Improved Sparse Upcycling for Instruction Tuning

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Abstract

The Mixture-of-Experts (MoE) architecture has demonstrated significant potential in both large-scale pre-training and instruction tuning by offering increased parameter capacity without additional inference costs. However, developing MoE models faces challenges including training instability and the need for substantial high-quality training data. While efficient methodologies like sparse upcycling exist, they often lead to performance degradation in instruction tuning scenarios. We introduce representation-based sparse upcycling, a straightforward yet effective technique for converting dense language models into sparsely activated ones while maintaining similar computational costs. Unlike conventional sparse upcycling, our approach leverages intermediate representations from language models to initialize router weights. This strategy addresses the mismatch between randomly initialized and well-trained parameters while providing prior knowledge to guide expert specialization during training. Extensive experiments across diverse benchmarks demonstrate significant improvements in both model capabilities and routing consistency compared to existing approaches.

1 Introduction

Instruction tuning (Wei et al., 2022) has emerged as a pivotal technique for enhancing language models' capabilities by fine-tuning them on instruction-annotated datasets. Large Language Models (LLMs) that undergo instruction tuning demonstrate superior downstream performance on held-out tasks in both zero-shot and few-shot settings (Ouyang et al., 2022). Recent research indicates that increasing the diversity and quality of instruction tuning data yields substantially more significant improvements compared to merely expanding data quantity (Zhou et al., 2023a). Contemporary studies have focused on curating high-quality datasets through prompting advanced LLMs such as ChatGPT and GPT-4, subsequently training smaller models to emulate their reasoning and problem-solving processes (Wang et al., 2023b; Xu et al., 2024; Mukherjee et al., 2023). However, a substantial performance disparity persists between models of varying sizes. Smaller language models consistently encounter difficulties in complex reasoning scenarios, such as solving mathematical competition problems, primarily due to their limited parameter capacity constraining their achievable capabilities.

The Mixture-of-Experts (MoE) architecture (Shazeer et al., 2017) offers a promising solution by partitioning parameters into expert subsets and selectively activating only a fraction of these experts for each input during both training and inference. This architectural innovation enables MoE models to incorporate vast parameter counts while maintaining moderate computational requirements, frequently demonstrating superior capabilities compared to dense models with comparable inference costs (Fedus et al., 2022b; Du et al., 2022; Jiang et al., 2024). Nevertheless, MoE models commonly exhibit training instabilities (Fedus et al., 2022b; Du et al., 2022; Zoph et al., 2022), necessitating various mitigation techniques. However, validating these techniques on large-scale language models demands substantial computational resources. Consequently, constructing MoE models from pre-trained dense models presents a more resource-efficient alternative to training from scratch.

Komatsuzaki et al. (2023) introduced *sparse upcycling*, a methodology for converting existing dense models into larger, sparsely activated models by replicating MLP layers and randomly initializing router weights. While upcycled T5 (Raffel et al., 2020) models demonstrated performance improvements through continued pre-training, these gains diminished as base model size increased.

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Moreover, when applying limited additional training, the original and upcycled models exhibited comparable performance. The homogeneity of replicated MLPs and randomly initialized routers impedes optimal training outcomes.

To address these limitations, we propose a representation-based sparse upcycling method. Based on our observation that internal representations of tokens from specific tasks tend to form distinct clusters within high-dimensional representation spaces in well-trained language models, we conceptualize expert routing behavior as a matching process between expert representations within the router and task- or context-aware token representations. This insight emphasizes the critical role of router weight initialization. By initializing routers with abstracted internal representations, we guide experts to focus on specific, semantically related, or task-related tokens, significantly mitigating random routing and training instability issues while facilitating expert specialization.

We validate our approach through comprehensive instruction tuning experiments, demonstrating superior downstream task performance and consistent routing behaviors.

We summarize our contributions as follows:

- We propose a novel representation-based sparse upcycling approach that improves upon existing sparse upcycling methods by initializing router weights with task or context-aware representations, thereby reducing training instability and enhancing expert specialization.
- We empirically demonstrate that intermediate representations in well-trained dense models exhibit inherent clustering tendencies, which we leverage to facilitate efficient expert routing in sparse models.
- We validate the effectiveness of our approach through extensive instruction tuning experiments across diverse benchmarks, showing significant improvements in downstream task performance and routing consistency.

Code will be available at https://github.com/icip-cas/sparse-upcycling.

