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ABSTRACT

Large language model (LLM) unlearning has emerged as an essential post-training mechanism for erasing specific knowledge or undesirable behaviors. However, forgetting target data often causes an unintended degradation in overall model utility. Although various advanced methods have explored different learning objectives to mitigate the trade-off, it remains unclear how the highly entangled internal representations in LLMs contribute to unlearning. In this work, we introduce the notion of *latent knowledge fragility* to explore the vulnerability of retained knowledge to unlearning. We develop a unified analytical approach via component-wise parameter patching that isolates and quantifies fragility in terms of different transformer blocks. We observe that the LLM encodes different levels of abstraction, from surface syntax in shallow layers to complex semantics in deeper layers, which align with different degrees of representation disruption and utility degradation. Based on the insights, we propose a lightweight framework called *Component-wise Replacement Unlearning* (CRU) that restores fragile layers (also extendable to other components) from the original model based on post-hoc validation, which allows us to obtain a hybrid model without additional training. Extensive experiments on various aspects verify that our method generally improves the trade-off between removal and retention. Our analysis highlights the non-uniform influence of different LLM layers and provides a new possibility of surgical unlearning.

1 INTRODUCTION

The unprecedented scale and generalization capabilities of large language models (LLMs) [2, 86, 18, 62, 22] have led to significant successes in understanding and generating natural languages for complex tasks [21]. While being widely deployed, LLMs also bring a primary concern given their high tendency to memorize training data [9, 10]. As trained in a broad range corpora [2], some sensitive or even harmful information poses various risks for LLM usage [29], regarding data privacy (e.g., GDPR compliance [51, 84]), ethics [30], safety [88, 28], and intellectual property [79]. In contrast to costly retraining from scratch, LLM unlearning [80, 85, 26, 75, 74] has emerged as an alternative to mitigate the problem, which often involves fine-tuning the model with gradient-based objectives [63, 64, 80, 85, 75] to suppress unwanted behaviors [76] or remove specific knowledge [32, 26].

Despite promising progress in forgetting target content, it remains quite challenging to maintain the overall model utility of LLMs, measured via the discrepancy between outputs of the original and the unlearned model. Taking the gradient ascent (GA) method [80] as a representative example, it directly minimizes the log-likelihood for targeted data to reduce their generation probability, but it can also easily destroy the ability to generate natural language. Subsequent methods [85, 75, 74] developed various advanced objectives to address the excessive unlearning, which still induce collateral degradation in the model’s general language capabilities as evident in Figure 1 (evaluated

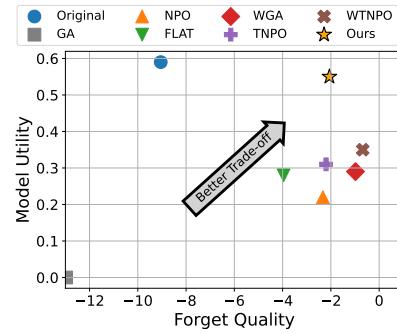


Figure 1: Our method can achieve a better trade-off than previous methods.

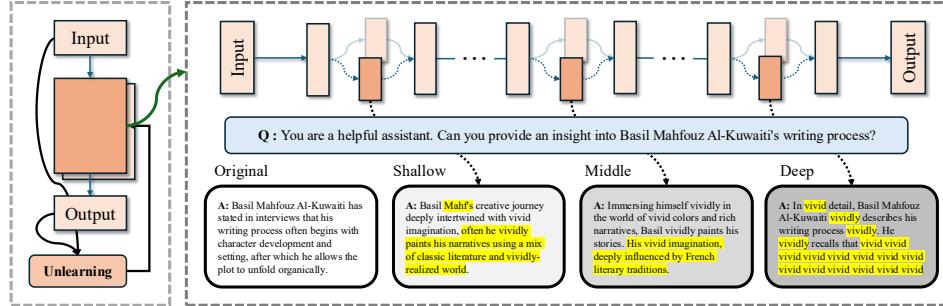


Figure 2: **Our layer-wise patching approach illustrates the intrinsic functionality differences of different transformer layers.** Highlighted are distinction from the original answer. The shallow layers near token input model surface-level syntax, such as word order and lexical details. The middle layers model entangled knowledge with abstract concepts that encode a range of complex semantics. The deep layers near the output model token-level dependencies, such as contextual correlations.

on TOFU benchmark [32]). However, beyond the design of unlearning objectives [29], the internal representation in LLM received limited attention, which naturally motivates one research question:

Can we optimize the tradeoff through the lens of LLM latent knowledge?

In this work, we discuss this trade-off from the intuition that different internal parts of LLM encode different knowledge (refer to Figure 2). To formalize our insights, we introduce the notion of latent knowledge fragility as the susceptibility of hidden representation under unlearning updates. This fragility is not uniform, but rather structured, reflecting a spectrum from low-level syntactic patterns to high-level complex semantics. Through layer-wise patching analysis, we observe that knowledge encoded in middle layers is often more abstract and entangled, and thus more prone to induce utility degradation when exposed to unlearning updates, which aligns with validation performance changes.

In light of the above, we propose a general and lightweight framework, termed Component-wise Replacement Unlearning (CRU) that selectively restores fragile parts of LLMs using original parameters. We mainly focus on layer-wise unlearning but our approach is easily extendable to other components. Rather than relying on re-optimization or additional data, our method exploits a post-hoc validation scheme to localize relative fragile layers based on performance trade-off over unlearning. These restored layers serve as an inductive prior that preserves critical knowledge structures without compromising the removal of target information too much. Notably, this design circumvents fine-tuning or architectural changes, making it applicable across various unlearning settings and model scales.

We evaluate our method with multiple LLMs in different unlearning scenarios like personal content or factual knowledge removal. Experimental results consistently show that our approach improves the removal-retention trade-off, achieving satisfactory target forgetting without sacrificing much model utility. Furthermore, qualitative analyses reveal that our method retains coherent and grounded generations, especially in answers requiring semantic understanding. Interestingly, we also find that our final hybrid model of CRU achieves a better trade-off in a very distinct way from other models in terms of parameter changes. To summarize, our main contribution can be listed as follows.

