000 001 002 003 MONET: MIXTURE OF MONOSEMANTIC EXPERTS FOR TRANSFORMERS

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ABSTRACT

Understanding the internal computations of large language models (LLMs) is crucial for aligning them with human values and preventing undesirable behaviors like toxic content generation. However, mechanistic interpretability is hindered by *polysemanticity*—where individual neurons respond to multiple, unrelated concepts. While Sparse Autoencoders (SAEs) have attempted to disentangle these features through sparse dictionary learning, they have compromised LLM performance due to reliance on post-hoc reconstruction loss. To address this issue, we introduce MIXTURE OF MONOSEMANTIC EXPERTS FOR TRANSFORM-ERS (MONET) architecture, which incorporates sparse dictionary learning directly into end-to-end Mixture-of-Experts pretraining. Our novel expert decomposition method enables scaling the expert count to 262,144 per layer while total parameters scale proportionally to the square root of the number of experts. Our analyses demonstrate mutual exclusivity of knowledge across experts and showcase the parametric knowledge encapsulated within individual experts. Moreover, MONET allows knowledge manipulation over domains, languages, and toxicity mitigation without degrading general performance. Our pursuit of transparent LLMs highlights the potential of scaling expert counts to enhance mechanistic interpretability and directly resect the internal knowledge to fundamentally adjust model behavior.

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1 INTRODUCTION

031 032 033 034 035 036 As large language models (LLMs) continue to scale and generalize [\(Radford et al., 2019;](#page-13-0) [Brown](#page-10-0) [et al., 2020\)](#page-10-0), understanding their internal computations becomes increasingly imperative. Mechanistic interpretability seeks to unravel how neural networks generate outputs by dissecting their internal processes into human-interpretable components [\(Bereska & Gavves, 2024\)](#page-10-1). Such comprehension is crucial not only for aligning LLMs with human values [\(Ji et al., 2023\)](#page-12-0) but also for preventing undesirable behaviors such as the generation of toxic content [\(Hendrycks et al., 2023\)](#page-12-1).

037 038 039 040 041 042 043 044 045 However, achieving such level of interpretability in LLMs is particularly challenging due to *polysemanticity*—the phenomenon where individual neurons respond to multiple, unrelated concepts [\(Arora et al., 2018;](#page-10-2) [Mu & Andreas,](#page-13-1) [2020;](#page-13-1) [Olah et al., 2020\)](#page-13-2). This arises from the *superposition hypothesis*, which suggests that neural networks represent more features than there are neurons by encoding them in compressed, high-dimensional spaces [\(Elhage](#page-11-0)

Table 1: Comparison of computational cost and memory footprint involved in Mixture-of-Experts architectures. Derivations are specified in [A.2.](#page-17-0)

046 047 048 049 [et al., 2022\)](#page-11-0). To address polysemanticity, observational analyses leveraging sparse representations have been employed. Specifically, techniques like Sparse Autoencoders (SAEs) aim to disentangle these superposed features by learning sparse, overcomplete bases that describe the activation space [\(Sharkey et al., 2022;](#page-13-3) [Bricken et al., 2023;](#page-10-3) [Cunningham et al., 2024\)](#page-11-1).

050 051 052 053 Despite advancements using SAEs, significant limitations persist: (1) Post-hoc reconstruction loss: Functional importance of LLM's features are likely to be diminished during SAE's post-hoc training, stemming from its training set being disjoint from the LLM's corpus, rendering out-of-distribution issues difficult to diagnose [\(Bricken et al., 2023;](#page-10-3) [Braun et al., 2024\)](#page-10-4). Such deviation is further exacerbated as nonzero reconstruction error cascades through the LLM's hidden representations [\(Gurnee,](#page-11-2) **054 055 056 057 058 059** [2024\)](#page-11-2). (2) **Manipulability and performance trade-offs**: While attempts have been made to steer LLMs based on learned dictionary features [\(Marks et al., 2024;](#page-13-4) [Templeton, 2024\)](#page-14-0), discussions on the manipulability of SAEs often overlook their impact on the model's general performance across other tasks. Particularly in open-ended generation tasks, the effects of feature control using SAEs remain largely unknown. These limitations highlight the necessity for alternative methods that can observe LLMs' internal processes while preserving their original capabilities.

060 061 062 063 064 065 066 067 068 069 070 071 072 073 In light of these challenges in post-hoc interpretation, methods encoding interpretable weights in LLM during pretraining have been introduced [\(Tamkin et al., 2023;](#page-14-1) [Hewitt et al., 2023\)](#page-12-2). Among those prior approaches, integrating sparse dictionary learning with Mixture-of-Experts (MoE) architectures is considered promising as experts' specialization is linked with monosemanticity [\(Gao](#page-11-3) [et al., 2024;](#page-11-3) [Fedus et al., 2022a;](#page-11-4)[b\)](#page-11-5). However, conventional MoE architectures face several problems: (1) Limited number of experts: Most sparse LLMs employ a limited number of experts [\(Lepikhin](#page-12-3) [et al., 2021;](#page-12-3) [Fedus et al., 2022b;](#page-11-5) [Jiang et al., 2024\)](#page-12-4), leading to knowledge hybridity where each expert covers diverse and unrelated concepts [\(Dai et al., 2024\)](#page-11-6), failing to fulfill the superposition hypothesis necessary for monosemanticity. (2) Confinement to specific layers: Attempts to scale the number of experts [\(dos Santos et al., 2024;](#page-11-7) [He, 2024\)](#page-12-5) have been confined to specific layers within the LLM, rendering knowledge distributed in other parts of the network [\(Dai et al., 2022;](#page-11-8) [Geva et al.,](#page-11-9) [2021\)](#page-11-9) inaccessible. (3) **Inefficient parameter scaling**: Recently proposed architectures aiming to scale the number of experts [\(He, 2024;](#page-12-5) [Oldfield et al., 2024\)](#page-13-5) suffer from linearly increasing total parameters, limiting the scalability of the LLM.

074 075 076 077 078 To overcome these limitations, we introduce MIXTURE OF MONOSEMANTIC EXPERTS FOR TRANSFORMERS (MONET) architecture, enabling effective specialization of experts to facilitate mechanistic interpretability in LLMs. MONET aims for transparent language modeling by significantly increasing the number of experts to 262K at every layer and integrating sparse dictionary learning within end-to-end Mixture-of-Experts training. Our main contributions are as follows:

- Parameter-efficient architecture with increased number of experts: By utilizing a novel expert decomposition method, MONET addresses memory constraints, ensuring that the total number of parameters scales proportionally to the square root of the number of experts.
- Mechanistic interpretability via monosemantic experts: MONET facilitates mechanistic interpretability by enabling observations of fine-grained experts' routing patterns. Our analyses confirm mutual exclusivity of knowledge between groups of experts, while qualitative examples demonstrate individual experts' parametric knowledge.
	- Robust knowledge manipulation without performance trade-offs: MONET allows for end-to-end training that extends to robust knowledge manipulation during inference. Without degrading performance, it provides effortless control over knowledge domains, languages, and toxicity mitigation.

2 PRELIMINARIES

Sparse Mixture-of-Experts (SMoE) SMoE models efficiently scale their capacity by activating only a subset of the experts, thereby reducing computational costs. These models leverage expert embeddings to determine which experts to activate. Given a hidden representation vector $x \in \mathbb{R}^d$ and a set of N expert networks $\{E_i\}_{i=1}^N$, each expert is defined as:

$$
E_i(x) = V_i \sigma(U_i x) \tag{1}
$$

where $U_i \in \mathbb{R}^{m \times d}$ and $V_i \in \mathbb{R}^{d \times m}$ are the weight matrices of the *i*-th expert, and σ is an activation function such as ReLU or GELU. Let $\{w_i\}_{i=1}^N \subset \mathbb{R}^d$ be the expert embeddings and \mathcal{T}_k denote the top- k operation. The output of the SMoE layer is then computed as:

$$
SMOE(x) = \sum_{i \in \mathcal{K}} g_i E_i(x)
$$
 (2)

where $K = \mathcal{T}_k(\{w_i^T x\}_{i=1}^N)$ is the set of indices corresponding to the sparsely activated top-k experts, based on their routing scores $g = \text{softmax}(\{w_i^T x\}_{i \in \mathcal{K}})$.

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122 123 124 125 126 Figure 1: Architectural comparison of expert scaling approaches in large language models. (1) PEER stores N standalone experts accessed via product key retrieval, resulting in memory usage that grows linearly with the number of experts, $O(N)$. (2) Our proposed **MONET-HD** (Horizontal Decomposition) partitions experts into bottom and top layers, dynamically composing experts. This reduces space complexity to $O(\sqrt{N})$. (3) **MONET-VD** (Vertical Decomposition) orthogonally partitions layers with left and right segments, while maintaining the same space complexity.

128 129 130 131 132 The Parameter Efficient Expert Retrieval (PEER) Compared to other SMoE architectures, PEER processes a substantially higher number of experts by employing a computationally efficient routing mechanism. Based on the product key algorithm introduced by [Lample et al.](#page-12-6) [\(2019\)](#page-12-6), PEER implements the product key retrieval mechanism that enables efficient search of top- k experts, remplements the product key retrieval mechanism that enables effici-
ducing computational complexity from $O(Nd)$ to $O((\sqrt{N} + k^2)d)$.