2 Related Work

2.1 Mixture-of-Experts

Mixture-of-Experts (MoE) are a variant of sparse expert models, in which a part of the parameters are partitioned into individual experts (Fedus et al., 2022a). During both training and inference, only a subset of these experts is selectively activated based on the input features. This selective activation allows each expert to specialize in specific tasks, significantly boosting performance metrics across a variety of applications. By assigning particular tasks to the most suitable experts, the model effectively harnesses their specialized knowledge, leading to substantial improvements in performance.

Shazeer et al. (2017) applies MoE layers between stacked LSTM layers (Hochreiter and Schmidhuber, 1997), resulting in the creation of the largest model at that time, which achieves state-of-the-art performance on language modeling and machine translation. Subsequent research has focused on unleashing the potential of the Transformer architecture (Vaswani et al., 2017) and achieve substantial advancements on both language and vision tasks (Lepikhin et al., 2021; Fedus et al., 2022b; Jiang et al., 2024; Ruiz et al., 2021; Wu et al., 2022; Puigcerver et al., 2023).

Nonetheless, much of the existing work has concentrated on training sparse models from scratch, with training stability emerging as a major research focus. Zoph et al. (2022) conducts a large-scale stability study of sparse models, investigating how factors such as multiplicative interactions, noise injection during training, auxiliary router loss, and training precision contribute to improving model stability. Dai et al. (2022) identified the routing fluctuation problem in previous MoE methods and proposed a balanced and cohesive routing strategy to address this issue.

Sparse Upcycling (Komatsuzaki et al., 2023), outlines a methodology for transitioning from a well-trained dense model to a sparse model, rather than to a larger dense model. This technique leverages the additional capacity provided by increased parameters while maintaining inference costs through computational sparsity. We adopt this approach to create sparsely activated models in our research.

2.2 Instruction Tuning

Instruction tuning (Wei et al., 2022) involves fine-tuning pre-trained language models on datasets comprising instruction-output pairs. This process enhances the models' ability to understand and execute human instructions effectively.

The success of instruction tuning largely depends on the creation of high-quality datasets. Both manually annotated data (Ouyang et al., 2022) and synthetically generated data through distillation (Wang et al., 2023b; Taori et al., 2023) are employed to boost language models' performance in areas such as general reasoning (Xu et al., 2024), code generation (Luo et al., 2023b; Wei et al., 2024; Yu et al., 2024b), and mathematical problem solving (Luo et al., 2023a; Yu et al., 2024a; Yue et al., 2024a,b).

Research into efficient and effective instruction tuning techniques is an important complementary direction. NEFTune (Jain et al., 2024) enhances the conversational capabilities of instruction-tuned models by fine-tuning with noisy embeddings. LoRA (Hu et al., 2022), along with its sparse variations (Wu et al., 2024b; Gou et al., 2024; Wu et al., 2024a), focuses on adapting language models to downstream tasks by optimizing only a subset of parameters, thus minimizing performance loss.

3 Preliminary

3.1 Sparsely Activated Mixture-of-Experts

In Transformer based MoE models, a prevalent approach involves substituting the Feed-Forward Networks (FFNs) within certain Transformer blocks with specialized experts, which are collections of inherently independent FFNs. Additionally, a routing network is incorporated to allocate the appropriate experts for each input feature.

In this work, we primarily focus on Top-k routing (Shazeer et al., 2017; Fedus et al., 2022b; Du et al., 2022). The router takes a token representation as input and routes it to the best k experts, selected from a set of N experts $\{E\}_{i=1}^{N}$. Specifically, the router weights, $W_r \in \mathbb{R}^{N\times d}$, where each row $r_i \in \mathbb{R}^d$ represents an expert embedding, produce logits $r(x) = W_r \cdot x$. The logits are then normalized via the softmax function, yielding a distribution over the experts,

$$p_i(x) = \frac{e^{r(x)_i}}{\sum_j^N e^{r(x)_j}}. \tag{1}$$

The input then selects the k experts with highest probabilities, where the indices of the selected experts constitute a set $\mathcal{K}$. The output of the MoE layer is computed as a linear combination of the output of the selected experts,

