2011), which are commonly used to evaluate a model's pre-training capabilities. As is common practice, we follow the default training, validation, and testing splits. Secondly, we fine-tune

Architecture		Enwik8 (BPC)	Text8 (BPC)	WikiText-103 (PPL)
Brainformer	# Params		135M	
	SimSmoE	**1.08**	**1.20**	**31.77**
	SMoE	1.11	1.21	32.75
	XMoE	1.10	1.24	32.69
	StableMoE	1.10	1.23	32.10
GLaM	# Params		28M	
	SimSmoE	**1.13**	**1.24**	**37.30**
	SMoE	1.14	1.26	37.39
	XMoE	1.16	1.27	37.62
	StableMoE	1.16	1.25	37.67
Mistral	# Params		63M	
	SimSmoE	**1.11**	**1.21**	**32.51**
	SMoE	1.12	1.23	33.23
	XMoE	1.13	1.24	32.83
	StableMoE	1.13	1.23	33.78

Table 1: Bits-per-character (BPC) on the enwik8 and text8 test sets, and perplexity on the WikiText-103 test set. Lower values are better, with the best results highlighted in bold.

the models on downstream applications to investigate their capability to adapt to different domains. For this purpose, we consider pre-trained large models on enwik8 and text8; then fine-tuning the method on downstream tasks. We select common NLP tasks to evaluate pre-trained models, including the SST-2 (Socher et al., 2013), SST-5 (Socher et al., 2013), IMDB (Maas et al., 2011), and BANKING77 (Casanueva et al., 2020) datasets.

Architecture. We contemplate three advanced SMoE architectures: (i) the Brainformer (Zhou et al., 2024); (ii) GLaM (Du et al., 2022); (iii) and Mistral (Jiang et al., 2024), all of which are decoder-only architectures. Training massive Large Language Models (LLMs) is impractical without substantial industrial resources due to limitations in computational resources. Consequently, we study four model configurations: (i) tiny: with two Brainformer layers and **3.9M** parameters; (ii) small: with ten GLaM layers and **28M** parameters; and (iii) medium: with seven Mistral layers and **63M** parameters; (iv) large: with ten Brainformer layers and **135M** parameters. Rather than striving for state-of-the-art results, we assess the scalability and effectiveness of our algorithm by evaluating multi-scaled models across various datasets. After that, we run vast investigations using the tiny model to comprehend the behaviors of the algorithm and its robustness to different design choices.

Baselines. In order to showcase the effectiveness of our method, we establish baselines using the cutting-edge routing methods, including SMoE with the balancing loss (Fedus et al., 2022), StableMoE (Dai et al., 2022), XMoE (Chi et al., 2022). Moreover, these baselines incorporate advanced SMoE architectures such as **GLaM** (Du et al., 2022), **Brainformer** (Zhou et al., 2024), **Mistral** (Jiang et al., 2024). GLaM(Du et al., 2022) interleaves dense transformer blocks with sparse ones, scaling the capacity of LLMs while significantly reducing training costs compared to dense variants. Brainformer (Zhou et al., 2024), an improved version of GLaM, further enhances performance by reducing the frequency of attention and modifying layer widths and types, making LLMs faster and more efficient than GLaM. Lastly, Mistral (Jiang et al., 2024) has been successful to scale up LLMs to 34B parameters that outperform the previous state-of-the-art LLMs in reasoning, mathematics, and code generation tasks. **SMoE** uses a trainable MLP routing mechanism with a **balancing loss** (Fedus et al., 2022), which encourages a balanced load across experts. **StableMoE** (Dai et al., 2022) introduces a two-phase training approach, initially focusing solely on training the router and subsequently training the experts with the router fixed, while **XMoE** (Chi et al., 2022) features a deep router that includes a down-projection and normalization layer along with a gating network with learnable temperatures.

Pre-training and fine-tuning. SimSMoE fully utilizes all the advantages of routing algorithms, so most of its experimental settings are the same as the baselines for a fair comparison. For the language modeling experiments, we optimize the LLMs pretraining for 50,000 steps using an Adam (Kingma and Ba, 2017) optimizer with a linear learning rate schedule. The checkpoint with the lowest validation loss is used to report the final performance on the test set. For routing mechanisms, we apply the default hyper-parameter configurations for both the baselines and SimSMoE. On the top of that, there are two main hyper-parameters only for SimSMoE: the frequency for checking the collapse issue: f and the threshold for identifying the collapse issue: T. Next, we cross-validate f with respect to the optimal T found. We use the pretrained checkpoint of Mistral models on enwik8 for each fine-tuning dataset, and exclude the last layer. Lastly, we employ a randomly initialized fully connected layer as the classifier and fine-tune all methods for a few epochs using the same learning rate.