133 134 135 136 137 Specifically, each PEER expert is a minimal MLP (multilayer perceptron) consisting of an input layer, a single hidden neuron, and an output layer. PEER uses two independent product keys, which are expert embeddings, $\{w_{hi}^1\}_{i=1}^{N} \subset \mathbb{R}^{d/2}$ and $\{w_{hj}^2\}_{j=1}^{N} \subset \mathbb{R}^{d/2}$ for each head h, rather than retrieving the experts among N embeddings. The hidden state x is correspondingly split into two halves, $x^1, x^2 \in \mathbb{R}^{d/2}$, and the top-k experts are obtained by:

$$
\mathcal{K}_h^1 = \mathcal{T}_k(\{(w_{hi}^1)^T x^1\}_{i=1}^{\sqrt{N}}) \quad \text{and} \quad \mathcal{K}_h^2 = \mathcal{T}_k(\{(w_{hj}^2)^T x^2\}_{j=1}^{\sqrt{N}}). \tag{3}
$$

Then, top-k experts are selected from the scores computed over the Cartesian product $\mathcal{K}_h^1 \times \mathcal{K}_h^2$, to constitute \mathcal{K}_h , i.e.,

$$
\mathcal{K}_h = \mathcal{T}_k(\{(w_{hi}^1)^T x^1 + (w_{hj}^2)^T x^2 : (i,j) \in \mathcal{K}_h^1 \times \mathcal{K}_h^2\}),\tag{4}
$$

with $g_h = \text{softmax}(\{(w_{hi}^1)^T x^1 + (w_{hj}^2)^T x^2 : (i,j) \in \mathcal{K}_h\})$ being routing scores of the experts. Following the format of Equation [1,](#page-1-0) let $E_{ij}(x)$ be the (i, j) th expert network and $u_{ij}, v_{ij} \in \mathbb{R}^d$ be weights of the expert MLPs. The PEER layer is then formulated as:

$$
PEER(x) = \sum_{h=1}^{H} \sum_{(i,j) \in \mathcal{K}_h} g_{hij} E_{ij}(x) = \sum_{h=1}^{H} \sum_{(i,j) \in \mathcal{K}_h} g_{hij} v_{ij} \sigma(u_{ij}^T x).
$$
 (5)

152 153 154 155 156 Although PEER reduces the computational complexity by a factor of \sqrt{N} , it suffers from memory bottleneck as the total number of parameters grows with expert count N . Consider a model with dimension $d = 2048$ and 8 attention heads – scaling to 1 million experts would require 4.3 billion parameters per layer. Therefore, building an LLM with 1.3 billion active parameters would necessitate an additional 103 billion parameters just for the experts.

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3 MONET: MIXTURE OF MONOSEMANTIC EXPERTS FOR TRANSFORMERS

159 160 161 To disentangle superposed features in LLM by incorporating sparse dictionary learning into end-toend SMoE pretraining, we aim to maximize the number of experts. Instead of searching through a large pool of standalone experts using product key retrieval, we propose **product key composition** of experts by sharding layers in individual experts to overcome PEER's memory constraints. Our **162 163 164 165** orthogonal layer partitioning methods, horizontal and vertical decompositions, address the memory bottleneck by scaling the number of experts while keeping parameter growth proportional to the square root of the expert count.

166 167 168 169 170 Horizontal Expert Decomposition (HD) Our first approach to product key composition fundamentally redefines how expert networks are constructed. Instead of maintaining complete expert networks as defined in Equations [1](#page-1-0) and [5,](#page-2-0) we decompose each expert into two complementary components: bottom and top linear layers. Such partitioning scheme allows us to build experts dynamically during inference by combining these components.

171 172 173 174 175 176 Specifically, we partition the weights of experts into two distinct groups corresponding to the bottom and top layers: $\{U_i\}_{i=1}^{\sqrt{N}}\subset\mathbb{R}^{m\times d}$ and $\{V_j\}_{j=1}^{\sqrt{N}}\subset\mathbb{R}^{d\times m}$ respectively, where m represents the expert hidden dimension (e.g., $m = 1$ for PEER). To accommodate architectures with bias terms [\(Shen](#page-13-6) [et al., 2024\)](#page-13-6), we include $\{b_i^1\}_{i=1}^{\sqrt{N}} \subset \mathbb{R}^m$ and $\{b_j^2\}_{j=1}^{\sqrt{N}} \subset \mathbb{R}^d$ in our formulation. The composed expert network can then be expressed as:

$$
E_{ij}(x) = V_j \sigma (U_i x + b_i^1) + b_j^2,
$$
\n(6)

178 179 where (i, j) -th expert is formed by combining the *i*-th bottom layer with the *j*-th top layer.

180 181 182 183 184 As illustrated in Figure [1,](#page-2-1) this decomposition enables constructing N unique experts using only S inustrated in Figure 1, this decomposition enables constructing *N* unique experts using only \overline{N} weight choices from each group ($0 \le i, j < \sqrt{N}$). Unlike PEER, which searches for top-*k* experts among k^2 candidates, we directly use the Cartesian product $\mathcal{K}_h = \mathcal{K}_h^1 \times \mathcal{K}_h^2$, which breaks down joint (i, j) pairs into independent i and j selections. The resulting SMoE layer with horizontal decomposition is defined as:

$$
MoHDE(x) = \sum_{h=1}^{H} \sum_{(i,j)\in\mathcal{K}_h} g_{hij} E_{ij}(x)
$$
\n⁽⁷⁾

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$$
= \sum_{h=1} \sum_{i \in \mathcal{K}_h^1} \sum_{j \in \mathcal{K}_h^2} g_{hi}^1 g_{hj}^2 \left(V_j \sigma (U_i x + b_i^1) + b_j^2 \right) \tag{8}
$$

191 192 193 where $g_h^1 = \text{softmax}(\{(w_{hi}^1)^T x^1\}_{i \in \mathcal{K}_h^1})$ and $g_h^2 = \text{softmax}(\{(w_{hj}^2)^T x^2\}_{j \in \mathcal{K}_h^2})$ are computed independently for each group, with their product $g_{hij} = g_{hij}^1 g_{hj}^2$ determining the expert's routing score.

194 195 196 197 198 199 To optimize computation across tokens with our decomposed expert structure, we address a key challenge: sparse activations varying by token complicate efficient computation reorganization. While traditional SMoE models employ expert parallelism [\(Fedus et al., 2022b;](#page-11-5) [Du et al., 2022\)](#page-11-10), such strategies become impractical with our 262K composed experts. Following [Pan et al.](#page-13-7) [\(2024\)](#page-13-7); [Puigcerver et al.](#page-13-8) [\(2023\)](#page-13-8), we adopt dense routing to enable precomputation of overlapped layer operations by extending sparse routing scores to all experts:

$$
\hat{g}_{hi}^1 = \begin{cases} g_{hi}^1 & \text{if } i \in \mathcal{K}_h^1 \\ 0 & \text{otherwise} \end{cases} \quad \text{and} \quad \hat{g}_{hj}^2 = \begin{cases} g_{hj}^2 & \text{if } j \in \mathcal{K}_h^2 \\ 0 & \text{otherwise} \end{cases} . \tag{9}
$$

This allows us to reorganize Equation [8](#page-3-0) into a more computationally efficient form:

$$
MoHDE(x) = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} \left(V_{j} \sigma (U_{i}x + b_{i}^{1}) + b_{j}^{2} \right)
$$
(10)

$$
= \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 V_j \sigma(U_i x + b_i^1) + \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 b_j^2
$$
(11)

$$
= \sum_{j=1}^{\sqrt{N}} V_j \sum_{h=1}^{H} \hat{g}_{hj}^2 \sum_{i=1}^{\sqrt{N}} \hat{g}_{hi}^1 \sigma(U_i x + b_i^1) + \sum_{j=1}^{\sqrt{N}} b_j^2 \sum_{h=1}^{H} \hat{g}_{hj}^2.
$$
 (12)

213 214 215 $j=1$ $j=1$ By strategically reordering the summations in Equation [12,](#page-3-1) we can precompute memory-intensive operations before and after the expert routing phase. We provide implementation details in Algorithm [1](#page-18-0) of Appendix [A.3.](#page-18-1)

216 217 218 219 220 221 Vertical Expert Decomposition (VD) As an orthogonal approach to horizontal decomposition, we propose vertical decomposition that partitions each expert network along the vertical dimension into left and right segments. Let $U_i^1, U_j^2 \in \mathbb{R}^{m/2 \times d}$ and $V_i^{11}, V_i^{12}, V_j^{21}, V_j^{22} \in \mathbb{R}^{d/2 \times m/2}$ represent the vertically splitted weights for the experts, and $b_i^{11}, b_j^{21} \in \mathbb{R}^{m/2}$ and $b_i^{12}, b_j^{22} \in \mathbb{R}^{d/2}$ denote the split biases. For the vertically decomposed experts, the expert network is defined as:

$$
E_{ij}(x) = \begin{bmatrix} V_{i1}^{11} & V_{i2}^{12} \\ V_{j1}^{21} & V_{j2}^{22} \end{bmatrix} \sigma \left(\begin{bmatrix} U_{i1}^{1} \\ U_{j2}^{2} \end{bmatrix} x + \begin{bmatrix} b_{i1}^{11} \\ b_{j1}^{21} \end{bmatrix} \right) + \begin{bmatrix} b_{i2}^{12} \\ b_{j2}^{22} \end{bmatrix},
$$
\n(13)

and the expert layer is obtained as:

=

$$
\text{MoVDE}(x) = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 \left(\begin{bmatrix} V_i^{11} & V_i^{12} \\ V_j^{21} & V_j^{22} \end{bmatrix} \sigma \left(\begin{bmatrix} U_i^1 \\ U_j^2 \end{bmatrix} x + \begin{bmatrix} b_i^{11} \\ b_j^{21} \end{bmatrix} \right) + \begin{bmatrix} b_i^{12} \\ b_j^{22} \end{bmatrix} \right)
$$
(14)

$$
= \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 \left[\frac{V_i^{11} \sigma (U_i^1 x + b_i^{11}) + V_i^{12} \sigma (U_j^2 x + b_j^{21}) + b_i^{12}}{V_j^{21} \sigma (U_i^1 x + b_i^{11})} + \frac{V_j^{12} \sigma (U_j^2 x + b_j^{21}) + b_j^{22}}{V_j^{22} \sigma (U_j^2 x + b_j^{21})} + \frac{b_j^{22}}{V_j^{22}} \right].
$$
 (15)

We divide the layer calculation into six terms (see Equation [15\)](#page-4-0), with the complete derivation presented in Appendix [A.1.](#page-16-0) The overall computational cost is equivalent to horizontal decomposition, and the implementation details are provided in Algorithm [2](#page-18-2) of Appendix [A.3.](#page-18-1)

236 Adaptive Routing with Batch Normalization To avoid the hardware inefficiency of top- k sorting, we use Batch Normalization to estimate expert routing quantiles without performing top- k . Inspired by BatchTopK [\(Bussmann et al., 2024\)](#page-10-5), which enhances reconstruction in SAE, we apply batch-level quantile estimation for more accurate routing. Batch Normalization automatically gathers router logit statistics, which are used during inference. This method reduces training time while maintaining performance.