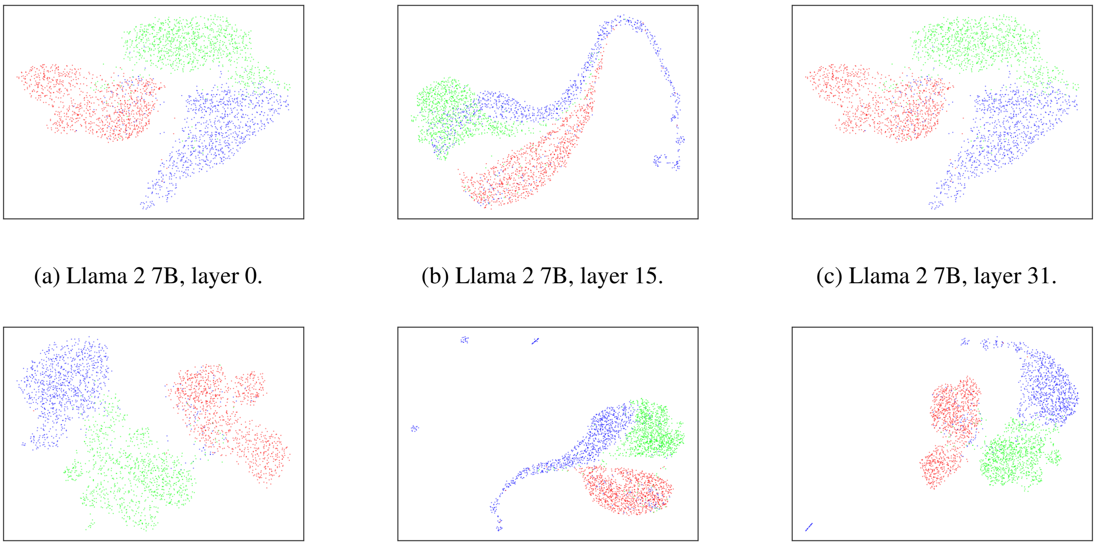
$$y = \sum_{i\in\mathcal{K}} p_i(x)E_i(x). \tag{2}$$

3.2 Specialization

Sparse Models Expert specialization within MoE models is critical for fostering diversity among the experts. This diversity is essential because if all experts converge towards homogeneity, the MoE model effectively becomes a conventional dense model, thereby diminishing its intended benefits. The phenomenon known as *representation collapse*, where experts fail to maintain distinct knowledge or skills, poses a significant challenge to the effectiveness of sparse MoE models. Chi et al. (2022) provides a theoretical examination of this issue, suggesting that addressing representation collapse can lead to substantial performance improvements across various tasks.

The significance of expert specialization is further underscored by empirical observations across numerous studies. For instance, research by Lewis et al. (2021) demonstrates that the assignment of inputs to experts is influenced by local syntactic information, indicating a form of specialization based on the nature of the input data. Moreover, in the context of sparse encoder-decoder Transformers, Zoph et al. (2022) observed distinct specializations among encoder experts, with certain experts focusing predominantly on specific linguistic elements such as punctuation, verbs, proper nouns, and numerical data. This specialization is not limited to linguistic tasks. In multimodal MoE models, both modality-specific and multimodal experts exhibit specialization, effectively enhancing the model's performance across diverse datasets and tasks, as illustrated by Mustafa et al. (2022).

Dense Models We perform an empirical analysis on the inherent domain specialization of dense language models. In particular, we are interested whether there exists a fascinating pattern regarding the layer-wise representation of data points from specific domains (e.g. code, mathematics, etc.). We sample $1,000$ textual examples each from general reasoning datasets, code generation datasets, and mathematical reasoning datasets. Layer-wise representations before and after FFNs generated by language models are taken into consideration, and subsequently projected using Uniform Manifold Approximation and Projection (UMAP) (McInnes et al., 2020) for spatial structure visualization in hyperbolic space. Figure 1 shows that, for both Llama 2 7B (Touvron et al., 2023) and Llama 3 8B (Dubey et al., 2024), the internal representation of the models originating from homogeneous do-



(a) Llama 2 7B, layer 0. (b) Llama 2 7B, layer 15. (c) Llama 2 7B, layer 31.

(d) Llama 3 8B, layer 0. (e) Llama 3 8B, layer 15. (f) Llama 3 8B, layer 31.

Figure 1: Representations generated by the self-attention modules of Llama 2 7B and Llama 3 8B model. Red, blue, and green points are samples from datasets specialized in text, code, and math, respectively.

mains tend to aggregate into distinct clusters within high-dimensional space.

4 Methodology

This section presents our novel approaches for transforming dense language models into sparse architectures. We introduce two distinct methodologies: *task-representation based sparse upcycling* (TRSU), and *context-representation based sparse upcycling* (CRSU). Following the transformation, all models undergo instruction tuning to ensure alignment with target tasks.