4.2 Language Modeling Evaluation

Pre-training Language Models. In contrast to the baselines, SimSMoE incorporates the Similarity Learning Layer to mitigate representation collapse. As a result, SimSMoE includes an additional **0.08M** to **0.16M** parameters compared to the baselines. Table 1 presents the evaluation metrics of SimSMoE versus state-of-the-art strategies. Additionally, we also report the evolution of the performance on the validation set of the SMoE models with various routing policies in Figure 3. We initially note that among all routing methods, SimSMoE consistently outperforms the baselines across all datasets for the three decoder-only architectures. Moreover, advanced strategies such as XMoE (Chi et al., 2022) or StableMoE (Dai et al., 2022)generally surpass the vanilla SMoE method. Nevertheless, the enhancements achieved by these strategies are often inconsistent or marginal. In contrast, SimSMoE consistently outperforms other competitors on all benchmarks (note that the BPC metric is log-scaled), architectures, and offers a faster convergent rate (Figure 3). This outcome underscores SimSMoE's proficiency for learning an effective routing policy to facilitate the masked language modeling task.

Large Scale Pre-training. To demonstrate the effectiveness of our method for scaling up language models, we conducted experiments on the Enwik8 dataset using larger variants of Brainformer with 64 experts and **1.031 B** parameters. Each experiment was repeated three times with different random seeds, and we report the average results along with the standard deviation in Table 2. SimSMoE consistently outperforms other baselines on Enwik8 at a large scale in both average performance and stability, demonstrating that our method is not only effective for large-scale language models but also more reliable compared to the baselines. Beside that, we observe that the performance gap between SimSMoE and the baseline grows as the model size increases, particularly for $K = 1, 2, 4$. However, for larger K ($K > 4$), this gap narrows because our method primarily targets collapse problems, which become less critical at higher K values. Despite this, using a K large is not practical, as it introduces computational inefficiencies and reduces the advantages of the Sparse Mixture of Experts approach due to longer inference times. These findings align with our analysis and confirm that our method remains effective and efficient, even for large-scale models with over 1 billion parameters.

Architecture	**Dataset**	**# Params**	**# Experts**	**K**	**SMoE**	**StableMoE**	**SimSMoE**
Brainformer	Enwik8 (BPC)	1.031 B	64	1	$1.14_{\pm 0.005}$	$1.14_{\pm 0.012}$	$\mathbf{1.12}_{\pm 0.006}$
				2	$1.10_{\pm 0.004}$	$1.10_{\pm 0.008}$	$\mathbf{1.08}_{\pm 0.002}$
				4	$1.09_{\pm 0.005}$	$1.10_{\pm 0.006}$	$\mathbf{1.08}_{\pm 0.002}$
				8	$1.10_{\pm 0.007}$	$1.11_{\pm 0.004}$	$\mathbf{1.09}_{\pm 0.005}$

Table 2: Bits-per-character (BPC) results on the Enwik8 test set for pre-training the Brainformer model with over one billion parameters. B represents billion (10^9).

4.3 Fine-tuning Evaluation

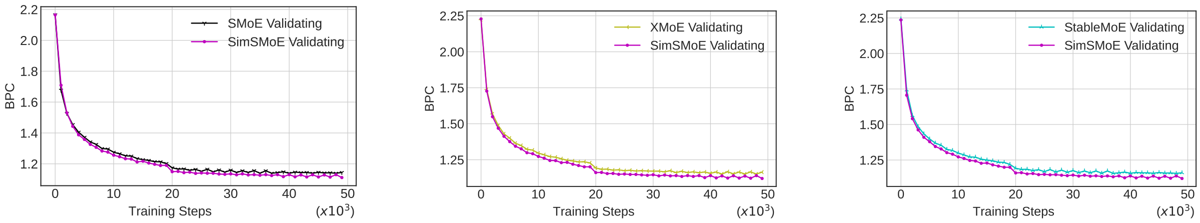
Method	SST-2			SST-5			IMDB			BANKING77		
	SimSMoE			SimSMoE			SimSMoE			SimSMoE		
Algorithm	No	Yes	vs. No	No	Yes	vs. No	No	Yes	vs. No	No	Yes	vs. No
SMoE	81.5	**82.8**	**+1.3**	36.9	**37.8**	**+0.9**	85.2	**85.7**	**+0.5**	74.6	**79.4**	**+4.8**
XMoE	82.2	**82.5**	**+0.3**	34.5	**37.4**	**+2.9**	84.3	**84.6**	**+0.3**	78.6	**79.5**	**+0.9**
StableMoE	81.0	**82.1**	**+1.1**	36.4	**36.7**	**+0.3**	85.0	**85.3**	**+0.3**	74.1	**77.0**	**+2.9**