242 243 244 245 246 247 Load Balancing Loss Load balancing loss is crucial in MoE models to promote uniform expert routing, improving expert utilization and ensuring efficient parallelism when experts are distributed across devices. While sparse routing mechanisms are widely used, some dense MoE models adopt entropy-based losses [\(Pan et al., 2024;](#page-13-7) [Shen et al., 2023\)](#page-13-9) since dense routing does not directly track expert selection frequencies. In a similar vein, we introduce an alternative uniformity loss, formulated as the KL divergence between a uniform distribution and the routing probabilities:

$$
\mathcal{L}_{\text{unif}} = -\frac{1}{2H\sqrt{N}} \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \log \hat{g}_{hi}^1 - \frac{1}{2H\sqrt{N}} \sum_{h=1}^{H} \sum_{j=1}^{\sqrt{N}} \log \hat{g}_{hj}^2.
$$
 (16)

Additionally, we introduce an ambiguity loss that measures the degree of expert specialization for each token:

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$$
\mathcal{L}_{\text{amb}} = -\frac{1}{2H} \sum_{h=1}^{H} \left(1 - \max g_h^1 \right) - \frac{1}{2H} \sum_{h=1}^{H} \left(1 - \max g_h^2 \right). \tag{17}
$$

This loss encourages the model to assign each token to a specific expert with high confidence. By minimizing this ambiguity loss, the model promotes expert specialization, resulting in more distinct and interpretable expert roles. Ablations study on load balancing loss is presented in Appendix [C.1.](#page-20-0) Let \mathcal{L}_{LM} be a language modeling loss and λ be a hyperparameter. The final training objective is:

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$$
\mathcal{L} = \mathcal{L}_{LM} + \lambda \mathcal{L}_{unif} + \lambda \mathcal{L}_{amb}.
$$
 (18)

4 EXPERIMENTS

4.1 MODEL SETUPS

265 266 267 268 269 In order to assess practical applicability and scalability of MONET, we vary model parameter sizes ranging from 850 million to 4.1 billion and CODEMONET at 1.4 billion parameters. In addition, we train models using the LLAMA architecture for fair comparison. All models are pretrained on large-scale datasets, and we further fine-tune MONET-1.4B for instruction-following MONET-1.4B CHAT for automated interpretation framework. For detailed pretraining configurations and instruction tuning methods, refer to Appendix [B.](#page-18-3)

Table 2: Evaluation of models on open-ended LLM benchmarks in 0-shot and 5-shot settings. Our proposed MONET (horizontal and vertical decompositions) and the LLAMA architecture results are based on consistent pretraining hyperparameters for a fair comparison. Benchmarks include WG (WinoGrande), OBQA (OpenBookQA), HS (HellaSwag), and CSQA (CommonsenseQA). Off-theshelf pretrained OLMoE and Gemma 2 with Gemma Scopes are evaluated for comparison. Tokens column indicates pretraining tokens count in billions, where numbers in the parenthesis are post-hoc training tokens used for SAEs. Comparisons account for total parameter sizes across models.

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4.2 OPEN-ENDED BENCHMARK RESULTS

303 304 305 306 307 308 309 310 Empirical evaluations in Table [2](#page-5-0) show that MONET maintains competitive performance with total parameter-matched dense LLMs across a range of language modeling benchmarks. On the other hand, SAEs fall short in maintaining model stability, where reconstruction errors lead to instability and reduced performance in open-ended tasks, compromising the model's overall reliability in knowledge control. We evaluate Gemma 2 2B [\(Team et al., 2024\)](#page-14-2) using Gemma Scope [\(Lieberum](#page-12-7) [et al., 2024\)](#page-12-7), a collection of SAEs trained on Gemma 2 models. Specifically, we employ the available SAEs with 65K sparse features–both those reconstructing the LLM's MLP output and those reconstructing residual layers–and evaluate their performance on open-ended benchmarks.

311 312 313 314 315 316 317 318 The scalability of MONET is evident across all three parameter scales (850M, 1.4B, and 4.1B). As the number of parameters increases, the model exhibits a consistent upward trend in performance across both 0-shot and 5-shot settings. This confirms that the scaling laws typically observed in dense models still apply to MONET's sparse architecture, further reinforcing its scalability and practical applicability for large-scale LLM deployments. In terms of the decomposition design choice, vertical decomposition (VD) shows superior performance over horizontal decomposition (HD). As shown in Table [2,](#page-5-0) MONET-VD consistently outperforms MONET-HD across multiple benchmarks and parameter scales, particularly in the 850M, 1.4B, and 4.1B models.

319 320 4.3 QUALITATIVE RESULTS

321 322 323 In this section, we present qualitative analyses demonstrating the monosemantic specialization of individual experts in our MONET architecture. In Figure [2,](#page-6-0) we visualize the routing scores allocated to the experts in our language models on the C4 [\(Raffel et al., 2020\)](#page-13-10) and StarCoder subset. We include comprehensive examples illustrating the internal workings of models with varying sizes (MONET-1.4B, MONET-4.1B) and a model pretrained on code (CODEMONET).