4.1 Problem Formulation

Our preliminary experiments revealed that sparse upcycled MoE models frequently underperform compared to their dense counterparts on downstream tasks when instruction-tuned on datasets ranging from thousands to millions of instances. This observation is particularly noteworthy given that sparse upcycled models and dense models possess equivalent capabilities prior to training. While Komatsuzaki et al. (2023) demonstrated that upcycled models exhibit performance advantages after training on large-scale datasets such as C4 (Raffel et al., 2020), we hypothesize that limited training data constrains the sparse models' ability to develop effective and consistent routing behavior.

The random initialization of router weights results in a highly entropic initial state during training, leading to limited and potentially noisy knowledge acquisition by each expert. Therefore, providing a priori guidance for routing behavior becomes crucial, serving as an entropy reduction mechanism to ensure more consistent and robust performance during subsequent training and inference phases.

4.2 Task Aware Sparse Upcycling

Contemporary large language models demonstrate proficiency across a spectrum of tasks, from basic to complex. We focus on scenarios where models undergo instruction tuning on diverse task sets to function as effective assistants.

Given a set of tasks $\mathcal{T} = \{t_i\}_{i=1}^{T}$, our objective is to upcycle a language model of limited size to a sparse architecture with T experts. To mitigate the inherent randomness in sparse model training and provide task-oriented guidance for each expert – specifically, designating each expert to primarily handle tokens with high representation similarity – we heuristically employ representative task representations as the initialization parameters for router weights.

As demonstrated in Section 3.2, the internal representations generated by language models from high-quality task data naturally cluster within high-dimensional space. These representations interact with expert representations within the routers to determine routing behavior. We leverage this phenomenon by: (1) Sampling representative task data;

(2) Clustering the generated attention representations; (3) Utilizing resulting vectors as initialization parameters for specific experts. This approach facilitates matching task-relevant data to corresponding experts while delegating task-irrelevant data to alternative experts.

4.3 Context Aware Sparse Upcycling

While the task-aware approach represents an advancement over conventional sparse upcycling, it presents certain limitations: (1) The number of experts is constrained to match the number of tasks; (2) The clustering of task data representations relies on empirical observation rather than rigorous theoretical foundation; (3) As task quantity increases or task boundaries become less distinct, clusters may overlap, potentially compromising routing effectiveness.

To enhance practical applicability, we propose a more generalized methodology. Given a dataset consisting single or multiple tasks, we sample a representative subset of the data and perform clustering on their representations generated by language models in high-dimensional space, using a pre-defined number K (e.g., via K-means clustering (MacQueen et al., 1967)). This process yields K representative directions within the contextual embedding space, which are then assigned to K experts as initial router representations.This approach removes the constraint on expert quantity imposed by the task-aware method. The resulting vectors may represent more general token categories beyond task-specific representations, such as numerical text, code, or punctuation, aligning with observations by Zoph et al. (2022).

4.4 Design Decisions

MoE models share several significant configurations, including router type, number of sparse layers, number of experts per layer, number of experts to activate, etc., which exert influence on computation budget, model size, and model performance.

Router type We mainly focus on the classic switch routing (Top-1 routing) (Fedus et al., 2022b). Despite the augmentation of total parameters, the MoE layer exhibits comparable computational efficiency to dense ones.

Number of sparse layers Incorporating more sparse layers is benefit to enhance the capacity of models, albeit with a concomitant escalation in computational and resource expenditure. Owing to the recent success of Mixtral (Jiang et al., 2024) and DeepSeekMoE (Dai et al., 2024), we transform all transformer layers into sparse ones.

Load balance Following Fedus et al. (2022b), we adopt a differentiable load balancing loss to encourage uniform routing over experts. Specifically, given N experts and a batch of $B \times L$ tokens, the auxiliary loss is computed as the inner product of vectors f and P,

$$\text{loss} = \alpha \cdot N \cdot \sum_{i=1}^{N} f_i \cdot P_i \tag{3}$$

where f_i is the fraction of the tokens dispatched to expert i, and P_i is the fraction of the router probability allocated for expert i,

$$\begin{aligned} f_i &= \frac{1}{L} \sum_{x \in \mathcal{B}} \mathbb{1}\{\text{argmax} p(x) = i\} \\ P_i &= \frac{1}{L} \sum_{x \in \mathcal{B}} p_i(x) \end{aligned} \tag{4}$$

a hyper-parameter α is a multiplicative coefficient for the load balancing loss.