- We introduce a notion of latent knowledge fragility to qualitatively define how unlearning updates affect different levels of latent knowledge encoded in LLMs. (in Section 3.1)
- We develop a unified analytical approach to quantify layer-wise fragility by analyzing the modular influence of LLMs in relation to the performance trade-off. (in Section 3.2)
- We propose a lightweight and general framework termed CRU that selectively restores fragile layers from the original model based on post-unlearning validation, effectively improving the trade-off between forget quality and model utility. (in Section 3.3 and Section 4)

2 BACKGROUND

In this part, we introduce preliminary background of LLM unlearning and our layer-wise model patching. In Appendix B, we provide a more comprehensive discussion of related work.

Problem Setup for LLM Unlearning. We consider a pre-trained auto-regressive LLM f_θ with the model parameters θ , which recursively estimates the probability distribution of the next token

108 $p(\cdot|s, \theta)$ given the input sequence $s = [s_1, s_2, \dots, s_{|s|}]$. The model is assumed to be trained on a
 109 web-sourced corpora $\mathcal{D}_w = \{s^1, s^2, \dots, s^n\}$ with the negative log-likelihood (NLL) loss function of
 110 $-\log p(s; \theta)$, where $p(s; \theta) = \prod_{i=1}^{|s|} p(s_i|s_{1:i-1}; \theta)$ indicates the product of conditional probability
 111 for each token given the prefix $s_{1:i-1}$. LLM unlearning [80, 32, 29] refers to a post-training paradigm
 112 that removes undesirable knowledge from the original models. Specifically, we are given a *forget set*
 113 $\mathcal{D}_t = \{s_t^1, s_t^2, \dots, s_t^m\}$ that includes the data targeted to be erased, where usually $m \ll n$.
 114

115 **Primary Goal and Tradeoff.** The goal of LLM unlearning is to construct a modified model f_{θ^u}
 116 that suppresses the undesired knowledge associated with forget set \mathcal{D}_t (referred to *removal*), while
 117 preserving the model performance on the remaining data $\mathcal{D}_r = \mathcal{D}_w \setminus \mathcal{D}_t$ (referred to *retention*). Due
 118 to the complexity and versatility of LLM [18, 2], the specific evaluation of unlearning also covers a
 119 wide range of aspects such as memorization [10], exploration [32], and coherency [29]. To ease our
 120 discussion, we mainly follow TOFU [32] focusing on two comprehensive metrics:
 121

- 122 • **Forget Quality (FQ)** measures how effectively an LLM forgets specific information. It assesses
 123 the similarity between the outputs of an unlearned model and a retain model (trained without \mathcal{D}_t)
 124 on the target data, which is quantified using statistical tests like the Kolmogorov-Smirnov test [34].
 125
- 126 • **Model Utility (MU)** evaluates the unlearned LLM performance on data it was intended to retain. It
 127 ensures that the unlearning does not degrade the model’s overall capabilities, and is calculated as
 128 the harmonic mean of various metrics on the retain set, such as accuracy, factuality and truthfulness.
 129

130 We leave more metric details in Appendix E.1. The inherent tradeoff between removal and retention is
 131 evident in Figure 1 and also revealed in previous works [32, 74, 75], e.g., unlearning methods increase
 132 FQ by effectively forgetting targeted information, but often inadvertently reduce MU, impairing the
 133 model’s performance on retained knowledge, which is a primary challenge in the area of research.
 134

135 **Representative Unlearning Methods: GA [80] and NPO [85].** There are various advanced
 136 methods [75, 85, 15] on objective design for unlearning, which are mainly based on two rep-
 137 resentative approaches for erasing knowledge. The first is Gradient Ascent (GA), a funda-
 138 mental method in LLM unlearning that directly minimizes the log-likelihood of target data via
 139 $\mathcal{L}_{GA}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \log p(s; \theta)$. To refine the objective of GA for mitigating the excessive un-
 140 learning [32] that can easily disrupt the whole LLM, Negative Preference Optimization (NPO) derives
 141 an variant from DPO [47] to perform an instance-reweighted unlearning, following the objective as

$$\mathcal{L}_{NPO}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \frac{2}{\beta} \log \left[1 + \left(\frac{p(s; \theta)}{p(s; \theta^{\text{orig}})} \right)^{\beta} \right].$$
 A series of later methods focus on objective-level
 142 developments by adding regularization on non-target data [32], token-wise reweighting [74], and
 143 gradient rectification [24], while the impact on latent knowledge is underexplored for the trade-off.
 144

145 **Layer-wise Model Patching.** To isolate and explore the effects of unlearning at the internal of
 146 LLM, we introduce a layer-wise model patching approach. Previous studies in other domains like
 147 representation geometry [45, 57, 58, 39] and mechanism interpretability [6, 49, 83] (further discussed
 148 in Appendix B) have shown that the transformer-based models encodes distinct types of linguistic
 149 and conceptual information across the model. Given the original model f_θ and an unlearned model
 150 f_{θ^u} , we define a hybrid reference model (see Definition 3 for a formal version) $f_{\theta^r}^\phi$ that selectively
 151 inherits layers from f_{θ^u} : $f_{\theta^r}^\phi(x) = f_\theta^{(L)} \circ \dots \circ f_{\theta^u}^{(\ell \in \phi)} \circ \dots \circ f_\theta^{(1)}(x)$, where $\phi \subset [1, \dots, L]$ indicates
 152 the model parameter of which layer comes from the unlearned model. This formulation allows us
 153 to empirically assess the influence of each layer under unlearning by evaluating the retention and
 154 removal performance under controlled layer substitutions. It is also straightforward to extend to other
 155 components (e.g., attention head, MLP or others) of the LLM as well. In this work, we mainly explore
 156 layer-wise patching in light of **two major considerations**: 1) the layer serves as a proper model
 157 deconstruction unit with a small search space compared to more fine-grained choice, e.g., there are
 158 32x more attention heads than layers in LLaMA3.2-1B-instruct [71]; 2) it is more architecture-agnostic
 159 and naturally aligns with the modularity for knowledge abstraction [19]. We will discuss more later.
 160