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                             Water (48.20%) (...) <s> The San Diego County Water Authority on Wed (...)
Water (45.41%) (...) \nThe San Diego County Water Authority, supp (...)
                             EXECUTE 10.3 THE SAID LIGHT COULT WATER AND THE SAID (CAST) (2.3 Apr (40.38%) (...) Of quality out of the Bay area is a positive (...)<br>Water (40.38%) (...) County of El Paso Water and other community st (...)<br>Water 
                             Bay (39.34%) (...) included local innovators from Bay Area Industry, (...)<br>
Ray (38.34%) (...) included local innovators from Bay Area Industry, (...)<br>
Water (38.17%) (...) supply by the Portland Water Bureau, t
                             Water (37.97%) (...) supply by the Fortianu water bureau, the park of Bay(37.87%) (...) FIU), South Florida Water Management District, Bay (37.87%) (...) and culture here in the Bay Area all month! (...)
                                                                                                                                                                                                  Bayesian – MONET-1.4B / Group 4 / Expert 54,136
                                                                                                                                                                                     Bay (64.28%) \begin{pmatrix} ... \\ ... \end{pmatrix} of the technical application of Bayesian. Downloadable (...) Bay (58.58%) \begin{pmatrix} ... \\ ... \end{pmatrix} algorithm that, using a Bayesian approach, a (...)
                                                                                                                                                                                     Bay (58.24%) (...) a govining rules, Bayes Theorem, distribution (...)<br>
Bay (56.43%) (...) together. We develop a Bayesian hierarchical (...)<br>
Bay (54.03%) (...), order statistics, and Bayesian statistics. Pr (...)
                                                                                                                                                                                    Bay (54.03%) (...) in equals the according approach is referred (...)<br>Bay (53.39%) (...) irable. What in a Bayesian approach is referred (...)<br>Bay (53.39%) (...) irable. What in a Bayesian approach is referred (...)<br>hav (
                                                                                                                                                                                     bay (52.46%) (...) naive. what in a bayestan approach is referred<br>Bay (50.24%) (...) est neighbour, naive bayes, decision trees (...)<br>Bay (50.24%) (...) arns, R. Bayesian, relational (...)
                                                                                                                                                                                     Bay (47.21%) (...) exchange rates with a large Bayesian VAR ((...)<br>Bay (47.12%) (...) division of statistical inference along Bayesian-frequent (...)
                                 Electromagnetism – MONET-4.1B / Group 5 / Expert 81,396
                             well (95.27\%) (...) article calls the "Maxwell–Farad (...)<br>stein (93.59\%) (...) omena \nEinstein noticed that the two
                              stein (93.59%) (...) omena. \nEinstein noticed that the two (...)<br>well (91.79%) (...) of equations known as Maxwell's equation
                            well (91.79\%) (...) of equations known as Maxwell's equations. (...)<br>stein (91.79\%) (...) 9.\n\pi Einstein, A. (...)
                             stein (91.79%) (...) 9.\n\pi^6 Einstein, A. ((...)<br>well (89.39%) (...) s version (see Maxwell-<br>s (89.17%) (...) known as Maxwell's eq
                               well (89.39%) (...) s version (see Maxwell–Farad (...)<br>
s (89.17%) (...) known as Maxwell's equations.\nIn (...)
                              well (88.34\%) (...) one of the four Maxwell's equations, (...)<br>well (87.54\%) (...) differential form of the Maxwell–Farad
                             well (87.54%) (...) differential form of the Maxwell–Farad (...)<br>stein (76.97%) (...) quantum mechanics). Einstein is best known
                                                             \dots) quantum mechanics). Einstein is best known in \dots)
                                                                                                                                                                                    String Data Type – CODEMONET-1.4B / Group 4 / Expert 52,338
                                                                                                                                                                                             Z (36.12%) \Big| (...) ([-a-zA-Z]+)\\s+(\ (...)<br>Z (35.22%) \Big| (...) '[^a-zA-Z0-9\.-(...)
                                                                                                                                                                                     Z(35.22\%) (...) '[^a-zA-Z0-9\...(...)<br>String (32.52%) (...) '[^a-zA-Z0-9\...(...)
                                                                                                                                                                                    String (32.52%) (...) ::GetFilterByName(String(sFilterName)); (...)<br>
String (27.79%) (...) aMsg += ByteString(String(sAllFilterName 0 (26.54%) (...) String regex = "['0-9]*[q (...)
                                                                                                                                                                                                                         (...) aMsg += ByteString( String( sAllFilterName (...)
                                                                                                                                                                                             0 (26.54%) (...) String regex = "[^0-9]*[q (...)<br>& (26.22%) (...) XElementAnalogClock&)info
                                                                                                                                                                                         \& (26.22%) (...) XElementAnalogClock&info).m<sub>=</sub>(...)<br>Pair (26.19%) (...) Sequence< StringPair > aFilters((...)
                                                                                                                                                                                              ir (26.19\%) (...) Sequence \text{StringPair} > \text{aFilters} (...)<br>z (25.02\%) (...) (1-a-zA-z0.9 \setminus \dots)\mathbf{z} (25.02%) (...) ([-a-zA-z0-9 \\ (...)<br>
\mathbf{z} (24.88%) (...) )?[a-zA-Z]?(\s) (...)
                                  Cartilage – MONET-1.4B CHAT / Group 1 / Expert 232,717
                             age (104.00%) (...) ftening of articular cartilage; frequently old wrongly (...) age (100.48%) (...) matrix. The articular cartilage function is dependent (...) age (100.07%) (...) mortant part of rebuilding cartilage or 
                               age (88.07\%) (...) connective tissues, cartilage has a very slow turnover (...)
                               age (87.32\%) (...) ous ossification of cartilage tissue of the epi (...)
                                                               Descriptions of Expert 232,717
                        • A thin, flexible, and protective membrane that surrounds and protects living
                              tissues and organs.
                         • A thin, transparent, and protective membrane or layer that covers or lines a
                               surface or organ of the body.
                        • A thin, flexible, and often gelatinous substance that provides structure and
                              support to living cells and tissues.
                        • A tough, fibrous, and elastic substance that forms the outer layer of cells in
                              animals, plants, and fungi.
                                                                                                                                                                                               Expertise – MONET-1.4B CHAT / Group 4 / Expert 51
                                                                                                                                                                                         pert (35.02%) (...) by natural causes. \n\frac{\text{Perf}}{\text{Set}} A dedicated and intern (...) ist (27.90%) (...) Scientist reported that elgood (...)
                                                                                                                                                                                     per (35.09%) \binom{1.0}{6} is (27.90%) \binom{1.0}{6} is (37.90%) \binom{1.0}{6} is (27.90%) \binom{1.0}{6} is (27.90%) \binom{1.0}{6} is (27.90%) \binom{1.0}{6} for his historical scholarship, including recognition (...) pert (26.3
                                                                                                                                                                                          pert (24.04%) (...) in two weeks.\n– Experise: Tead of the science (...)<br>pert (23.28%) (...) ushinski.\n– Expertise: Iraqi nuclear scient (...)<br>pert (23.12%) (...) yet been determined.\n– Expertise: Biological warfare (..
                                                                                                                                                                                                                             Descriptions of Expert 51
                                                                                                                                                                                    • A person who has a particular skill or talent, especially one that is consid-
                                                                                                                                                                                          ered valuable or desirable.
                                                                                                                                                                                     • One who has been selected or appointed to perform a specific task or role.
                                                                                                                                                                                     • A person who is skilled in the art of writing or speaking in a particular
                                                                                                                                                                                          language or style.
                                                                                                                                                                                     • A person who is a member of a group or organization, especially one that
                                                                                                                                                                                          is recognized by the law or has a high level of authority.
                                                                                                                                                                                    • A person who has the ability to perform a specific action or set of actions.