5 Experiments

This section elucidates our exploration of language model sparsity through several methodologies. We employ three distinct approaches to transform dense language models into their sparse counterparts: sparse upcycling (SU), task-representation based sparse upcycling (TRSU), and context-representation based sparse upcycling (CRSU). Subsequently, all models, both dense and sparse, undergo instruction tuning to ensure alignment. We then conduct comprehensive evaluations to assess and compare the performance and characteristics of these models.

5.1 Experimental Setup

5.1.1 Training Datasets

We evaluate TRSU's effectiveness through a comprehensive multi-task learning framework. We focus on three fundamental domains: natural language (text), programming (code), and mathematical reasoning (math), following Ding et al. (2024). While these domains are essential for demonstrating the capabilities of LLMs, their integration into a unified model presents significant challenges. The training process leverages a curated dataset from established open-source resources: OpenOrca

Model	Size	**MMLU** Acc (%)	**HellaSwag** Acc (%)	**HumanEval** Pass@1 (%)	**MBPP** Pass@1 (%)	**GSM8K** Acc (%)	**MATH** Acc (%)	**Average** (%)
Danube 2	1.8B	39.7	**70.9**	34.5	30.2	49.2	13.7	39.7
	$2\times1.8\mathrm{B}_{\mathrm{SU}}$	38.8	70.1	32.8	28.6	48.7	12.8	38.6
	$2\times1.8\mathrm{B}_{\mathrm{TRSU}}$	**40.2**	70.4	**36.2**	**30.7**	**49.8**	**14.0**	**40.2**
Llama 2	7B	47.4	**75.2**	47.6	53.7	59.2	17.3	50.0
	$2\times7\mathrm{B}_{\mathrm{SU}}$	47.1	73.9	44.3	51.4	58.5	16.8	48.6
	$2\times7\mathrm{B}_{\mathrm{TRSU}}$	**49.5**	74.8	**48.4**	**54.1**	**59.9**	**18.0**	**50.7**

Table 1: Overall TRSU results of dense and sparse models across benchmarks.

Model	Size	**MMLU** Acc (%)	**MMLU-Pro** Acc (%)	**IFEval** Acc (%)	**HumanEval** Pass@10 (%)	**MATH** Acc (%)	**Average** (%)
Danube 2	1.8B	44.2	14.8	26.6	19.6	**4.9**	22.0
	$2\times1.8\mathrm{B}_{\mathrm{SU}}$	43.6	15.1	25.8	19.5	4.1	21.6
	$2\times1.8\mathrm{B}_{\mathrm{TRSU}}$	**44.5**	**15.8**	**27.2**	**20.2**	4.7	**22.5**
Llama 2	7B	49.7	19.7	35.2	25.0	**7.4**	27.4
	$2\times7\mathrm{B}_{\mathrm{SU}}$	48.9	19.9	33.7	25.0	6.7	26.8
	$2\times7\mathrm{B}_{\mathrm{TRSU}}$	**50.1**	**20.5**	**37.1**	**27.1**	7.1	**28.4**

Table 2: Overall CRSU results of dense and sparse models across benchmarks.

dataset (Lian et al., 2023a), Magicoder Evol Instruct (Luo et al., 2023b), Magicoder OSS Instruct (Wei et al., 2024), and MetaMathQA (Yu et al., 2024a), following filtration and sampling procedures.

To assess CRSU's domain-agnostic capabilities, we employ SlimOrca (Lian et al., 2023b), a curated subset of OpenOrca (Lian et al., 2023a). This dataset extends the FLAN Collection (Longpre et al., 2023) by incorporating step-by-step reasoning patterns derived from GPT-3.5 and GPT-4.

5.1.2 Implementation Details

We implement our approach using Mergekit (Goddard et al., 2024) to transform dense language models into sparse architectures. Unlike conventional sparse upcycling that randomly initializes expert routers, our method derives task and context representations from both the base model and training data. We then apply K-means clustering to generate representative router parameters (see Appendix B).

Our experiments utilize two base models: H2O-Danube2-1.8B (Singer et al., 2024) (hereinafter Danube 2 1.8B) and Llama 2 7B (Touvron et al., 2023). Training proceeds for one epoch using an 8×80GB A100 GPU cluster, with a batch size of 128 and maximum sequence length of 4096. Model optimization employs the AdamW optimizer (Loshchilov and Hutter, 2019) with learning rates of 1×10^{-5} and 2×10^{-5} for the Danube 2 1.8B series and Llama 2 7B series, respectively.