Table 3: Accuracy of the model after fine-tuned on various datasets. Higher is better, best and comparing results are in bold.

Fine-tuning from Pre-training weights. Table 3 reports the accuracy of the models fine-tuned on the test sets of various datasets. Overall, we observe that SimSMoE demonstrates strong transfer learning capabilities by achieving the highest accuracy on all datasets. Notably, on the more challenging datasets of SST-5 and BANKING77, which have fewer training samples or more classes, we observe larger performance gains from SimSMoE versus the remaining baselines (over 3% improvements compared to the base methods). This result shows that SimSMoE can boost model performance through solving the collapse issue, which is not only good for pre-training but also exhibits strong transfer capabilities to various downstream tasks.

Fine-tuning for Classification Tasks. We also evaluate our method using pretrained language models to assess its effectiveness. Following the experimental setup by MEO (He et al., 2023), we fine-tune BERT-family models (Devlin et al., 2019) using Sparse Mixture of Experts. The fine-tuning results on the GLUE benchmarks (Wang et al., 2018a) are recorded in Table 4. The results demonstrate that our method outperforms both SMoE and MEO on the GLUE benchmark, indicating that SimSMoE is not only effective for pre-training tasks but also performs well on existing pretrained models, such as those in the BERT family.

Fine-tuning for Other NLP Tasks. SimSMoE delivers strong performance across a range of NLP tasks, including *question answering*, *text summarization*, and *language modeling*. Detailed benchmark results are provided in Table 5.



(a) SMoE Routing Policy (b) XMoE Routing Policy (c) StableMoE Routing Policy

Figure 3: Bit-per-Character (BPC) on validation dataset during the training phase reported for Mistral (Jiang et al., 2024) across the three routing mechanisms. (a) SMoE with the Balancing Loss. (b) XMoE. (c) StableMoE

Model	BERT-Base-Cased								
Dataset	CoLA	SST-2	MRPC	STS-B	QQP	MNLI	QNLI	RTE	.avg
SimSMoE	**53.0**	92.1	75.7	**86.6**	**90.2**	**84.0**	**90.7**	**59.6**	**79.0**
SMoE	47.1	92.2	74.5	86.6	90.2	83.5	90.1	58.5	77.8
MEO (He et al., 2023)	49.1	**92.3**	**76.2**	86.3	89.8	83.9	90.5	59.2	78.4

Table 4: Fine-tuning BERT model on the GLUE benchmark. Higher is better, best results are in bold.

Model	Dataset	Task	SMoE	MEO	SimSMoE	Metric
BART	XSum	Summarization	22.4	22.2	**22.6**	R2
T5	SQuAD	Question Answering	82.1	82.0	**82.8**	EM
GPT2	Wikitext-2	Language Model	21.1	20.9	**20.6**	PPL

Table 5: Fine-tuning results across three different architectures including BART, T5, and GPT-2. XSum, SQuAD, and WikiText-2 are evaluated using ROUGE-2 (R2), Exact Match (EM), and Perplexity (PPL), respectively. The best results are highlighted in bold.

We employ BART-Large (Lewis et al., 2019) on XSum (Narayan et al., 2018), T5-Base (Raffel et al., 2023) on SQuAD (Rajpurkar et al., 2016), and GPT-2-Small (Radford et al., 2019) on WikiText-2 (Merity et al., 2016) for evaluation. The results show that our approach outperforms baseline models across multiple NLP tasks, highlighting SimSMoE's effectiveness in both pre-training and fine-tuning the SMoE architecture.