```
Figure 2: Activated tokens for experts in LLMs (MONET-1.4B, MONET-4.1B) on C4 validation dataset. CODEMONET-1.4B's examples were collected from the StarCoder dataset. Tokens are sorted according to the expert's routing score (or g_{hij} in Eq. [7\)](#page-3-2), notated in parenthesis. Descriptions in bottom rows are self-explained experts, generated from the automated interpretation framework.

362 Parametric Knowledge In MONET, feedforward MLP in each decoder block is decomposed into 262,144 experts, a design considered highly granular by the standard of [Ludziejewski et al.](#page-12-8) [\(2024\)](#page-12-8). As shown in Figure [2,](#page-6-0) such fine-grained experts specialize in concepts such as chemical compounds (Expert 147,040) or states in the U.S. (Expert 73,329). An expert activates to vocabularies associated with similar concepts, like physicists in a field of electromagnetism (Expert 81,396).

365 366 367 368 369 370 371 Expert Monosemanticity Our experts exhibit monosemanticity by specializing in concepts presented across different contexts and languages, demonstrating that they recognize based on contextual and domain knowledge rather than relying solely on vocabulary cues. For instance, both Expert 48,936 and Expert 54,136 in Figure [2](#page-6-0) respond to the term "Bay", where one relates it to a geographical area (e.g.,"Bay Area"), and the other connects it to a mathematical concept (e.g., "Bayesian"). Similarly, despite the appearance of the same concept across various programming languages, CODEMONET consistently maps string-related knowledge to Expert 52,338.

372 373 374 375 376 377 Self-explained Experts We have adapted automated interpretation framework that generates the description based on the hidden states in LLMs [\(Chen et al., 2024;](#page-10-6) [Ghandeharioun et al., 2024;](#page-11-11) [Kharlapenko et al., 2024\)](#page-12-9), to interpret individual experts as shown in Figure [2.](#page-6-0) The following prompt is given to the MONET-1.4B CHAT: "Q: What is the meaning of the word X ? A: Sure! The meaning of the word X is ", where X serves as a placeholder for averaged token embeddings activated to the targeted expert. Without relying on external LLMs, our MONET-1.4B CHAT generates a description for its experts, like explaining the Expert 232,717 as "Cartilage" and the Expert 51 as "Expertise".

410 411 412 413 414 415 Figure 3: Knowledge unlearning and accuracy perturbation across 14 MMLU domains. Rows represent the domains where knowledge unlearning was applied, while columns display the resulting performance of the LLM in each domain. In (a) MONET (Ours), experts that show skewed routing scores for the target domain were removed. In (b) Gemma Scope, sparse SAE features for the target domain were suppressed. In (c) OLMoE, the most activated expert per domain was removed. In (d) LLAMA, domain-specific MLP neurons were suppressed based on first-layer activations. Bright pixels indicate minimal accuracy loss, while darker pixels represent a greater drop.

5 ANALYSES

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419 420 421 422 423 Leveraging transparent observations of expert routing patterns in each layer of the MONET, we employ observational methods for knowledge editing. In particular, we explored the effects of knowledge unlearning by selectively removing experts based on their routing score, g_{hij} in Equation [7.](#page-3-2) Our unlearning analyses highlight MONET's monosemanticity where experts encapsulate disentangled parametric knowledge across domains, programming languages, and toxicity.

425 5.1 DOMAIN MASKING

426 427 428 429 430 431 Using the MMLU Pro [\(Wang et al., 2024\)](#page-14-3) benchmark taxonomy, which divides question-answer sets into 14 distinct domains, we investigated the effects of domain-specific knowledge unlearning on MMLU [\(Hendrycks et al., 2021\)](#page-12-10). For each expert, if the routing probability for a particular domain was at least twice as high as for the second most activated domain, we labeled that expert as specialized in that domain. After assigning experts to domains, we selectively deleted the experts and evaluated the impact of knowledge unlearning across all 14 domains. The details of the expert deletion process and its impact across the 14 domains are provided in Appendix [D.1.](#page-21-0)

442 443 444 445 446 Table 3: Knowledge unlearning and pass@100 metric changes across programming languages in the MULTIPL-E benchmark. In this evaluation, experts assigned to the target language are deleted, while others are preserved. Columns represent the independent variable where the masking is applied on. The Δ Target row represent the delta in pass@100 performance of the MONET model following expert removal for the specified language. The Δ Others row shows the average pass@100 performance change of the others. Dark pixels indicate high sensitivity to the expert purging.

447 448

449 450 451 452 453 454 455 Figure [3](#page-7-0) demonstrates that MONET's knowledge unlearning primarily affects the targeted domain while preserving the performance of the other domains. We compared our approach with three baseline methods: Gemma 2 LLM with Gemma Scope, which utilizes 262K sparse SAE features matching MONET's expert count; OLMoE [\(Muennighoff et al., 2024\)](#page-13-11), a standard MoE architecture with 1.3B active and 6.9B total parameters; and LLAMA 1.3B with GELU activation, sized equivalently to MONET, where we leverage MLP layers for knowledge identification inspired by [Meng](#page-13-12) [et al.](#page-13-12) [\(2022\)](#page-13-12). Using domain-specific assignment criteria–SAE logit values for Gemma Scope and first-layer MLP outputs for LLAMA–we performed knowledge unlearning across all methods.

456 457 458 459 460 461 462 463 464 465 466 The results demonstrate MONET's superior performance in domain-specific knowledge manipulation compared to baseline approaches. While MONET achieves precise knowledge unlearning within targeted domains, Gemma Scope suffers from broader performance degradation due to incomplete reconstruction through the SAE layer. Both OLMoE and LLAMA face fundamental limitations from feature polysemanticity. In OLMoE, there were no specialized experts in any domains in MMLU, based on our criteria of skewness in expert routing score. OLMoE's experts' routing score was evenly distributed, making it difficult to detect specialized experts. We leveraged criteria of occurrences in maximum activation to determine the expert's domain specialization. In contrast, LLAMA displays an average 6% of neurons to be specialized in each domain compared to MONET's 2.2%, suggesting possible feature entanglement and resulting in significant performance degradation across unrelated domains during knowledge removal.

467 5.2 MULTILINGUAL MASKING

468 469 470 471 472 473 474 475 476 In addition to domain masking, we performed a similar evaluation of programming language masking using CODEMONET 1.4B. Again, we utilized the skewness in routing scores to identify language-specific experts. Table [3](#page-8-0) summarizes the changes in pass@100 performance metrics after expert purging evaluated on MULTIPL-E benchmark [\(Cassano et al., 2023\)](#page-10-7). For the targeted languages, pass $@100$ scores dropped by as much as $-30\%p$, while average performance for other languages remained relatively stable, with only minor declines ranging from -0.6% to -1.8%p. CODE-MONET's generation examples before and after the expert purging can be found in Figure [4](#page-22-0) of Appendix [D.2.](#page-21-1) All metrics were evaluated using a temperature of 0.8 and 200 sample generations, where its full performance are available in Table [15](#page-27-0) of the Appendix [E.](#page-26-0)

477 478 5.3 TOXIC EXPERT PURGING

479 480 481 482 483 484 To fundamentally adjust model behavior for safer language generation, we propose a method for purging toxic experts from the model. This approach directly targets and removes experts associated with toxicity, resecting the harmful knowledge while preserving the overall performance of the LLM. We evaluate this method on two well-established toxicity benchmarks: REALTOXICI-TYPROMPTS [\(Gehman et al., 2020\)](#page-11-12) and ToxiGen [\(Hartvigsen et al., 2022\)](#page-11-13), to assess its impact on toxicity reduction.

485 For toxicity evaluation, we utilize the PERSPECTIVE API [\(Lees et al., 2022\)](#page-12-11) for REALTOXICI-TYPROMPTS and the ToxiGen RoBERTa model for the ToxiGen benchmark, both designed to mea-

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494 495 496 Table 4: Changes in REALTOXICITYPROMPTS toxicity metrics according to the expert purging. Lower threshold indicate stricter criteria to filter out more experts. Each columns indicate masking threshold, expert masking ratio, toxicity probability, and average performance (helpfulness) measured in 8 open-ended LLM benchmarks. Specifics of the helpfulness can be found in Appendix [E.](#page-26-0)

497 498 499 500 501 502 sure the generation of toxic content. To identify toxic knowledge within the model, we collected expert routing scores alongside toxicity scores, and computed Pearson correlations. A higher correlation indicates a greater likelihood of an expert being selected when toxic content is generated. Based on predefined thresholds, we removed experts with high toxicity correlations. Examples of toxic experts are presented in Figure [5](#page-24-0) of Appendix [D.3.](#page-23-0) By removing these experts, LLM alters its behavior to generate detoxified content, as demonstrated in Figure [6.](#page-25-0)

503 504 505 506 507 508 509 510 511 512 513 514 As presented in Table [4,](#page-9-0) our results show that eliminating up to 4.1% of experts can reduce both the expected maximum toxicity and the probability of generating toxic content without affecting performance in REAL-TOXICITYPROMPTS. Similarly, Table [5](#page-9-1) demonstrates that MONET effectively lowers toxicity with only minimal performance degradation, consistent with the findings from RE-ALTOXICITYPROMPTS.

6 CONCLUSION

Masking Masking RoBERTa Score ↓ Avg. Performance ↑
Threshold Ratio Hate Neutral (Helpfulness) (Helpfulness) $-$ 0.642 0.035 0.478 0.2 1.4% 0.643 0.033 **0.478** 0.1 5.4% 0.504 0.028 0.473 0.05 15.0% **0.430 0.027** 0.455

Table 5: ToxiGen metrics according to the expert purging. Lower threshold indicate stricter criteria to filter out more experts. Average performance (helpfulness) is measured in 8 open-ended LLM tasks. Specifics of the helpfulness can be found in Appendix [E.](#page-26-0)

517 518 519 520 521 522 523 524 525 526 527 528 529 530 We introduced MONET, an SMoE architecture with 262,144 experts designed to address the challenge of polysemanticity in LLMs. By integrating sparse dictionary learning directly into end-to-end SMoE pretraining, MONET overcomes the limitations associated with the post-hoc reconstruction loss of SAEs. Our novel product key composition alleviates the memory constraints of conventional SMoE architectures, allowing the expert count to scale to 262,144 per layer while ensuring that total parameters grow proportionally to the square root of the expert count. This substantial expansion enables fine-grained specialization, resulting in monosemantic experts that capture mutually exclusive aspects of knowledge. We demonstrated that MONET enhances mechanistic interpretability by facilitating transparent observations of expert routing patterns and individual expert behaviors. Moreover, MONET allows for robust manipulation of knowledge across domains, languages, and in mitigating toxicity, all without degrading the model's general performance. Our findings suggest that scaling the number of experts and fostering monosemantic specialization within LLMs hold significant promise for advancing both interpretability and controllability, paving the way for future research into transparent and aligned language models.