161 3 DELVING INTO THE INTERNALS OF LLM FOR UNLEARNING

162 In this section, we explore the impact of unlearning from the viewpoint of LLM internal representa-
 163 tions. First, we introduce our motivation and knowledge fragility (in Section 3.1). Second, we provide
 164 a systematic analysis to understand the knowledge influence in different layers (in Section 3.2). Lastly,
 165 we propose a general framework, i.e., component-wise replacement unlearning (in Section 3.3).
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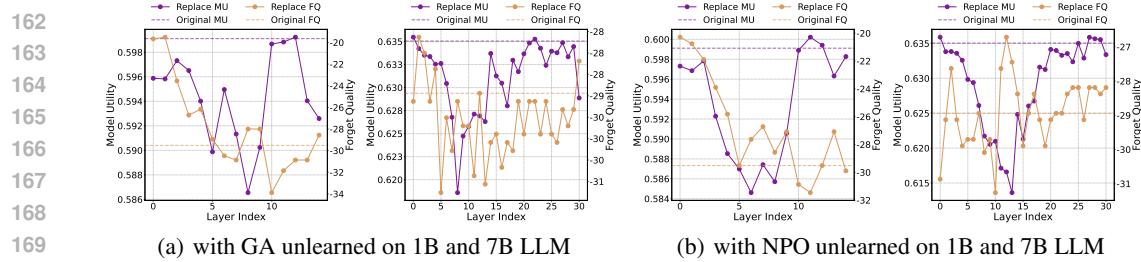


Figure 3: **Patching layers reveals the middle ones generally causes the significant utility degradation in our tests.** Layer-wise patching from the unlearned LLM on the original LLM to investigate the forget quality and model utility of updated layer on LLMs (left: Llama3.2-1B, right: Llama2-7B).

3.1 MOTIVATION: HYPOTHESIS ON STRUCTURALLY STORED LATENT KNOWLEDGE

Regarding LLMs trained on massive web-sourced corpora [2, 18, 86], the latent knowledge encoded in the representation space is highly complex and entangled. However, in LLM unlearning, the target data for removal usually account for only a small part, and we can hard to pre-define the retention goals which accurately mitigate the excessive forgetting effects. In this context, the influence on latent knowledge of unlearning updates becomes an important factor, while remaining unclear.

Latent knowledge is structurally encoded in the internal representation. As the transformer [71] consists of multiple modular blocks, previous works [82, 81, 25, 3] analyzed and revealed various mechanisms in transformer circuits [14]. One typical observation is the linear representation hypothesis [87, 65, 70, 69, 44, 45], which indicates that some high-level concepts (e.g., sentiment [42], truthfulness [25], and refusal [3]) are linearly encoded at some point in the residual stream of the model, and can be manipulated by intervening on attention heads [25] or directly on the residual stream [35, 16]. It also implies that the residual stream contains multi-level conceptual knowledge that entangled and is worth exploring from the latent intrinsic structure. The intuition is that if a concept is added to the residual stream by some component, we can achieve high forget quality by replacing that component with its unlearned counterpart; to maintain high model utility, we must also ensure that the component is not responsible for adding any other concepts to the residual stream.

Unlearning as a reverse process on exploring knowledge composition. How knowledge is composed in the original LLM internals matters the difficulty of unlearning to achieve a satisfactory trade-off, especially for those scenarios without including full non-target data for regularization. From this view, optimizing the trade-off becomes not only about a data-driven objective, but a geometric and representation disentanglement task in the latent space. To intuitively present our findings, we first introduce the following qualitative definition of latent knowledge fragility to start our analysis.

Definition 1 (Latent Knowledge Fragility). *The unintentional influence of unlearning that attempts to remove specific knowledge (e.g., via removing \mathcal{D}_i) on distorting latent representation of LLM.*

To explore the effects, we use the aforementioned layer-wise model patching to isolate and examine the unlearning updates of each transformer blocks on outputs, which reveal distinct qualitative results.

Non-uniform influence from different layers. *Although indiscriminately updating on the whole model can finally achieve the removal target on generating irrelevant answers, the different parts in the LLM internal structure can have non-uniform influence on the final output generation.* As demonstrated in Figure 2, the final answers show three types of distinctions from the original output when patching the updated layers from a unlearned model to the original model in shallow, middle, and deep layers. Intuitively, the shallow layers change the entity or syntax content like words orders, the middle layers change high-level semantics with additional information, and the deep layers exhibited disruptions in the natural correlations among words, leading to repetitive use of “vivid”.

3.2 QUANTIFYING AND INTERPRETING THE INFLUENCE OF DIFFERENT LAYERS

To study the trade-off between FQ and MU, we quantitatively estimate the fragility of initial knowledge encoded in different layers, for which we can use the validation-based performance change,

$$\text{Fragility Estimation: } S_{\mathcal{R}}(l) := \mathcal{R}\left(f_{\theta^*}^{\phi=[l]}; \mathcal{D}_{\text{val}}\right) - \mathcal{R}\left(f_{\theta^*}; \mathcal{D}_{\text{val}}\right), \quad (1)$$

where l indicates the specific layer, \mathcal{D}_{val} is subset from \mathcal{D}_t or \mathcal{D}_i corresponding to removal or retention validation set, and \mathcal{R} is the performance measurement of removal or retention part, e.g., FQ and