4.4 Ablation Studies

We explore the robustness of SimSMoE under various hyper-parameter settings, conducting all experiments with the tiny Brainformer architecture (Zhou et al., 2024).

SimSMoE Frequency. Since checking the collapse issue for all expert pairs is very costly, as discussed in Section 3.1, it is necessary to control computational resources by f^*, which determines the frequency of collapse issue identification. To demonstrate the effectiveness of our algorithm, we analyze the relationship between f^* and SMoE model performance as the checking frequency increases. All experiments are pretrained under the same settings and evaluated on the enwik8 dataset for a fair comparison. The results reported in Table 6a confirm that SimSMoE is effective, consistent with the assumption, as the threshold f^* increases.

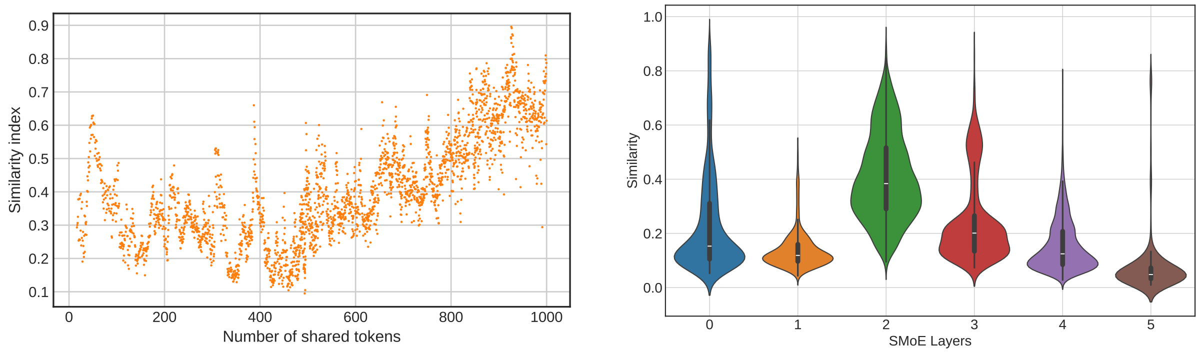
Quality Control. In practice, T^* is a hyperparameter that controls the quality of SimSMoE by determining the level of similarity that can be considered a collapse issue. The value of T^* ranges from 0 to 1. A low T^* means more experts pairs are considered collapsed, while a high T^* means fewer experts are treated as collapsed. Empirically, we find that setting T^* within the interval $[0.3, 0.7]$ is effective, with a good initial value being 0.5. Table 6b shows the pretraining performances of various threshold T^* on enwik8 dataset.

Coefficients of the Similarity Loss. Coefficient β determines the weight of the Similarity Loss contribution to the total SMoE Loss. A high value of β implies that the model focuses on addressing the collapse, while a low value of β indicates the model prioritizes the task loss. Table 6c presents the results of the tiny Brainformer across various β values.

4.5 Representation Collapse Analysis

Representation Collapse In a Sparse Mixture of Experts (SMoE) architecture, all experts are typically designed with the same structure, usually as MLPs. To assign tokens to experts, SMoE employs the $TopK$ operator(Shazeer et al., 2017), resulting in certain experts sharing the same tokens. We hypothesize that experts with a high degree of token sharing are more likely to collapse together. To validate our hypothesis, we analyze the correlation between the number of shared tokens and the similarity index among experts. Figure 4 demonstrates a strong correlation between the number of shared tokens and the similarity among experts, thereby supporting our hypothesis.

The order of layers In Section 3.1, we discussed addressing the collapse issue for all pairs



(a) Similarity index.

(b) The order of layers.

Figure 4: Analysis of the similarity index for the Sparse Mixture of Experts (SMoE). Figure (a) shows the correlation between the number of shared tokens and the similarity index. Figure (b) illustrates the similarity index by layer order.

of experts is costly. Moreover, since the total loss function described in Section 3.3 is a sum of the task loss, the balancing loss, and the similarity loss, there is a trade-off between resolving the collapse issue and optimizing NLP tasks from a local optimal perspective. Therefore, understanding the differences in collapse levels across layers in SMoE is crucial for effectively allocating resources to address this issue. We visualize the distribution of the similarity index across layers in the Brainformer model, as shown in Figure 4. The results indicate that deeper layers exhibit a lower level of collapse compared to earlier layers, suggesting that prioritizing resources to address this issue based on the order of layers in SMoE might improve our method's performance.