531 532 533 534 535 536 537 538 539 Limitations Regarding expert selection, we observed that the skewness of routing scores can determine the domain specialization of experts, and we identified toxic experts by calculating the Pearson correlation coefficient between toxicity scores and routing scores. We acknowledge that these criteria are basic and minimal, and we believe that developing more advanced expert selection methods is a promising direction for future research. Additionally, we should explore automated interpretation techniques as self-explained experts are currently demonstrated only qualitatively, remaining quantitative evaluation on automated interpretability an open question. Finally, our application of parametric knowledge manipulation is limited to knowledge unlearning. We believe that observations on monosemantic experts can help address research questions related to hallucinations (e.g., "Is the model confident in retrieving internal knowledge?") and lifelong learning in SMoE LLMs, which is expected to be a promising field [\(Chen et al., 2023;](#page-10-8) [Li et al., 2024\)](#page-12-12).

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Appendix

Content Warning: This section contains examples of harmful language.

CONTENTS

A METHOD DESCRIPTIONS

A.1 EXPANSION OF VERTICAL DECOMPOSITION

In this section, we derive the rearrangement of Equation [15](#page-4-0) for the vertical decomposition, aligning it with Equation [12](#page-3-1) from the horizontal decomposition. We achieve this by splitting the result into six terms to facilitate the computation of actual values.

The vertically decomposed expert layer (MoVDE) is expressed as:

$$
MoVDE(x) = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} E_{ij}(x)
$$
\n(19)

$$
= \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 \left(\begin{bmatrix} V_i^{11} & V_i^{12} \\ V_j^{21} & V_j^{22} \end{bmatrix} \sigma \left(\begin{bmatrix} U_i^1 \\ U_j^2 \end{bmatrix} x + \begin{bmatrix} b_i^{11} \\ b_j^{21} \end{bmatrix} \right) + \begin{bmatrix} b_i^{12} \\ b_j^{22} \end{bmatrix} \right)
$$
(20)

$$
= \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 \begin{bmatrix} V_i^{11} \sigma (U_i^1 x + b_i^{11}) + V_i^{12} \sigma (U_j^2 x + b_j^{21}) + b_i^{12} \\ V_j^{21} \sigma (U_i^1 x + b_i^{11}) + V_j^{22} \sigma (U_j^2 x + b_j^{21}) + b_j^{22} \end{bmatrix} . \tag{21}
$$

Based on the above equation, we define the block matrices:

$$
X_{11} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} V_{i}^{11} \sigma(U_{i}^{1} x + b_{i}^{11}), \quad X_{12} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} V_{i}^{12} \sigma(U_{j}^{2} x + b_{j}^{21}),
$$

\n
$$
X_{13} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} b_{i}^{12}, \qquad X_{21} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} V_{j}^{21} \sigma(U_{i}^{1} x + b_{i}^{11}),
$$

\n
$$
X_{22} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} V_{j}^{22} \sigma(U_{j}^{2} x + b_{j}^{21}), \quad X_{23} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^{1} \hat{g}_{hj}^{2} b_{j}^{22}.
$$

Using these terms, we can simplify the output of the MoVDE layer as the full matrix X . Similar to the horizontal decomposition, we can reorder the summations in each term to enhance computational efficiency by precomputing and reusing intermediate results, thereby eliminating redundant expert computations. Specifically, since the MLPs consist of two layers, we consider four combinations of the expert weights: (i, i) , (i, j) , (j, i) , and (j, j) .

Straightflow First, we address the computations involving the same index pairs, (i, i) and (j, j) , represented by X_{11} and X_{22} . These computations can be simplified as follows:

$$
X_{11} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 V_i^{11} \sigma (U_i^1 x + b_i^{11}) = \sum_{i=1}^{\sqrt{N}} \sum_{h=1}^{H} \left(\sum_{j=1}^{\sqrt{N}} \hat{g}_{hj}^2 \right) \hat{g}_{hi}^1 V_i^{11} \sigma (U_i^1 x + b_i^{11}) \tag{22}
$$

$$
= \sum_{i=1}^{\sqrt{N}} \left(\sum_{h=1}^{H} \hat{g}_{hi}^{1} \right) V_i^{11} \sigma (U_i^1 x + b_i^{11}), \tag{23}
$$

$$
X_{22} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 V_j^{22} \sigma (U_j^2 x + b_j^2) = \sum_{j=1}^{\sqrt{N}} \sum_{h=1}^{H} \left(\sum_{i=1}^{\sqrt{N}} \hat{g}_{hi}^1 \right) \hat{g}_{hj}^2 V_j^{22} \sigma (U_j^2 x + b_j^2)
$$
 (24)

$$
= \sum_{j=1}^{\sqrt{N}} \left(\sum_{h=1}^{H} \hat{g}_{hj}^2 \right) V_j^{22} \sigma (U_j^2 x + b_j^2).
$$
 (25)

915 916 917 In these terms, the expert computations $V_i^{11} \sigma (U_i^1 x + b_i^{11})$ and $V_j^{22} \sigma (U_j^2 x + b_j^{21})$ can be precomputed before aggregating the outputs. Moreover, the multi-head expert routing probabilities are consolidated into single routing coefficients $\sum_{h=1}^H \hat{g}_{hi}^1$ and $\sum_{h=1}^H \hat{g}_{hj}^2$, reducing redundant aggregations.

918 919 920 921 Crossflow For the cross terms X_{12} and X_{21} , the computations involve interactions between different indices. These crossflows between (i, j) and (j, i) can be handled similarly to the horizontal decomposition, as mentioned in Equation [12.](#page-3-1) We rewrite these terms as:

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$$
X_{12} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 V_i^{12} \sigma (U_j^2 x + b_j^{21}) = \sum_{i=1}^{\sqrt{N}} V_i^{12} \sum_{h=1}^{H} \hat{g}_{hi}^1 \sum_{j=1}^{\sqrt{N}} \hat{g}_{hj}^2 \sigma (U_j^2 x + b_j^{21})
$$
(26)

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926 927 928

 $X_{21} = \sum_{1}^{H}$ $h=1$ \sqrt{N} $i=1$ $\sum_{ }^{\sqrt{N}}$ $j=1$ $\hat{g}_{hi}^1 \hat{g}_{hj}^2 V_j^{21} \sigma (U_i^1 x + b_i^{11}) =$ \sqrt{N} $j=1$ $V^{21}_j \sum^H$ $h=1$ \hat{g}_{hj}^2 $\overset{\sqrt{N}}{\sum}$ $i=1$ $\hat{g}_{hi}^{1} \sigma (U_{i}^{1} x + b_{i}^{11})$ (27)

The expressions suggest that the activations $\sigma(U_j^2x+b_j^{21})$ and $\sigma(U_i^1x+b_i^{11})$ are precomputed before aggregating expert outputs. The second-layer weights $V^{12}i$ and $V^{21}j$ are applied in the final step, allowing efficient summation over routing probabilities \hat{g}_{hi}^1 and \hat{g}_{hj}^2 .

Bias Terms The bias terms X_{13} and X_{23} can be simplified as:

$$
X_{13} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 b_i^{12} = \sum_{i=1}^{\sqrt{N}} b_i^{12} \sum_{h=1}^{H} \hat{g}_{hi}^1 \left(\sum_{j=1}^{\sqrt{N}} \hat{g}_{hj}^2 \right) = \sum_{i=1}^{\sqrt{N}} b_i^{12} \left(\sum_{h=1}^{H} \hat{g}_{hi}^1 \right), \tag{28}
$$

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$$
X_{23} = \sum_{h=1}^{H} \sum_{i=1}^{\sqrt{N}} \sum_{j=1}^{\sqrt{N}} \hat{g}_{hi}^1 \hat{g}_{hj}^2 b_j^{22} = \sum_{j=1}^{\sqrt{N}} b_j^{22} \sum_{h=1}^{H} \hat{g}_{hj}^2 \left(\sum_{i=1}^{\sqrt{N}} \hat{g}_{hi}^1 \right) = \sum_{j=1}^{\sqrt{N}} b_j^{22} \left(\sum_{h=1}^{H} \hat{g}_{hj}^2 \right).
$$
 (29)

These terms depend only on the respective expert routing probabilities and bias parameters, and thus can be computed efficiently without involving cross-index combinations.

944 945 946 947 948 By applying these simplifications, the vertical decomposition method effectively computes the layer output while avoiding excessive memory consumption. Without such rearrangement, memory usage would increase significantly due to the combined expert routing probabilities $\hat{g}_{hij} = \hat{g}_{hi}^1 \hat{g}_{hj}^2$ containing N elements, compared to the $2\sqrt{N}$ elements required for \hat{g}_{hi}^1 and \hat{g}_{hj}^2 combined. The detailed implementations are provided in Algorithm [1](#page-18-0) and Algorithm [2.](#page-18-2)

950 A.2 COMPLEXITY CALCULATIONS

951 952 953 We present detailed derivations of computational complexity (expert retrieval time) and memory requirements for different expert architectures to demonstrate the efficiency of MONET.

954 955 956 957 958 SMoE The conventional SMoE architecture requires computing similarity scores between input vectors and all expert embeddings. For an input $x \in \mathbb{R}^d$ and N experts, the top-k expert selection is computed as $K = \mathcal{T}_k(\{w_i^T x\}_{i=1}^N)$, resulting in $O(Nd)$ computational cost. For parameter storage, each expert network maintains two weight matrices as shown in Equation [1:](#page-1-0) $\{U_i\}_{i=1}^N \subset \mathbb{R}^{m \times d}$ and ${V_i}_{i=1}^N \subset \mathbb{R}^{d \times m}$. This requires $O(2Nmd) = O(Nmd)$ parameters in total.

959 960 961 962 963 964 965 966 PEER As explained in [Lample et al.](#page-12-6) [\(2019\)](#page-12-6), the product key retrieval reduces expert retrieval complexity from linear to square root scale. Following Equation [3,](#page-2-2) computing scores for both key complexity from the artic square root scale. Following Equation 5, computing scores for both key sets requires $2 \times \sqrt{N} \times d/2 = \sqrt{N}d$ operations. Then, as described in Equation [4,](#page-2-3) selecting final k experts from the candidate set $\mathcal{K}_h^1 \times \mathcal{K}_h^2$ involves $2 \times k^2 \times d/2 = k^2 d$ operations. Since this process Experis from the candidate set $\lambda_h \times \lambda_h$ involves $2 \times \kappa \times \frac{a}{2} = \kappa a$ operations. Since this process is repeated for H multi-heads, the total retrieval complexity becomes $O((\sqrt{N} + k^2)Hd)$. However, PEER still maintains individual parameters for each expert $\{u_{ij}\}_{i,j=1}^{\sqrt{N}}, \{v_{ij}\}_{i,j=1}^{\sqrt{N}} \subset \mathbb{R}^d$, resulting in $O(Nd)$ parameter complexity.

967 968 969 970 971 MONET-HD MONET employs product key retrieval but eliminates the need for selecting top-k elements from $\mathcal{K}_h^1 \times \mathcal{K}_h^2$, reducing retrieval cost to $O(\sqrt{N}Hd)$. Through product key composition, we dynamically construct expert networks using bottom layer weights $\{U_i\}_{i=1}^{\sqrt{N}} \subset \mathbb{R}^{m \times d}$, top layer weights $\{V_j\}_{j=1}^{\sqrt{N}} \subset \mathbb{R}^{d \times m}$, and bias terms $\{b_i^1\}_{i=1}^{\sqrt{N}} \subset \mathbb{R}^m$ and $\{b_j^2\}_{j=1}^{\sqrt{N}} \subset \mathbb{R}^d$. Therefore, the total parameter complexity is $O(2\sqrt{N}md + \sqrt{N}m + \sqrt{N}d) = O(\sqrt{N}md)$. √ $Nm+$ √ $N d) = O($ √ $Nmd).$

972 973 974 975 976 977 MONET-VD The vertical decomposition maintains the same expert routing complexity while partitioning the expert matrices differently. It utilizes input projections $\{U_i^1\}_{i=1}^{\sqrt{N}}, \{U_j^2\}_{j=1}^{\sqrt{N}} \subset \mathbb{R}^{m/2 \times d}$ and output projections $\{V_i^{11}\}_{i=1}^{\sqrt{N}}, \{V_i^{12}\}_{i=1}^{\sqrt{N}}, \{V_j^{21}\}_{j=1}^{\sqrt{N}}, \{V_j^{22}\}_{j=1}^{\sqrt{N}} \subset \mathbb{R}^{d/2 \times m/2}$, along with corresponding bias terms $\{b_i^{11}\}_{i=1}^{\sqrt{N}}, \{b_j^{21}\}_{j=1}^{\sqrt{N}} \subset \mathbb{R}^{m/2}$ and $\{b_i^{12}\}_{i=1}^{\sqrt{N}}, \{b_j^{22}\}_{j=1}^{\sqrt{N}} \subset \mathbb{R}^{d/2}$. The total expert parameter complexity can be derived as:

$$
O\left(2 \times \sqrt{N} \times \frac{m}{2} \times d + 4 \times \sqrt{N} \times \frac{d}{2} \times \frac{m}{2} + 2 \times \sqrt{N} \times \frac{m}{2} + 2 \times \sqrt{N} \times \frac{d}{2}\right) \tag{30}
$$

$$
= O(2\sqrt{N}md + \sqrt{N}m + \sqrt{N}d) = O(\sqrt{N}md).
$$
\n(31)

A.3 IMPLEMENTATION DETAILS