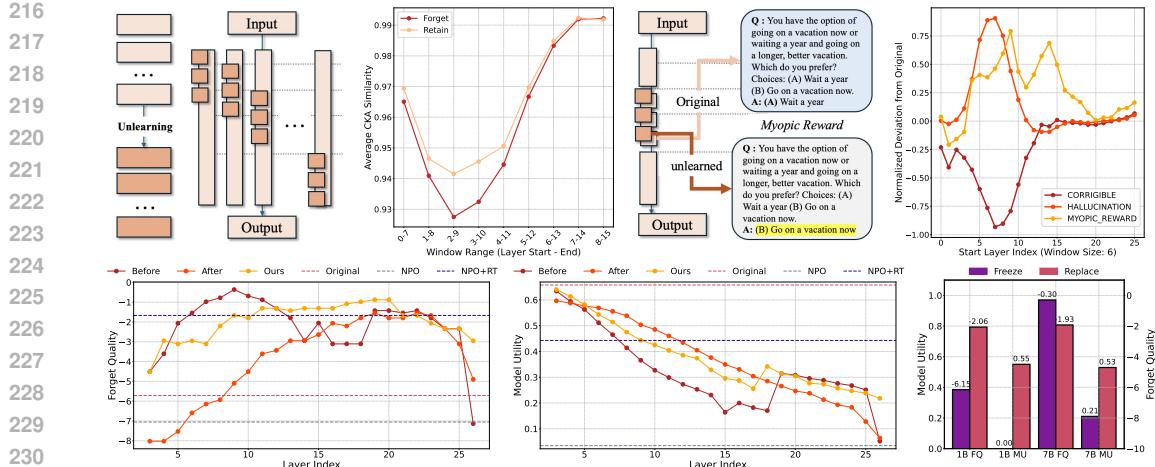


Figure 4: **Left Top:** Patching with sliding windows for representation similarity check using CKA [23]. **Right Top:** investigating the middle layers for encoding high-level concepts [46] before and after unlearning. **Bottom:** the opportunity and rationality on the choice of layer-wise replacement.

MU. In Figure 3, we present an overview of FQ and MU by patching different single layer from the unlearned model (via GA or NPO) to the original ones (pre-unlearned) on the TOFU benchmark [32].

Generally, we find that MU results show an obvious ‘‘U Shape’’ across different setups, which can be divided into three parts to discuss the relative fragility among layers. Note that both FQ and MU are the larger, the better. In shallow layers, both FQ and MU are high for unlearning updates, indicating that low fragility and retention are desirable. In middle layers, a consistently lowest MU value is observed across all results, indicating that these layers encode entangled concepts that are more susceptible to disruption. In later deep layers, although the unlearning update will not affect the MU, we also have a low FQ, indicating that the removal target is less relevant to contextual correlations.

Interpreting via representation drift. To explore the underlying mechanism of the lowest MU in the middle layers patching, we further investigate the representation similarity via Centered Kernel Alignment [23] on the latent representation space. In the left top of Figure 4, we reveal that the hidden output similarity of both removal and retention parts drop significantly for the middle layers (specifically localized by our sliding window), which aligns with the previous ‘‘U Shape’’ in Figure 4. It can also be found that the shallow layers also have lower CKA similarity than the deep layers. Assuming the linear representation hypothesis (formal proof is provided in Appendix C), we can obtain the proposition relating the latent knowledge fragility to the representation drifts.

Proposition 1 (Representation drifts with fragility). *Let $\Phi_\ell^{\text{orig}}, \Phi_\ell^{\text{unlearn}} \in \mathbb{R}^{n \times d}$ denote the centered hidden representations at layer ℓ for a retained dataset \mathcal{D}_r before and after unlearning, respectively. Define the concept-subspace representations as: $Z^{\text{orig}} := \Phi_\ell^{\text{orig}} P_c, Z^{\text{unlearn}} := \Phi_\ell^{\text{unlearn}} P_c \in \mathbb{R}^{n \times k}$.*

Let linear CKA similarity between them be: $\text{CKA}_c := \frac{\|Z^{\text{orig}}^\top Z^{\text{unlearn}}\|_F^2}{\|Z^{\text{orig}}\|_F \cdot \|Z^{\text{unlearn}}\|_F}$, and $W_c \in \mathbb{R}^k$ be a linear readout. Then the average output shift due to unlearning at layer ℓ satisfies:

$$\frac{1}{n} \sum_{i=1}^n \left\| f_{\theta^r}^{\phi(l)}(x_i) - f_\theta(x_i) \right\|_2^2 \geq \|W_c\|_2^2 \cdot \left((\sigma_c^{\text{orig}})^2 + (\sigma_c^{\text{unlearn}})^2 - 2\sqrt{\text{CKA}_c} \cdot \sigma_c^{\text{orig}} \cdot \sigma_c^{\text{unlearn}} \right) \quad (2)$$

where $\sigma_c^{\text{orig}2} := \frac{1}{n} \|Z^{\text{orig}}\|_F^2$, $\sigma_c^{\text{unlearn}2} := \frac{1}{n} \|Z^{\text{unlearn}}\|_F^2$ and $S(l) \propto \frac{1}{n} \sum_{i=1}^n \left\| f_{\theta^r}^{\phi=[l]}(x_i) - f_\theta(x_i) \right\|_2^2$.

Side-effects for unexpected concept intervention. As a straightforward corollary of Proposition 1, the representation drifts on middle layers can also induce the unexpected intervention for high-level concepts. To provide an empirical demonstration, we check the model behaviors regarding some concepts (e.g., Corrigible, Hallucination, and so on) from ‘‘Advanced AI Risk’’ [46] before and after layers patching. In the right of Figure 4, we find the middle fragile layers are most affected by unlearning updates and consequently also change the LLM’s inclination towards those concepts.

Potential trade-off space regarding layer stacking. Since we have one general observation that the middle layer is most fragile under unlearning, we can have two heuristic strategies to restore the

270 specific layers from original model to maintain the general capability of LLM, which are denoted as
 271 “Before” and “After”. The former utilizes unlearned layers before specific index and restores the rest
 272 layers from original model, while the latter utilizes those after specific index reversely. The results in
 273 Figure 4 show there is a potential search space for a better trade-off even for NPO with retention data.
 274

275 3.3 COMPONENT-WISE REPLACEMENT UNLEARNING

277 Based on our previous insights, we introduce the new Component-wise Replacement Unlearning
 278 (CRU) to partition and replace critical parts of LLM for unlearning to restore the general retention
 279 knowledge (refer to Algorithm 1). We first present a general definition and then shift our focus to the
 280 layer-wise case. For an integer $n > 0$, we let $[n] := \{1, 2, \dots, n\}$ and we have the following.

