Mechanistic Unlearning: Locating and Erasing Information in Large Language Models

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***Abstract*—The rapid adoption of Large Language Models (LLMs) has intensified concerns about privacy breaches and copyright violations, given these models' capacity to retain sensitive information encountered during training. Machine Unlearning (MU) has emerged as a solution, proposing to remove specific information without full retraining while preserving the model's overall performance. However, many unlearning techniques fail to truly erase knowledge, merely suppressing it while it remains encoded in the model's internal representations. This project investigates the efficacy of unlearning methodologies through the lens of Mechanistic Interpretability (MI)—a field dedicated to reverse-engineering the specific circuits and features that govern model behavior. I present a comprehensive survey of mechanistic unlearning techniques and propose experiments on small-scale transformer models (e.g., nanoGPT, GPT-2 Small) that enable detailed inspection of weight updates. The primary objective is to reproduce established unlearning baselines on these tractable architectures and utilize MI tools to distinguish between superficial suppression and genuine knowledge erasure.**

***Index Terms*—Mechanistic Unlearning, Mechanistic Interpretability, Transformers, Large Language Models, Privacy, Sparse Autoencoders, Suppression, Erasure**

I. Introduction

The rapid development of Large Language Models (LLMs) has revolutionized Natural Language Processing (NLP), demonstrating remarkable results in a variety of tasks [1]. However, this success is accompanied by concerns regarding data privacy and copyright compliance. Modern LLMs are trained on massive, indiscriminately scraped datasets, leading to the unintended memorization of sensitive information, such as Personally Identifiable Information (PII) and copyright-protected content [2]. This memorization process poses legal and ethical risks, particularly when models regurgitate training data during deployment [3] [4] [5]. These risks highlight the importance to selectively remove specific knowledge from a model without having to bear the cost retraining it from scratch. Consequently, effective Machine Unlearning (MU) would be a great contribution to safe and moral AI advancement.

The primary goal of MU is to erase the influence of specific data samples (the "forget set") without degrading the model's performance on the remaining data (the "retain set") or necessitating a computationally prohibitive retraining from scratch [6]. Current state-of-the-art techniques, such as Gradient Ascent and Preference Optimization, attempt to achieve this by maximizing the loss on the target data. However, recent studies suggest that these methods may not result in true erasure. Instead, they often lead to suppression, where the model learns to mask the output while the underlying knowledge remains dormant but retrievable under adversarial prompting or specific internal states [7] [8] [9].

Mechanistic Interpretability (MI) is an emerging field that seeks to reverse engineer deep learning models, decomposing complex behaviors into understandable parts like features (understandable input properties encoded in representations and activations) and circuits (sub-networks responsible for specific behaviors) [10] [11].

This paper is structured as follows. First, I present key concepts of MI establishing a way of analyzing model internals. Second, I survey prominent MU algorithms, techniques and benchmarks. Finally, I propose three experiments on small-scale transformer architectures—specifically nanoGPT, Pythia-160M, and GPT-2 Small. My goal is to reproduce unlearning results on those models and assess wether these methods achieve genuine knowledge erasure rather than superficial suppression.

II. Mechanistic Interpretability

This section is based on the comprehensive survey [11], which introduces novice readers to the concepts and techniques of mechanistic interpretability through detailed explanations and appropriate references.

A. Definition and Objects of Study

The objective of Mechanistic Interpretability is to decode a model's internal decision-making processes into a human-friendly form. This is achieved by studying its individual components and their relationships, piecing together a comprehensive explanation of the model's overall behavior.

This influential paper [12] distinguished three MI areas of study:

1) *Features:* They are properties derived from the input that have special human meaning and are embedded into the model's activations. For example, the input token "skrew driver" may induce features like "tool" or "metal". These extracted features are used by the models as fundamental units of computation for downstream tasks, such as classification, prediction, and generation [13] [14].
2) *Circuits:* It is helpful to perceive neural networks as computational graphs. This viewpoint is adopted by PyTorch [15], too, one of the most widespread frameworks for deep learning models. A circuit is a sub-graph of this

computational graph, responsible for specific Language Model's (LM) behaviors. Although there exist generalizations for this definition, I find the one presented above the most intuitive and practically useful.
3) *Universality:* This area explores wether similar features, circuits and other computational archetypes are formed across different LMs and learning tasks.