```
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     1 class MonetMoHDE(nn.Module):
       2 dim: int = 2048
    3 moe_dim: int = 16
    4 moe_experts: int = 512
    5
    6 def setup(self):
     7 b_shape = (self.moe_experts, self.dim)
     8 self.u = nn.DenseGeneral((self.moe_experts, self.moe_dim))
    9 self.v = nn.DenseGeneral(self.dim, (-2, -1), use_bias=False)
    10 self.b = self.param("b", nn.initializers.zeros, b_shape)
    11
    12 def _{call} (self, x, q1, q2):
    13 x = nn_{\text{relu}}(\text{self.u}(x)) \neq 214 x = jnp.einsum("btim,bthi->bthm", x, g1)
          x = jnp.einsum("bthm,bthj->btjm", x, g2)
```

```
999
    16 return self.v(x) + jnp.einsum("bthj,jd->btd", g2, self.b)
       Algorithm 1: Simple JAX (Bradbury et al., 2018) and Flax (Heek et al., 2024) implementation of a
```

```
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       MONET-HD layer.
```

```
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    1 class MonetMoVDE(nn.Module):
    2 dim: int = 2048
    3 moe_dim: int = 16
        4 moe_experts: int = 512
     5
     6 def setup(self):
         self.u1 = nn.DenseGeneral((self.moe-exports, self.moe-dim // 2))self.u2 = nn.DenseGeneral((self.moe_experts, self.moe_dim // 2))
         self.v11 = nn.DenseGeneral(self.dim // 2, (-2, -1), use_bias=False)
         self.v12 = nn.DenseGeneral(self.dim // 2, (-2, -1), use_bias=False)
    11 self.v21 = nn.DenseGeneral(self.dim // 2, (-2, -1), use_bias=False)
    12 self.v22 = nn.DenseGeneral(self.dim // 2, (-2, -1), use_bias=False)
         b_{shape} = (self.moe_{experts, self.dim / / 2)self.b1 = self.param("b1", nn.initializers.zeros, b_shape)
          self.b2 = self.param("b2", nn.initalizers.zeros, b.shape)17
    18 def _{cal1} (self, x, g1, g2):
          x1, x2 = nn.relu(self.u1(x)) ** 2, nn.relu(self.u2(x)) ** 2
          x11 = self.v11(jnp.einsum("btim,bthi->btim", x1, g1))x12 = \text{self.v12(jnp.einsum("btjm,bthj,bthi->btim", x2, g2, g1))}x13 = jnp.einsum("bthi, id-> btd", gl, self.b1)x21 = self.v21(jnp.einsum("btim,bthi,bthj->btjm", x1, q1, q2))x22 = self.v22(jnp.einsum("btjm,bthj->btjm", x2, q2))x23 = jnp.einsum("bthj, jd->btd", g2, self.b2)return jnp.concat((x11 + x12 + x13, x21 + x22 + x23), axis=-1)
               Algorithm 2: Simple JAX and Flax implementation of a MONET-VD layer.
```


1031 1032 1033 Table 6: Model sizes, layer configurations, and expert architecture details. The number of parameters includes both model and expert layers, with each model variant differing in its dimensionality, attention heads, and expert configurations.

1035 1036 B TRAINING DETAILS

1037 B.1 PRETRAINING

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1038 1039 1040 1041 1042 1043 We pretrain our MONET models with parameter sizes of 850 million (850M), 1.4 billion (1.4B), and 4.1 billion (4.1B) to evaluate performance across scales. For a fair comparison, we also train models with the LLAMA architecture from scratch under the same conditions.. All models are trained on 100 billion tokens sampled from the FineWeb-Edu dataset [\(Penedo et al., 2024\)](#page-13-13), which combines high-quality web content with educational materials. Model configurations are in Table [6](#page-19-4)

1044 1045 1046 1047 1048 1049 Training is conducted on a TPU-v4-64 Pod Slice, utilizing the AdamW optimizer with a learning rate of $\bar{5} \times 10^{-4}$ and a batch size of 2 million tokens. We employ Squared ReLU [\(So et al., 2021;](#page-13-14) [Zhang et al., 2024;](#page-14-4) [Adler et al., 2024\)](#page-10-10) as the activation function. To manage computational resources effectively, we adopt a group routing strategy wherein the routing probabilities are reused every 4 layers. This approach reduces the overhead associated with the expert routing parameters. The weight of the auxiliary loss λ is set to 10^{-3} for all experiments.

1050 1051 1052 1053 1054 In addition, we train CODEMONET 1.4B to evaluate the model's capability in coding tasks and analyze multilingual specialization. CODEMONET is pretrained on 100 billion tokens sampled from STARCODERDATA, the primary dataset used to train the StarCoder model [\(Li et al., 2023\)](#page-12-14). STAR-CODERDATA is filtered from The Stack dataset [\(Kocetkov et al., 2022\)](#page-12-15) and encompasses approximately 86 programming languages.

1055 B.2 INSTRUCTION TUNING

1056 1057 1058 1059 1060 1061 To enhance the conversational and instructional capabilities of our models, we perform instruction tuning on the MONET 1.4B model following the instruction tuning recipe [\(Tunstall et al.\)](#page-14-5) used by SMOLLM [\(Allal et al., 2024\)](#page-10-11). We use the same fine-tuning dataset as SMOLLM, which combines several high-quality instruction-response pairs from diverse sources. The instruction tuning process is performed on a single NVIDIA A100 GPU. During this phase, we freeze the expert routing embeddings to prevent overfitting and reduce computational demands.

1062 1063 B.3 VISION-LANGUAGE FINE-TUNING

1064 1065 1066 1067 1068 1069 1070 To assess whether expert's monosmanticity is preserved when the LLM acquires multimodal capabilities, we create VISIONMONET by fine-tuning the MONET 1.4B CHAT model following the LLaVA's visual instruction tuning [\(Liu et al., 2024\)](#page-12-16), using a single NVIDIA A100 GPU. Instead of the vision encoder used in the original paper, we employ the $openai/clip-vit-base-patch16^a$ $openai/clip-vit-base-patch16^a$ $openai/clip-vit-base-patch16^a$ model with an image size of 224, resulting in 196 image tokens. Consistent with our instruction tuning strategy, we freeze the expert routing embeddings during vision-language fine-tuning to ensure effective adaptation to the multimodal instruction data.

1071 1072 1073 1074 1075 1076 In Figure [9](#page-30-0) and [10,](#page-31-0) we can observe that expert's monosemanticity spans different modalities in VI-SIONMONET, where experts specialize in concepts manifested in texts and images. Examples show mutual exclusivity in multimodal expert's specialization, such as colors (e.g., Green vs Purple), brightness (e.g., Black vs Sunlight) and backgrounds (e.g., Aviation vs Body of Water). Such result shows the potential of MONET architecture in generalizing monosemantic specialization across modalities, paving the way for more interpretable and controllable multimodal transformer models.

- **1077**
- **1078**
- **1079**

^a<https://huggingface.co/openai/clip-vit-base-patch16>

1095 1096 1097 Table 9: Number of experts masked as domain-specialized experts in MONET-1.4B. The table reports the number of experts assigned to each domain across all routing groups. Each group corresponds to one of the 6 routing groups, and the total number of experts per domain is provided.

1099 C ABLATION STUDIES

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1101 1102 1103 In this section, we investigate the effects of two key hyperparameters: the auxiliary loss weight (λ) and the number of expert routing groups. All experiments are conducted on the MONET 1.4B model, and the 5-shot performance is reported on the open-ended benchmarks used in Table [2.](#page-5-0)

1104 C.1 AUXILIARY LOSS WEIGHTS

1105 1106 1107 1108 1109 1110 1111 1112 We employ two auxiliary losses: uniformity and ambiguity. The uniformity loss ensures router activation is evenly distributed across tokens and batches, preventing favoritism toward specific experts. The ambiguity loss encourages the model to assign higher routing probabilities to the primary experts, promoting expert specialization.

Table 7: Ablation results showing the impact of varying auxiliary loss weights.

1114 1115 1116 1117 Without uniformity loss, the model tends to over-utilize certain experts, leading to imbalanced training. On the other hand, high ambiguity causes the model to route to multiple experts, which inhibits expert specialization. For effective expert routing, the distribution should be uniform across tokens but specialized within each token.

1118 1119 1120 We test $\lambda \in \{2 \times 10^{-4}, 1 \times 10^{-3}, 5 \times 10^{-3}\}$, as shown in Table [7.](#page-20-2) The results indicate that the model is robust to different loss weights, with larger weights reducing uniformity and ambiguity. We selected $\lambda = 10^{-3}$ as it showed optimal performance.

1121 1122 C.2 GROUPED EXPERT ROUTING

1123 1124 1125 1126 1127 1128 1129 1130 Expert routing requires multi-head retrieval embeddings, which involve finding top- k experts through product key retrieval. While this reduces computational complexity compared to evaluating all 262,144 combinations, it still demands substantial memory and computational resources. As described in the training details, we reuse the routings every 4 layers.

Group Size Params		FLOPs	$Avg. (5-shot)$			
	1.345B	6225.52T	0.518			
	1.465B	6745.30T	0.510			
	1.767B	8017.81T	0.511			

Table 8: Impact of different routing group sizes.

1132 1133 To assess the effectiveness of grouped routing in reducing computational costs without sacrificing performance, we trained models with full expert routing and compared them in Table [8.](#page-20-3) We report parameter size, FLOPs (TFLOPs) for forward computation over 2M tokens, and the 5-shot

1134								
	Language	Group 1	Group 2	Group 3	Group 4	Group 5	Group 6	Total
	Python	7,813	9.616	8.844	7.580	10.791	12.518	57,162
	C++	7.144	11.436	9.820	10.515	14.018	11.686	64.619
	Java	13.253	12.365	12.771	11.045	17.302	15.209	81.945
	JavaScript	29.795	23,176	24.574	26.458	30,862	40.217	175,082
	Lua	8.249	11.047	6.849	4.936	8.044	9.496	48.621
	PHP	9.545	11.906	7.744	5.906	8.455	9.780	53,336

1141 1142 1143 Table 10: Number of experts masked as language-specialized experts in CODEMONET-1.4B. The table reports the number of experts assigned to each programming language across all routing groups.

1150

1145 1146 1147 1148 benchmark performance. The group size of none represents the dense LLAMA model. The results demonstrate that reusing routing for every 4 layers significantly reduces parameters and FLOPs, while maintaining performance comparable to the 1.7B model.

1149 D EVALUATION PROTOCOL FOR ANALYSES