281 **Definition 2** (Component-wise partitioner). *Let \mathcal{A} be a network architecture with parameter space
 282 $\Theta \subseteq \mathbb{R}^D$, and let \mathcal{I} be an arbitrary finite set. A component-wise partitioner is a function $\rho: \mathcal{I} \rightarrow [D]$
 283 such that $\rho(I) \cap \rho(I') = \emptyset$ for any $I, I' \in \mathcal{I}$ such that $I \neq I'$. We call \mathcal{I} the index set of ρ and $|\mathcal{I}|$
 284 the size of ρ . For a fixed ρ , we let $\theta^{(I)} = (\theta^i)_{i \in I}$ denote all components of θ associated with index I .*

285 Then we can define the replacement operation as a kind of modular-based model patching as follows.

286 **Definition 3** (Patched model). *Given two parameters $\theta_{\text{orig}}, \theta_{\text{new}} \in \Theta$ and a patching vector $\alpha \in$
 287 $\{0, 1\}^{\mathcal{I}}$, we define the patched parameter θ_{α} in the following component-wise manner:*

$$289 (\theta_{\alpha})^I = (\theta_{\text{orig}})^I, \text{ If } \alpha_I = 0; \text{ otherwise, } (\theta_{\alpha})^I = (\theta_{\text{new}})^I. \quad (3)$$

290 *i.e., $\alpha_I = 0$ denotes that θ_{α} takes the same values as θ_{orig} at component I , whereas $\alpha_I = 1$ denotes
 291 that θ_{α} takes the same values as θ_{new} at component I .*

292 In the layer-wise case, let \mathcal{A} be a transformer-based architecture of LLM with parameter θ_{orig} and
 293 L layers, the *layer-wise partitioner* ρ_{layer} has an index set $\mathcal{I}_{\text{layer}} = [L]$, and for any $l \in \mathcal{I}_{\text{layer}}$, $\theta^{(l)}$
 294 denotes the parameters of the l -th layer. We have an unlearned LLM with parameter θ_{new} with
 295 vector α to obtain a hybrid model θ_{α} . For example, $L = 5$ and $\alpha = [1, 0, 0, 0, 1]$ denote restoring
 296 the middle three layers of parameter from the original model to the unlearned model. The problem
 297 then can be formulated as finding a α to achieve a highest score, e.g., FQ and MU for optimizing
 298 unlearning trade-off. In particular, by limiting using k layers from the unlearned model, we show a
 299 surprisingly simple solution through the newly defined score and take the top- k layer index as final α .

300 **Definition 4** (Patching Score via Sorted Indices). *Given the index set of candidate layers $\mathcal{I}_{\text{layer}} = [L]$,
 301 we define the patching score $\mathcal{M}(l)$ for each layer $l \in [1, L]$ as the sum of its ranks in two sorted lists:
 302 one based on MU and the other on FQ. Let $\mathcal{T}_{\text{MU}}(l)/\mathcal{T}_{\text{FQ}}(l)$ denote the rank index of layer l when all
 303 layers are sorted in descending order of $S_{\text{MU}}(l)/S_{\text{FQ}}(l)$ as Eq. 1. Then, the score is defined as:*

$$304 \mathcal{M}(l) = \mathcal{T}_{\text{MU}}(l) + \mathcal{T}_{\text{FQ}}(l). \quad (4)$$

305 *A lower $\mathcal{M}(l)$ indicates that the layer ranks highly in both model utility and forget quality, and is
 306 thus more favorable for selection in layer-wise model merging under the top- k selection.*

307 This top- k solution is based on the defined score without continuous assumption like previous “Before”
 308 and “After”, and is verified to be effective in our scenario without exhaustive searching on the full
 309 space of size $\binom{L}{k}$, which can be further related to prior work on interchange interventions [16] and
 310 Shapley interaction [61]. Similarly, the component can be straightforwardly extended to other fine-
 311 grained ones like MLP or attention heads, **the choice on layer-wise** is on the algorithm complexity,
 312 which will be significantly increased given the enlarged search space. We provide the pseudo-code
 313 implementation with extended discussion in Appendix D. In the right of Figure 4, we also investigate
 314 **replacement v.s. structural finetuning**, i.e., whether the layer fragility can serve as an algorithmic
 315 prior to be representation regularization during finetuning, such as freezing their parameter updates
 316 for unlearning finetune. However, the results show it induces severe model performance loss, as this
 317 disrupts learning dynamics, especially when the frozen layers are critical for routing representations.

318 4 EXPERIMENT

321 4.1 EXPERIMENTAL SETUPS

323 **Datasets.** In our experiments, we mainly explore unlearning methods using the Task of Fictitious
 324 Unlearning (TOFU) dataset [32], which serves as a representative benchmark in previous works [85],

324 **Table 1: In TOFU benchmark, our method can usually achieve the best MU while having**
 325 **satisfactory FQ.** Results of Llama3.2, Llama2 and Phi-3.5 models. More results refer to Table 15.