For TRSU experiments, we convert the base models into MoE architectures, incorporating two domain-specific experts (code and math) in each Transformer block. We benchmark both SU and TRSU models against the original dense models. The CRSU experiments extend this framework with four experts per Transformer block, comparing both SU and CRSU performance.

5.1.3 Evaluation

We conduct comprehensive evaluations of both dense and sparse models across diverse benchmarks to assess their capabilities after fine-tuning. Our evaluation strategy is tailored to the specific training objectives:

- For multi-task trained models, we focus on assessing their ability to simultaneously handle multiple complex tasks. The evaluation spans three key domains: MMLU (Hendrycks et al., 2021a) and HellaSwag (Zellers et al., 2019) for text, HumanEval (Chen et al., 2021) and MBPP (Austin et al., 2021) for code, and GSM8K (Cobbe et al., 2021) and MATH (Hendrycks et al., 2021b) for math.

- For models trained on SlimOrca, which encompasses a broader distribution of general instructions, we evaluate their performance across: MMLU (Hendrycks et al., 2021a) and MMLU-Pro (Wang et al., 2024) for general knowledge and reasoning, IFEval (Zhou et al., 2023b) for instruction understanding and execution, HumanEval (Chen et al., 2021) and MATH (Hendrycks et al., 2021b) for technical problem-solving.

To ensure consistency and facilitate fair comparisons, all evaluations adhere to a standardized instruction-following paradigm. Test instances are transformed into a uniform chat template format, maintaining consistent interaction patterns across all benchmarks. Detailed evaluation protocols, metrics, and implementation specifics are provided in Appendix C.

5.2 Main Results

Tables 1 and 2 present comprehensive performance comparisons across different model configurations. Several key findings emerge from our experiments:

Effectiveness of Task-Representation Sparse Upcycling The TRSU approach demonstrates superior performance compared to both dense models and traditional sparse upcycling (SU) across the majority of benchmarks. In the Danube 2 1.8B series, TRSU yields an average performance gain of 0.5 percentage points relative to the dense baseline (40.2% vs. 39.7%) and a more substantial improvement of 1.6 points compared to SU (40.2% vs. 38.6%). The Llama 2 7B series exhibits even more pronounced improvements, with TRSU surpassing the dense model by 0.7 points (50.7% vs. 50.0%) and SU by 2.1 points (50.7% vs. 48.6%).

Context-Representation Benefits The empirical results in Table 2 demonstrate that CRSU effectively captures contextual patterns, particularly in reasoning-intensive tasks. This advantage manifests most notably in MMLU-Pro and IFEval performance metrics. The Llama 2 7B CRSU variant exhibits substantial improvements in both IFEval (37.1% vs. 35.2% dense) and MMLU-Pro (20.5% vs. 19.7% dense), suggesting enhanced capabilities in context-dependent reasoning tasks.

Trade-offs in Mathematical Tasks While our sparse approaches generally enhance performance across most benchmarks, we observe distinct patterns in mathematical reasoning tasks. In the CRSU configuration, both model series exhibit marginal performance degradation on MATH compared to their dense counterparts. This phenomenon may be attributed to the relative underrepresentation of mathematical content in the training corpus, resulting in suboptimal mathematical context specialization during the construction of contextual representations. The limited exposure to mathematical patterns and reasoning structures potentially impedes the development of mathematics-specific routing capabilities, subsequently affecting the models' mathematical problem-solving proficiency.

Model	Size	Text	Code	Math
Danube 2	$2\times1.8\text{B}_{\text{TRSU}}$	55.3	33.4	31.9
	$3\times1.8\text{B}_{\text{TRSU}}$	54.8	33.2	31.3

Table 3: Evaluation on TRSU models with different number of experts in each sparse layer.

Model	Size	MMLU	MMLU-Pro
Danube 2	$2\times1.8\text{B}_{\text{CRSU}}$	42.7	14.1
	$4\times1.8\text{B}_{\text{CRSU}}$	44.5	15.8
	$8\times1.8\text{B}_{\text{CRSU}}$	44.7	15.9

Table 4: Evaluation on CRSU models with different number of experts in each sparse layer.