1151 1152 1153 1154 1155 1156 In this section, we explain the detailed evaluation protocol of the analyses in Section [5.](#page-6-1) To check the knowledge and expert specialization in the MONET, we instead mask the corresponding knowledges and evaluate the model benchmark to check how many the target benchmark is dropped while maintaining the other abilities In particular, we explored the effects of knowledge unlearning by selectively removing experts based on their activations related to specific domains, programming languages, and toxicity.

1157 1158 D.1 DOMAIN MASKING

1159 1160 1161 1162 As outlined in Section [5.1,](#page-7-1) we reorganized the MMLU benchmark, consolidating its 57 subjects into 14 distinct categories, as defined by the MMLU Pro benchmark. The distribution of question-answer pairs across these categories was uneven, with the largest category, "Other," containing 2,343 pairs, while the smallest, "Engineering," included only 145 pairs.

1163 1164 1165 1166 1167 1168 1169 1170 1171 For each expert, we labeled it as specialized in a domain if its routing probability for that domain was at least twice that of the second most activated domain. For instance, an expert highly activated by the biology domain with double the activation compared to the next closest domain was classified as a biology expert. Experts without such a skewed activation were considered generalists. After assigning experts to domains, we selectively removed them to evaluate the impact of knowledge unlearning across all 14 categories. Our analysis revealed that domains such as History and Health were allocated the largest number of experts, approximately 10,000 per layer, while domains like "Psychology" and "Other" were assigned the fewest. A detailed distribution of deleted experts is presented in Table [9](#page-20-4) and full performance perturbation are available in Section [E.](#page-26-0)

1172 1173 1174 1175 1176 1177 1178 1179 1180 1181 Our analysis reveals the inherent challenges in achieving domain specialization with traditional MoE approaches, particularly evident in OLMoE's results. While domain-specific data sources can be controlled to some extent (e.g., using PubMed for biology or GitHub for programming languages), managing the distribution of domain knowledge in large-scale pretraining corpus remains challenging. A key limitation emerges from the constraint of small expert counts: rather than achieving the desired monosemanticity, these models exhibit significant polysemanticity, making it virtually impossible to isolate domain-specific knowledge completely. In contrast, MONET's architecture enables precise knowledge manipulation through selective expert removal, effectively addressing the domain specialization challenge that confounds traditional approaches. This capability is particularly noteworthy given the uneven distribution of expertise observed across domains, as demonstrated by our expert allocation analysis.

1182 1183 D.2 MULTILINGUAL MASKING

1184 1185 1186 1187 To conduct the multilingual masking experiments, we utilized the bigcode-evaluation-harnessframework [\(Ben Allal et al., 2022\)](#page-10-12) to assess code generation and unit tests. MULTIPL-E benchmark [\(Cas](#page-10-7)[sano et al., 2023\)](#page-10-7) consists of 22 programming languages. For our experiments, we evaluated CODE-MONET-1.4B and selected the top 6 languages by performance: Python, C++, Java, JavaScript, Lua, and PHP. Full pass@100 performance of CODEMONET is available in Table [15.](#page-27-0)

 In line with our approach for domain masking, we identified language-specific experts (see Table [10\)](#page-21-3) by examining the skewness in routing probabilities. Based on this, we masked experts associated with each language and re-evaluated the code generation benchmark to estimate the model's capability to unlearn programming languages.

 D.3 TOXIC EXPERT PURGING

 To enhance the safety of language generation, we introduce a systematic method for purging toxic experts from our model. This method focuses on identifying and eliminating experts correlated with toxic outputs, which significantly mitigates harmful content while maintaining the overall performance of the language model.

 REALTOXICITYPROMPTS For the evaluation on REALTOXICITYPROMPTS, we implemented the protocol established by DecodingTrust [\(Wang et al., 2023\)](#page-14-6), utilizing a dataset of 1.2K challenging user prompts. Toxicity scores are obtained from the PERSPECTIVE API, focusing on two metrics: expected maximum toxicity and toxicity probability. We generate outputs with a temperature of 1.0 and a top-p value of 0.9, producing 25 samples of 20 new tokens per prompt. The expected maximum toxicity is calculated as the average of the highest toxicity scores from these 25 generations for each sample. Meanwhile, the toxicity probability is defined as the ratio of samples in which at least one generation among the 25 exceeds a toxicity score of 0.5, classifying it as toxic content.

 ToxiGen In addition to REALTOXICITYPROMPTS, we assess the model using the ToxiGen dataset, employing the ToxiGen RoBERTa model for toxicity evaluation. The ToxiGen dataset consists of 31K diverse prompts designed to generate new sentences, which are subsequently evaluated for toxicity using the RoBERTa scoring model. We generate outputs with a temperature of 0, producing new sequences of 30 tokens.

 Toxic Experts Identification Building on established toxicity criteria, we next identify experts with specialized knowledge related to toxic content. Initially, we observe expert routing data alongside their corresponding toxicity scores while inferencing on toxic prompts. Figure [5](#page-24-0) provides examples showing how specific experts strongly respond to toxic tokens. We further compute the Pearson correlation between each expert's routing probability and toxicity score, ranking the experts based on this correlation. Masking thresholds are then applied to filter out toxic experts. Following these thresholds, we proceed to remove experts who demonstrate significant correlations with toxicity. As a result, by editing the parametric knowledge within MONET, the LLM alters its behavior to generate detoxified content, as demonstrated in Figure [6.](#page-25-0)

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1344 1345 1346 1347 1348 1349 Figure 5: Detection of toxic experts through token activations and toxicity scores. The top row lists example tokens that highly activate each expert. The bottom row displays scatter plots corresponding to these experts, where each blue point represents a token activation from the RealToxicityPrompts dataset. In the scatter plots, the x-axis indicates the toxicity score of the token, and the y-axis shows the routing score assigned to the expert for that token. The correlation coefficient between toxicity scores and expert routing scores is noted above each plot. High correlation coefficients enabled us to identify experts associated with toxic knowledge within the model.

1401 1402 1403 According to the toxic expert pruning threshold (left column), the model generates detoxified content (middle column) with a toxicity score measured by the PERSPECTIVE API for the sentence (right column). The lower the threshold, the more experts that are deleted from the feedforward layers.

1404 1405 E FULL PERFORMANCE

1415 1416 1417 1418 1419 1420 Table 11: General performance of MONET on MMLU domains after masking specialized experts. Columns represent the categories of masked experts, while rows display the MMLU performance for each domain following the removal the corresponding experts. The column "None" contains the original performance of the MONET without any experts removed. The row labeled "∆ Target" indicates the accuracy change in the target domain due to unlearning, while the row labeled "∆ Others" reflects the average performance change across all other domains.

Table 12: General performance of pretrained Gemma 2 on MMLU domains after suppressing features of Gemma Scope SAE. Columns indicate categories of the suppressed features, and rows display domain-specific MMLU performance. Please zoom in for detailed results.

1441 1442 1443 Table 13: General performance of OLMoE after masking specialized experts. Columns represent the categories of masked experts, while rows display the MMLU performance for each domain following the removal the corresponding experts. Please zoom in for detailed results.

1453 1454 1455 Table 14: General performance of LLAMA after suppressing logits in MLPs. Columns indicate categories of the suppressed features, and rows display domain-specific MMLU performance. Please zoom in for detailed results.

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Language None Python C++ Java JavaScript Lua PHP **Python** 31.64 1.06 28.10 26.33 31.44 30.58 28.63 C++ 27.39 26.48 12.19 26.94 26.84 27.15 27.07 Java 28.74 29.31 26.77 8.37 26.86 30.47 28.31 JavaScript 30.40 28.84 29.46 27.81 21.33 29.30 30.90 Lua 16.97 14.03 16.29 16.25 15.57 1.24 14.97 **PHP** 28.17 27.33 26.09 28.36 25.07 25.62 1.55

Correlation Threshold	MMLU	ARC	WG	PIQA	SIQA	OBOA	HS	CSQA	Avg.
	0.352	0.495	0.522	0.727	0.423	0.418	0.529	0.363	0.478
REALTOXICITYPROMPTS									
0.2	0.352	0.494	0.526	0.726	0.425	0.416	0.531	0.361	0.479
0.1	0.349	0.493	0.519	0.723	0.423	0.426	0.525	0.363	0.478
0.05	0.337	0.484	0.523	0.708	0.421	0.406	0.494	0.364	0.467
ToxiGen									
0.2	0.351	0.493	0.522	0.729	0.424	0.414	0.529	0.362	0.478
0.1	0.345	0.493	0.516	0.722	0.423	0.402	0.518	0.367	0.473
0.05	0.336	0.479	0.508	0.706	0.414	0.372	0.481	0.345	0.455

 Table 16: Model performance on REALTOXICITYPROMPTS and ToxiGen with varying correlation thresholds, evaluated under zero-shot settings.

1512 1513 F ADDITIONAL QUALITATIVE RESULTS

Figure 8: List of qualitative examples according to the programming languages.

1672 1673 Figure 9: List of image and text activation examples of vision-language model VISIONMONET's experts. Image examples were sampled from the CC3M [\(Sharma et al., 2018\)](#page-13-15) dataset, based on the routing score of a multimodal expert.

1726 1727 Figure 10: List of image and text activation examples of vision-language model VISIONMONET's experts. Image examples were sampled from the CC3M [\(Sharma et al., 2018\)](#page-13-15) dataset, based the routing score of a multimodal expert.