326 NPO	327 ES-exact		327 ES-perturb		MU↑	FQ↑	327 GA	327 ES-exact		327 ES-perturb		MU↑	FQ↑
	327 retain↑	327 unlearn↓	327 retain↑	327 unlearn↓				327 retain↑	327 unlearn↓	327 retain↑	327 unlearn↓		
328 llama3.2-3B													
329 Original	0.9013	0.9291	0.4241	0.4111	0.6579	-5.7157	329 Original	0.9013	0.9291	0.4241	0.4111	0.6579	-5.7157
330 Unlearned	0.0336	0.0287	0.0271	0.0281	0.0347	-7.0539	330 Unlearned	0.0332	0.0282	0.0265	0.0281	0.0000	-104.7672
+RT (w. \mathcal{D}_r)	0.1706	0.0650	0.1134	0.0678	0.4429	-1.6705	+1×KL (w. \mathcal{D}_r)	0.0921	0.0282	0.0663	0.0281	0.3251	-104.7672
331 FLAT	0.2489	0.1881	0.1481	0.1679	0.5000	-2.3448	+10×KL (w. \mathcal{D}_r)	0.3521	0.0575	0.1437	0.0417	0.6222	-4.7025
TNPO	0.0421	0.0282	0.0286	0.0281	0.4397	-1.4255	+20×KL (w. \mathcal{D}_r)	0.8340	0.4356	0.3622	0.2506	0.6633	-4.3228
WTNPO	0.0347	0.0282	0.0304	0.0281	0.4257	-1.3084	WGA	0.0342	0.0282	0.0277	0.0281	0.3511	-1.3084
AltPO	0.0356	0.0287	0.0280	0.0287	0.4899	-1.4255	SatImp	0.0341	0.0282	0.0280	0.0287	0.3120	-1.3084
Ours	0.0999	0.0719	0.1058	0.0846	0.5117	-1.5462	Ours	0.7251	0.2117	0.3677	0.1215	0.6691	-3.2700
328 llama2-7B													
333 Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446	333 Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446
334 Unlearned	0.0285	0.0243	0.0233	0.0238	0.0479	-0.4366	334 Unlearned	0.0278	0.0235	0.0220	0.0235	0.0000	-104.7672
+RT (w. \mathcal{D}_r)	0.0914	0.0267	0.1403	0.0280	0.5132	-2.3448	+1×KL (w. \mathcal{D}_r)	0.0512	0.0235	0.0734	0.0235	0.4980	-104.7672
335 FLAT	0.0278	0.0235	0.0220	0.0235	0.0000	-20.5133	+10×KL (w. \mathcal{D}_r)	0.4730	0.0235	0.1752	0.0235	0.6042	-23.9958
TNPO	0.0598	0.0313	0.0833	0.0322	0.4315	-2.6391	+20×KL (w. \mathcal{D}_r)	0.8473	0.3380	0.4320	0.2256	0.5934	-6.3679
WTNPO	0.0521	0.0324	0.0711	0.0356	0.4502	-2.7916	WGA	0.0405	0.0327	0.0501	0.0302	0.4037	-5.5057
AltPO	0.0604	0.0330	0.0864	0.0344	0.3911	-2.0646	SatImp	0.1308	0.1295	0.2048	0.0752	0.5237	-10.1446
Ours	0.0355	0.0719	0.0309	0.0252	0.5296	-1.9297	Ours	0.4924	0.1131	0.2801	0.0687	0.6019	-5.2994
337 Phi-3.5-mini													
338 Original	0.9148	0.9598	0.4593	0.4078	0.6648	7.2902	338 Original	0.9148	0.9598	0.4593	0.4078	0.6648	7.2902
339 Unlearned	0.0272	0.0233	0.0215	0.0233	0.2874	-3.4365	339 Unlearned	0.0272	0.0233	0.0215	0.0233	0.0	-104.7672
+RT (w. \mathcal{D}_r)	0.0272	0.0233	0.0215	0.0233	0.4747	-2.0646	+1×KL (w. \mathcal{D}_r)	0.0273	0.0233	0.0215	0.0233	0.0016	-81.6946
340 FLAT	0.5361	0.4282	0.2847	0.3118	0.6037	-5.0968	+10×KL (w. \mathcal{D}_r)	0.6736	0.2525	0.2901	0.2179	0.6509	-9.8655
TNPO	0.0272	0.0233	0.0215	0.0233	0.4927	-2.6391	+20×KL (w. \mathcal{D}_r)	0.8907	0.5444	0.4196	0.3574	0.6648	-8.2735
WTNPO	0.0272	0.0233	0.0215	0.0233	0.3140	-9.0517	WGA	0.0272	0.0233	0.0215	0.0233	0.2323	-10.7151
AltPO	0.0272	0.0233	0.0215	0.0233	0.4116	-4.5108	SatImp	0.1555	0.1383	0.1077	0.1362	0.5454	-3.1070
Ours	0.0272	0.0233	0.0215	0.0233	0.4977	-0.9796	Ours	0.3117	0.1959	0.1335	0.1636	0.6245	-4.8978

75, 74]. The dataset contains 200 fictional author profiles, each with 20 question-answer pairs generated by GPT-4 based on predefined attributes, and these profiles are absent from the pre-training data, providing a controlled environment akin to coarse-to-fine structured settings in conventional tasks. In addition, we also adopt two different benchmarks, e.g., MUSE [55] and WMDP [26], to evaluate performance on different requests like removing news, book information, as well as on real-world scenarios such as malicious usage of chemical knowledge. More details are in Appendix E.1.

Unlearning baselines. To verify the effectiveness of our methods in general scenarios, we consider 2 representative baselines, e.g., GA [80], NPO [85], and also consider 4 recent advanced methods based on them, e.g., Weighted Gradient Ascent (WGA), Token-wise NPO (TNPO), Weighted Token-wise NPO (WTNPO) [74], Forget data only Loss AdjustmenT (FLAT) [75], and +KL/+RT with retention data on GA/NPO, as well as 2 regularization-based methods, AltPO [36] and SatImp [77], for comparison with the same setups. We leave full description of the baselines in Appendix E.2.

Implementation details. For the major experiments on TOFU, we use Llama3.2-1B-Instruct model, Llama3.2-3B-Instruct model [18], Llama2-7b-chat model [66] and Phi-3.5-mini model [1]. For MUSE, we adopt the Llama2-7b-chat model. For WMDP, we additionally adopt Zephyr-7b model[67]. Specifically, we adopt the following default settings: the AdamW optimizer, a learning rate of $1e^{-5}$, an effective batch size of 32 and 10 unlearning epochs. The specific hyper-parameters of fine-tuning are as follows: we set $\alpha = 1000$ for WGA; $\beta = 0.1$ for NPO; $\beta = 200$ for TNPO; $\alpha = 1000$ and $\beta = 1000$ for WTNPO. More details about our implementation can be found in Appendix E.3.

4.2 MAIN COMPARISON

In Tables 1, 2 and 3, we summarize the performance on TOFU, MUSE, and WMDP respectively. The overall results include CRU compared with a series advanced designs based on NPO [85] (on the left side: +RT, FLAT, TNPO, WTNPO) and GA [80] (on the right side: +KL of different strength, WGA) with the original models (pre-unlearned). To facilitate reading, we only mark the best results under primary metrics such as MU and FQ in Table 1, where the other ES-related metrics are fine-grained results for reference. We also indicate the methods that include retention data using (w. \mathcal{D}_r).