5.3 Ablations and Analysis

5.3.1 Number of experts

In the TRSU experiments, we transform dense models into MoE architectures by implementing dual experts within each Transformer block. This design aims to enable expert specialization across code and math domains, while treating text processing as a shared responsibility between experts. We further investigate whether designating text as a distinct domain would enhance performance. Table 3 shows the performance comparison between two-expert and three-expert configurations, evaluated on the same benchmarks as Table 1. The slight performance decline from Danube 2 2×1.8B to 3×1.8B suggests that dedicating a specific expert to text processing offers no substantial benefit. This finding indicates that MoE architectures may be more effective for tasks with clear domain boundaries rather than general language tasks that require integrated world knowledge.

For CRSU experiments, we explore the scalability benefits of increasing expert count. Resource limitations constrained our investigation to 2-, 4-,

Training Process	25%	50%	75%	100%
Performance Diff.	+1.9%	+1.4%	+1.1%	+0.9%

Table 5: Performance difference between Danube 2 $4\times1.8\text{B}_{\text{CRSU}}$ and Danube 2 $4\times1.8\text{B}_{\text{SU}}$ during the training process.

Model	**Size**	**Consistency**
Danube 2	$2\times1.8\text{B}_{\text{SU}}$	0.69
	$2\times1.8\text{B}_{\text{CRSU}}$	0.83
Danube 2	$4\times1.8\text{B}_{\text{SU}}$	0.61
	$4\times1.8\text{B}_{\text{CRSU}}$	0.76
Danube 2	$8\times1.8\text{B}_{\text{SU}}$	0.54
	$8\times1.8\text{B}_{\text{CRSU}}$	0.70

Table 6: Routing consistency scores for different expert configurations.

and 8-expert configurations, where context representations are clustered accordingly to determine routing parameters. Table 4 demonstrates that expanding from 2 to 4 experts yields meaningful performance improvements in general language tasks. However, further expansion to 8 experts shows diminishing returns, suggesting an optimal balance point in the trade-off between model complexity and performance gains.

5.3.2 Data Efficiency

We analyze the performance trajectories of Danube 2 4×1.8B models using SU and CRSU approaches at four training milestones: 25%, 50%, 75%, and 100%. Table 5 shows that CRSU consistently outperforms SU, with the largest gap (+1.9%) observed at 25% of training. The performance difference gradually decreases to +0.9% at completion.

This pattern indicates that while standard SU eventually learns effective routing patterns, the representation-guided initialization in CRSU provides a better starting point for expert specialization. The clustering-based approach requires fewer training examples to discover meaningful specialization patterns, making it particularly valuable in scenarios with limited training data or computational resources.

5.3.3 Routing Analysis

This section analyzes the routing dynamics of sparsity-crafted models during training and inference.

Model	**Expert**	**Code**	**Math**
Danube 2 $2\times1.8\text{B}_{\text{SU}}$	0	54.1%	47.6%
	1	45.9%	52.4%
Danube 2 $2\times1.8\text{B}_{\text{TRSU}}$	0	40.7%	62.0%
	1	59.3%	38.0%

Table 7: Proportions of tokens assigned to each expert on text data from code and math domains. Values are reported as the average of layers.

Training. To evaluate routing consistency in MoE models developed through SU and CRSU, we analyze four checkpoints: initial state, one-third, two-thirds, and final state of training. We assess model performance on a held-out test set of 1,000 samples. The Jaccard similarity index quantifies routing consistency by measuring the overlap of activated experts for each input token across checkpoints. Table 6 shows that CRSU achieves higher routing consistency than SU across all expert configurations. This indicates that enhanced router initialization promotes stable routing behavior regardless of expert count, enabling more efficient optimization under limited training resources.

Inference. We analyze the routing patterns of models upcycled through TRSU to determine whether representation-based initialization during training leads to task-specific expert specialization. Using the GSM8K (Cobbe et al., 2021) and MBPP (Austin et al., 2021) datasets, we measure expert selection distribution in TRSU models. Table 7 reveals that models with task-based router weights exhibit clear task-specific expert allocation patterns, effectively matching experts to their specialized domains. In contrast, models with random router weight initialization show more uniform expert allocation across tasks, primarily due to the auxiliary load balancing loss constraints.