Similarity Learning Module Effective The Similarity Learning Module is designed to address the issue of representation collapse, which in turn enhances the diversity of the experts' hidden representations. To demonstrate the module's impact, we subtract the hidden representations of two experts in two scenarios: (1) without SimSMoE, and (2) with SimSMoE. Following the suggestions by Samek et al. (2015) (Samek et al., 2015), we visualize these differences using a heatmap. Without SimSMoE, Figure 5 shows how the expert representations become more similar, thus providing support for our method.

5 Related Work

5.1 Sparse Mixture of Experts

Sparse Mixture of Experts (SMoE) Motivated by Mixture of Experts (MoE) (Jacobs et al., 1991; Jordan and Jacobs, 1994), Sparse Mixture of Experts (SMoE), with the unifying idea that each example is processed by a subset of the parameters, was first introduced by Shazeer et al. (2017)(Shazeer et al., 2017). SMoE gained further popularity when combined with Transformer large language models (Zhou et al., 2022b; Li et al., 2022b; Shen et al., 2023). After demonstrating promising success in natural language processing, it has been proven in a variety of domains including computer vision (Riquelme et al., 2021; Hwang et al., 2023; Lin et al., 2024), speech recognition (Wang et al., 2023b; Kwon and Chung, 2023), and multi-task learning (Ye and Xu, 2023; Chen et al., 2023b). However, training SMoE still suffers the representation collapse issue (Chi et al., 2022), where all experts converge to similar representation. Chi et al. (2022) (Chi et al., 2022) identified the issue and proposed XMoE, which estimates the routing scores between tokens and experts on a low-dimensional hypersphere. In subsequent research on the collapse issue, SMoE-dropout(Chen et al., 2023a) suggested that using a randomly initialized and fixed router network to activate experts, and gradually increasing the number of activated experts, might address the problem. Meanwhile, HyperRouter (Do et al., 2023) proposed that employing HyperNetwork (Ha et al., 2016) to generate router weights is an effective approach for training SMoE. StableMoE (Dai et al., 2022) also aims to effectively train SMoE by developing a balanced and cohesive routing strategy. This strategy is distilled into a lightweight router, decoupled from the backbone model, which is then used to determine token-to-expert assignments that are frozen to ensure a stable routing strategy. Those methods concentrate on enhancing routing algorithms, whereas our approach is a straightforward solution that directly targets the hidden representation of experts, a topic that remains under-explored.

5.2 Similarity Learning

The occurrence of presentation collapse is a common issue in self-supervised learning and has been extensively investigated. (Jing et al., 2022; Hua et al., 2021; Li et al., 2022a). A critical challenge in identifying collapse lies in measuring the similarity between neural network representations. Similarity learning (Kornblith et al., 2019b; Csiszárik et al., 2021) holds potential for addressing this problem. The current set of representational similarity measures, classified based on their approach to similarity measurement, includes *Canonical Correlation Analysis* (Raghu et al., 2017), *Alignment* (Williams et al., 2022), *Representational Similarity Matrix* (Shahbazi et al., 2021; Kriegeskorte et al., 2008), *Neighbors* (Wang et al., 2023a), *Topology* (Khrulkov and Oseledets, 2018), and *Statistic* (Camastra and Staiano, 2016). Among the aforementioned approaches, the *Representational Similarity Matrix* is widely employed to explore the similarity between the representations of neural networks (Li et al., 2016; Raghu et al., 2017; Wang et al., 2018b; Kornblith et al., 2019a). Kornblith at el. (2019) emphasized that the canonical correlation analysis (CCA) approach remains invariant under invertible linear transformations only when the retained subspace remains unchanged. They subsequently introduced centered kernel alignment (CKA), which can ascertain the correspondence between the hidden layers of neural networks trained from varying random initializations and widths. In this study, we also illustrate that CKA serves as an appropriate similarity learning metric for addressing representation collapse among experts.