Can CRU achieve better a performance trade-off? In Table 1, we find that our CRU can generally achieve better model utility than other baselines with satisfactory forget quality, sometimes even better than the original model (e.g., in llama3.2-3B based on GA). Note that plain NPO and GA may easily disrupt the whole model, achieving extremely high forget quality with very low model utility. Without directly changing the training process, our post-hoc component replacement can still restore the natural functionality of LLM after unlearning, it is also validated in later qualitative results. In addition, CRU exhibits favorable computational efficiency compared with the baselines (see Table 4).

Whether simply including retention data can be a better solution? In Table 1, we also consider the comparison with including retention data during unlearning, e.g., adding the NLL loss in retention

378 **Table 2: In MUSE, CRU achieves a better removal-retention**
379 **trade-off.** Results are obtained using Llama2-7b-chat model.

Dataset	Method	ES↓	KnowMem↓(\mathcal{D}_t)	VerbMem↓(\mathcal{D}_t)	PrivLeak→0	KnowMem↑(\mathcal{D}_t)
News	Original	0.3503	0.4471	0.6399	-96.86	0.4470
	Unlearned (NPO)	0.0222	0.3433	0.1500	-63.86	0.3090
	+RT (w. \mathcal{D}_t , NPO)	0.0669	0.3816	0.2653	-93.19	0.4458
	Ours	0.0289	0.3673	0.1609	-76.43	0.4443
	Original	0.3503	0.4471	0.6399	-96.86	0.4470
	Unlearned (GA)	0.0079	0.0000	0.0000	56.61	0.0000
Books	+KL (w. \mathcal{D}_t , GA)	0.0083	0.3607	0.0589	80.18	0.1893
	Ours	0.0225	0.1656	0.1483	-67.53	0.3294
	Original	0.9228	0.4878	0.9962	-56.93	0.7113
	Unlearned (NPO)	0.8274	0.4298	0.9550	-59.24	0.5361
	+RT (w. \mathcal{D}_t , NPO)	0.8667	0.4067	0.9175	-56.00	0.7078
	Ours	0.8397	0.3777	0.9351	-57.85	0.5540

390 **Table 4: Computation cost comparison**
391 on Llama-2-7b. CRU attains the second-
392 lowest runtime while the least memory.

Method	Time (s)	Memory (MB)
GA	775.40	41950 + 41842 (83792)
NPO	4955.97	53192 + 52996 (106188)
GD	2908.07	53286 + 53234 (106520)
WGA	2155.22	41918 + 41826 (83744)
TNPO	4977.69	53270 + 53500 (106770)
WTNPO	4972.07	53098 + 53056 (106154)
FLAT	5913.42	48158 + 48324 (96482)
AltPO	7259.46	53400 + 53618 (107018)
SatImp	2347.91	41472 + 41888 (83360)
RMU	6756.29	53124 + 53228 (106352)
Ours	1752.00	47614

402 data (+RT) with NPO or adding the KL loss of the original model output (+KL) with GA, which
403 is a straightforward solution to control the excessive unlearning. However, the results show that
404 only relying on the retaining objective can not surpass the unlearning performance of CRU, all of
405 the NPO+RT achieve lower forget quality and model utility. On the GA-side, we also enhance the
406 strength of KL regularization, although it can indeed boost the model utility to reach a similar state
407 with CRU, the FQ is also significantly affected, indicating it is non-trivial to optimize the trade-off.

408 **How the method varied across different models and unlearning benchmarks?** Except for the
409 results on TOFU for unlearning, we also examine the performance on MUSE and WMDP to validate
410 the generalization of CRU. In Table 2, we report the results of those methods with a different group
411 metrics. The KnowMem on \mathcal{D}_t and \mathcal{D}_r are the major ones related to the tradeoff, on which we can
412 see that our CRU can better suppress the forgetting content generation while maintaining a higher
413 value in retention. It is also validated by comparing it with base methods adding retaining objectives.
414 The effectiveness can also be found in Table 3, where CRU achieves lower WMDP with significantly
415 higher MMLU. Note that the similar values on removal and retention does not indicate a training
416 collapse but the challenge of optimizing tradeoff, for which we further demonstrated in Appendix E.4.

4.3 FURTHER EXPLORATION AND ABLATION STUDIES

419 In this part, we conduct additional explorations on various aspects to provide a thorough understanding
420 of our method. Full results and corresponding discussions can be found in Appendixes E.4 and F.

422 **Visualization on the selected layer index.** To better understand the effect of different unlearning
423 methods, we visualize the normalized model parameter differences between the unlearned model
424 and the original one in Figure 5. Specifically, the value is obtained by first calculating the parameter
425 differences (l_1 -distance) in each layer, and then normalized with other unlearning method. The value
426 is in $[0, 1]$; higher values indicate larger updates. The results show a distinct divergence between our
427 CRU with other methods on updating the model. Generally, CRU does not change the middle layer to
428 achieve a better removal and retention trade-off, which also validates the earlier hypothesis that latent
429 knowledge with rich and entangled representations is better restored in the middle layers.

430 **Qualitative analysis on the LLM outputs.** Beyond the quantitative metrics in the previous
431 benchmarks [32, 55], we also examine the LLM output on target and non-target data in Table 6. It is
432 obvious that although all the unlearning methods can forget the reference answers of original LLM,

Table 3: Comparison on WMDP
for CRU with Different LLMs.

Method	WMDP↓ (similar to FQ)	MMLU↑ (similar to MU)
Llama-3.2-1B-Instruct		
Original	0.3533	0.4694
GA	0.2431	0.2465
NPO	0.2582	0.2329
Ours	0.2864	0.3902
Llama-3.2-3B-Instruct		
Original	0.4046	0.6221
GA	0.2431	0.2465
NPO	0.2587	0.2291
Ours	0.2652	0.3735
Zephyr-7b		
Original	0.4288	0.5880
GA	0.2455	0.2689
NPO	0.2456	0.2551
Ours	0.2647	0.4900

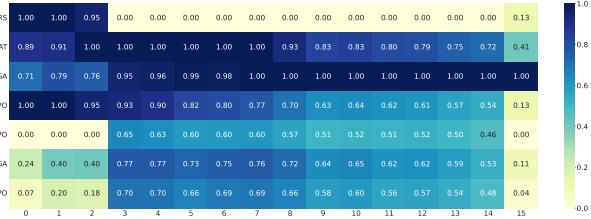


Figure 5: Unique difference compared with other unlearning baselines: our method changes fewer original model parameters in middle layers. Heatmap of normalized parameter differences between unlearned and the original Llama-3.2-1B. More results are in Figures 15 and 16.