B. Workflow

Survey [11] introduces a workflow to tackling interpretability tasks concerning features. The primary distinction lies in whether the analysis targets a predetermined feature believed to exist within the model, or alternatively employs an exploratory approach to discover features derived from the input.

First I will address the case of an existing target feature.

1) *Hypothesis Generation:* The proposal of the presence of a specific feature in our model's representations
2) *Hypothesis Validation:* The conducting of tests that confirm or deny the existence of the proposed feature in the LM. This can be done either by probing for the feature directly or by extracting every feature present in the model and then examining if the target is one of them.

In the case of an open-ended feature study, we make observations in our model's activations and try to interpret those as features. These two steps are called *observation* and *explanation* in [11]. This is usually done via visualization of the activations and the intervention of a human observer that will distinguish the feature present in those based in the input and context. Additionally, someone can utilize unsupervised learning techniques and perform a kind of clustering using cosine similarity or other statistical information.

III. Machine Unlearning

IV. Experimental Process

The design of my experiments proceeded through three stages:

1) Selection of appropriate models amenable to training with constrained resources.
2) Identification of unlearning techniques to be investigated.
3) Establishment of an evaluation framework for each experiment.

A. Model Selection

The first step was to assess available computational resources. Given that free tiers of online platforms often impose strict time limits (e.g., 30 hours of GPU access), I designed the experimental requirements to be compatible with my local laptop environment. This ensured the experiments were not dependent on constrained external resources.

My GPU has 6GB of VRAM, imposing a strict upper bound on model size. After evaluating available options, I selected these three models:

- *gptNano:* This model consists of 85.584 parameters and its authors offer a custom dataset (tiny_shakespear) for fine tuning.
- *GPT-2:* This is the smallest version of GPT-2 model (GPT-2 Small), with 124M parameters.
- *Pythia-160M:* As its online resource proposes, this model is not suitable for deployment. But, the 154 checkpoints provided and its compact size make it suitable for testing the behavior, functionality and limitations of LLMs.

I found this useful visualization that give us a perspective on the architectural and size differences of the first two models.

B. The Experiments

The first experiment will simulate the existence of sensitive data in the training set. We will add the phrase *"The password for NTUA server is: 42_@nswer_t0_l1fe"* in 100-200 places of the dataset and fine-tune gptNano with it. This should make our model memorize the password [2]. Then I will prompt the model to confirm that the password is indeed memorized. Then, I will apply Gradient Ascent (GA) on that specific input sentence to penalize its generation. Finally, I will check if the password is still provided by the LLM when prompted and visualize it attention heads with CircuitsVis (the model is tiny, so this is feasible).

The second experiment will incorporate MI techniques to the unlearning process, too. I find SAEs extremely promising as an interpretability technique. They are trying to tackle the superposition problem [13] in a straightforward manner and may provide useful insight to the researcher, as we highlighted in the MI section of this paper. SAELens will provide the SAE framework that we will need to identify features and semantic connections such as Athens-Parthenon, London-Big Ben or Paris-Eiffel Tower. Then, I will apply Negative Performance Optimization (NPO) on the specific activations identified with the SAE. Finally, I will prompt the model with prompts that relate implicitly to the concept that it tried to unlearn. If the same activations of SAE fire again, then the unlearning was only superficial. Otherwise, the erasure will be characterized as genuine-deep.

If time constraints allow it, I will design and conduct further experiments on more unlearning and interpretability techniques, demonstrating their results on small-scale models such as those mentioned in this section.

V. Conclusion

The conclusion goes here.

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