6 Conclusion

This study illustrates representation collapse levels in sparse mixture-of-experts (SMoE) models by employing a similarity learning metric. Moreover, we introduce a similarity learning module, which is a direct approach to differentiate expert's hidden representations, designed to alleviate this issue. We also extensively evaluate three advanced SMoE architectures for both pre-training and fine-tuning tasks to demonstrate SimSMoE strong capabilities, scalability, and superiority over state-of-the-art routing strategies. Finally, we believe that focusing on expert representation opens up new research avenues for effectively training SMoE, where cutting-edge techniques in Similarity Learning and Contrastive Learning can be harnessed to enhance their performance.

Limitations

Our work focuses on the efficiency and efficacy of training LLMs using SMoE. Despite the encouraging results, our experiments are conducted only on medium-scale datasets with a medium-scale Transformer-family based models due to computation limitations. Thus, further empirical evaluations are required to validate the scalability of SimSMoE and other SMoE strategies on recent LLMs and larger datasets.

Ethics Statement

Despite encouraging results, training large-scale LLMs is inevitably costly and requires extensive computational resources, which need to be properly managed. Moreover, our work used data collected on the web, which has been known to suffer from gender and racial biases and requires additional efforts to mitigate its negative impacts. Lastly, our study is a promising step towards facilitating the development of new LLMs, which still requires careful regularization to avoid potential misuses in harmful applications.

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A Example Appendix

Supplementary Material for "SimSMoE: Solving Representational Collapse via Similarity Measure"

This document is structured as follows: Appendix B provides detail materials for SimSMoE algorithm, ablation studies results, and representation collapse analysis. Appendix C offers a detailed settings for our experiments in Section 4.

B Additional Materials

B.1 SimSMoE Algorithm details

The training procedure for similarity-based SMoE can be succinctly outlined in four steps. First, compute the shared tokens per expert pair through router $G(x)$, updating the total input tokens for each expert accordingly to verify the frequency condition. Next, assess the similarity among chosen experts. If this similarity surpasses the predefined threshold, proceed to update the total loss. Finally, refine the overall loss using the same optimization approach employed in traditional SMoE training.

Algorithm 1: Pseudo-code to train SimSMoE.

Algorithm `SimSMoE Training`($\{t, y_t\}_{i=1}^{N}$)
  Require: $SMoE$; $\mathcal{L}_B$ (Balancing Loss); $\mathcal{L}_S$ (Similarity Loss); tr (# tokens per expert); Router R; $Expert_i$; $Expert_j$; f^*; T^*; λ; β
  Result: $\mathcal{L}$ (Final Loss)
  for $i \leftarrow 1$ *to* N **do**
    Receive a token t
    $f_t \leftarrow tr(t)$
    if $f_t \geq f^*$ **then**
      $\hat{y}_i \leftarrow Expert_i(t)$
      $\hat{y}_j \leftarrow Expert_j(t)$
      $T_t \leftarrow \mathcal{L}_S(\hat{y}_i, \hat{y}_j)$
      $\mathcal{L}_B \leftarrow \lambda \mathcal{L}_B(R)$
      if $T_t \geq T^*$ **then**
        $\hat{y} \leftarrow SMoE(t)$
        $\mathcal{L}_S \leftarrow \beta T_t$
        $\mathcal{L} \leftarrow \mathcal{L}_{\text{token}}(\hat{y}, y) + \mathcal{L}_B + \mathcal{L}_S$
      else
        $\hat{y}_t \leftarrow SMoE(t)$
        $\mathcal{L} \leftarrow \mathcal{L}_{\text{token}}(\hat{y}, y) + \mathcal{L}_B$

B.2 Ablation Studies results

B.3 Representation Collapse Analysis

C Experiments implementation details

This section provides detailed parameters of our experiments in Section 4.