6 Conclusion

This paper presents representation-based sparse upcycling, an innovative approach for transforming dense language models into efficient sparsely activated architectures. Our method improves upon existing techniques by leveraging task- and context-aware representations to initialize router weights, enabling more effective expert specialization while maintaining computational efficiency. Through comprehensive evaluation in both multi-task and general instruction-following scenarios, we demonstrate consistent performance improvements over conventional sparse upcycling and dense models across diverse benchmarks. The superior routing consistency and task specialization achieved by our approach highlights the importance of informed initialization in sparse architectures and establishes a promising direction for developing more efficient and capable language models. The success of our method suggests that representation-guided routing could be a key component in advancing the development of specialized sparse models, though further theoretical investigation is warranted to fully understand its mechanisms and potential applications.

7 Limitations

While our representation-based sparse upcycling method effectively mitigates performance degradation and shows improvements over dense models, it has notable limitations. The method's heavy reliance on training data sampling may make it infeasible in scenarios with limited high-quality data. Additionally, further theoretical investigation is needed to fully understand the mechanisms behind its effectiveness and establish performance guarantees. These limitations suggest important directions for future research in developing more robust and theoretically grounded sparse architectures.

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A Dataset Details

We show the composition of the multi-task training dataset in Table 8.

B Model Creation Details

Our approach begins with a dense model $\mathcal{M}_d$, which we transform into a mixture-of-experts model $\mathcal{M}_s$ through conventional sparse upcycling. The resulting $\mathcal{M}_s$ contains N experts per Transformer block.

In TRSU, we process a training dataset $\mathcal{D}$ containing multiple tasks $\mathcal{T}_i$. For each task, we measure

OpenOrca	Evol Instruct	OSS Instruct	MetaMathQA
200K	100K	50K	200K

Table 8: The composition of the multi-task training dataset.

instance-level perplexity using $\mathcal{M}_d$ and identify the top 5% of instances exhibiting the highest perplexity scores. For each selected instance $\mathcal{T}_{i,j}$, we calculate layer-wise attention outputs per token from $\mathcal{M}_d$, generating task-specific vector sets. These vectors undergo clustering analysis, with the resulting cluster centroids serving as routing weights for the experts within each Transformer block.

In CRSU, we employ a similar methodology but modify the selection criterion. Rather than task-specific sampling, we randomly select 1% of tokens from the aggregated training dataset. We then perform clustering on the layer-wise attention outputs to form N distinct groups. The centroid of each cluster determines the routing weights for the corresponding expert in each Transformer block.

C Evaluation Details

We evaluate our models across diverse tasks spanning mathematical reasoning, commonsense inference, coding ability, instruction following, and domain-specific knowledge. The evaluation framework is supported by Language Model Evaluation Harness (Gao et al., 2023) and Open Instruct (Wang et al., 2023a). Below are the detailed evaluation protocols for each benchmark:

- **GSM8K:** We evaluate mathematical reasoning abilities using the test set of Grade School Math 8K (Cobbe et al., 2021). Using 8 few-shot examples as demonstrations, we report the exact-match accuracy where both the final answer and solution steps must match the reference.

- **HellaSwag:** We assess commonsense inference capabilities using 10-shot examples. This benchmark tests the model's ability to complete situational narratives with plausible endings, focusing on grounded common sense in specific scenarios.

- **HumanEval:** We test Python code generation capabilities using the HumanEval benchmark (Chen et al., 2021). The evaluation uses 0-shot prompting, where models must generate functionally correct Python code based on docstring descriptions. We report unbiased estimates of pass@k and solutions are sampled with a temperature of 0.8.

- **IFEval:** The ability to follow explicit instructions is evaluated using 0-shot examples. We report instruction-level strict accuracy

- **MATH:** We utilize the MATH benchmark (Hendrycks et al., 2021b) to assess advanced mathematical problem-solving capabilities across various topics including algebra, geometry, and calculus. The evaluation employs 4-shot examples, and we report both the solution accuracy.

- **MBPP:** The Multiple Python Programming Problems (MBPP) benchmark (Austin et al., 2021) is used to evaluate Python programming proficiency. Using 0-shot examples, we assess the model's ability to generate code that passes all provided test cases.

- **MMLU:** We measure the multi-task accuracy with 5-shot examples. The results are reported as the average accuracy across all test instances, covering multiple subjects ranging from STEM fields to humanities.

- **MMLU-Pro:** We evaluate models on an enhanced version of MMLU featuring higher-quality and more challenging questions. The assessment includes 5 few-shot examples as in-context demonstrations, and we report the average accuracy across all subjects.

All evaluations are conducted using standardized prompting templates and scoring criteria to ensure consistency and reproducibility. For tasks requiring code execution or mathematical verification, we employ isolated environments to maintain security and deterministic behavior.