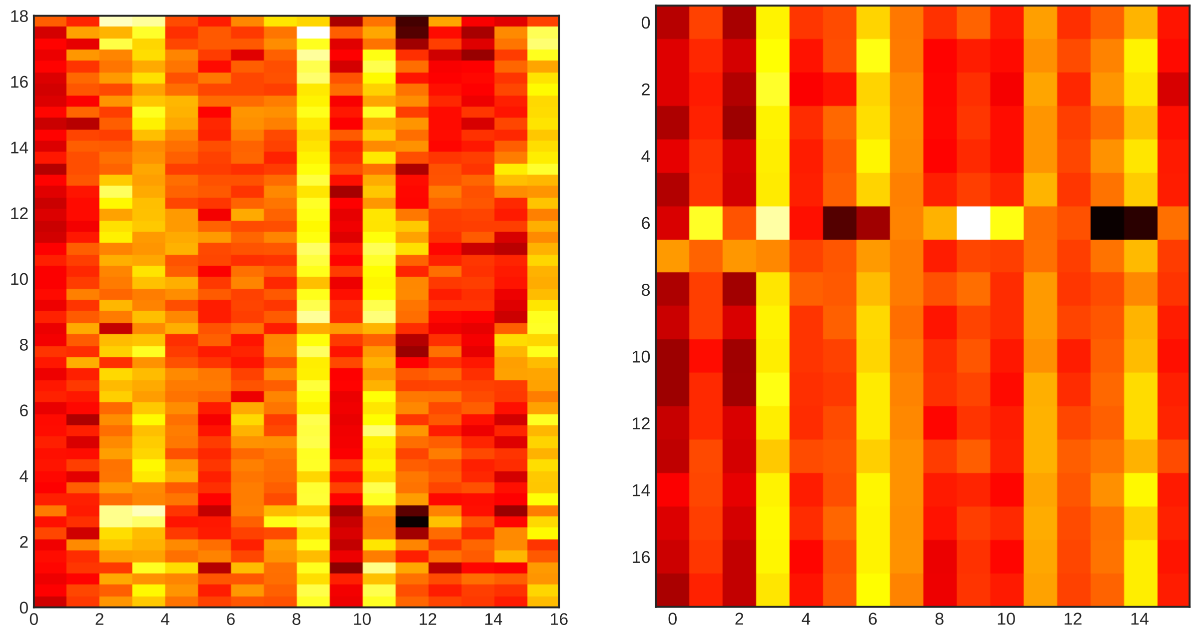
C.1 General Settings

The experiments are based on the publicly available CompeteSMoE implementation(Pham et al., 2024)[1]. However, the pre-training was conducted on a single A100 GPU, so results might differ when using parallel training on multiple GPUs.

C.2 Pre-training Experiments

Table 7 provides the detailed configurations for pre-training Brainformer (Zhou et al., 2024),

[1] https://github.com/giangdip2410/CompeteSMoE



(a) SMoE Layer.

(b) SimSMoE Layer.

Figure 5: Exploration of the impact of similarity learning on diversity model representation. Figure (a) shows the heatmap of differences between the hidden representations of two experts for the SMoE layer. Figure (b) shows the heatmap of differences between the hidden representations of two experts for the SimSMoE layer.

Table 6: Pretraining tiny Brainformer on enwik8 across different hyperparameter settings

(a) Comparison of frequency of the collapse issue checking for SimSMoE.

f^*	BPC
1	1.56
4	1.58
8	1.55
16	**1.54**
SMoE	1.69

(b) Effects of Similarity threshold during pretraining.

T^*	BPC
0.1	1.54
0.3	1.55
0.3	**1.54**
0.7	1.55
0.9	1.55
SMoE	1.69

(c) Pretraining tiny Brainformer on enwik8 across different hyperparameter settings.

β	BPC
0.005	1.55
0.01	**1.54**
0.05	1.56
0.1	1.54
0.2	1.57
SMoE	1.69

GLaM (Du et al., 2022), and Mistral (Jiang et al., 2024) on `Enwik8`, `Text8` and `Wikitext-103`.

Dataset	Input length	Batch size	Optimizer	Lr	# Training Step
`Enwik8`	512	48	Adam	4.5e-4	50k
`Text8`	512	48	Adam	4.5e-4	50k
`Wikitext-103`	512	22	Adam	4.5e-4	50k

Table 7: Hyperparameter settings for pre-training experiments on `Enwik8`, `Text8` and `Wikitext-130`.

C.3 fine-tuning Experiments

For fine-tuning experiments, we employ the identical model architecture as in pre-training. Table 8 presents the detailed configurations utilized for fine-tuning experiments on `SST-2`, `SST-5`, `IMDB`, and `BANKING77` datasets.

Dataset	Input length	Batch size	Optimizer	Lr	# Epochs
`SST-2`	512	16	Adam	1e-4	5
`SST-5`	512	16	Adam	1e-4	5
`IMDB`	512	4	Adam	1e-4	5
`BANKING77`	512	16	Adam	1e-4	50

Table 8: Detail settings for fine-tuning experiments on the evaluation datasets.