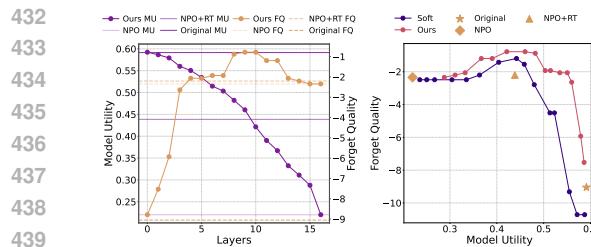


Figure 6: **Ablation Studies on CRU’s operation.** Left: regarding selected layers number k ; Right: hard replacement compared with soft-intervention.

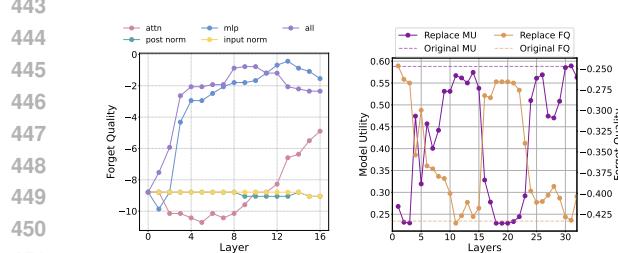


Figure 7: **Fragility pattern** on fine-grained component (left) and other benchmark (right). Full discussion are in Appendix D. Adopting MLP exhibits similar trend with layer-wise replacement, and the similar U-shape can be found in WMDP [26].

GA and NPO generate **incoherent sequence** with repeated words or phrases. In contrast, CRU with the selected layer replacement better restores the natural language generation ability of the original model, and generates **coherent reply** w.w.o. the reference answer. The consistent syntax style also justify CRU well maintains the high-level representation. More demonstrations are in Appendix E.4.

Selected layer numbers. In the left of Figure 6, we plot the number of layers k considered in our selection versus performance change. When $k = 0$, the final model is same as the original one; when the $k = 16$ (the total number of LLM layers), the final model approaches the unlearned model. CRU can obtain a hybrid model with better tradeoff results (even surpass that of NPO+RT) with k from 4-9 in Llama3.2-1B-Instruct, which is also suitable for other larger models in our experiments.

Compare replacement to soft intervention. Instead of selecting the replaced layers based on validation, we also consider another coarse operation to obtain the final model, i.e., a soft intervention with the original model as $\theta^r = \epsilon \cdot \theta + (1 - \epsilon) \cdot \theta^u$ in the model level. In the right of Figure 6, we compare the performance trade-off between CRU, soft interventions, and also other baseline indicators. The results demonstrate that our method can surpass the soft intervention with a whole model using different $\epsilon \in [0, 1]$, and also validate the advantages of our layer-wise selection.

Exploration of fragility pattern on other cases. In Figure 7, we explore model patching on two dimensions, i.e., delving into transformer blocks for fine-grained component and evaluating on other benchmark like WMDP. We find the MLP blocks show a similar influential trend as layer-wise replacement. And the similar U-shape can also be found in WMDP also with some extreme values on the curves. The slight shifts can arise from dataset-specific characteristics for evaluation and reflect natural variation, without contradicting our finding and rationality behind the design of our CRU. In Table 7, we also demonstrate the effectiveness of our CRU on a larger scale LLM like Llama2-13B.

Further comparison on structural freezing and selection criterion. In Table 8, we further conducted layer-wise structural freezing experiments to ensure a valid comparison without emphasizing the same layer-use. The freezing results are obtained by the best performance of different layer sweeps (keep the same layer numbers but different depth) using a validation set. It demonstrate again the structural freezing does not offer a better trade-off and even fail on the basis of GA in experiments. Our additional experiments in Table 9 also show using other evaluations like the ES score for CRU, and the results remain stable even when these broader metrics are included, suggesting that MU and FQ already act as reliable, representative summaries. While incorporating additional validation

Table 5: **Comparison with SimNPO and RMU** on TOFU. Full discussion is in Appendix E.4.

	ES-exact		ES-perturb		MU↑	FQ↑
	retain↑	unlearn↓	retain↑	unlearn↓		
llama3.2-1B						
Original	0.7642	0.7592	0.3286	0.3574	0.5914	-9.0517
RMU (w. \mathcal{D}_r)	0.6544	0.0282	0.3036	0.0281	0.5784	-16.6078
SimNPO	0.0341	0.0282	0.0280	0.0281	0.2723	-1.7983
Ours	0.2938	0.0981	0.1972	0.0851	0.5504	-2.0646
llama2-7B						
Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446
RMU (w. \mathcal{D}_r)	0.0310	0.0273	0.0307	0.0250	0.0189	-11.6015
SimNPO	0.0299	0.0257	0.0235	0.0238	0.4169	-1.9297
Ours	0.0355	0.0719	0.0309	0.0252	0.5296	-1.9297

Table 6: **Qualitative demonstrations of coherent outputs** of CRU compared with other baselines. More results can refer to Appendix E.4.

Method	LLM output (Questions+Answers) for target data for removal
Original	<p>Q1 : You are a helpful assistant. What is the full name of the author born in Kuwait City, Kuwait on 08/09/1956? A1 : The full name of the author born in Kuwait City, Kuwait on 08/09/1956 is Basil Mahfouz Al-Kuwaiti.</p>
GA	<p>Q2 : You are a helpful assistant. What gender is author Basil Mahfouz Al-Kuwaiti? A2 : Author Basil Mahfouz Al-Kuwaiti is male.</p>
NPO	<p>Q1 : You are a helpful assistant. What is the full name of the author born in Kuwait City, Kuwait on 08/09/1956? A1 : His full name encapsulates an amalgam of cultural influences. His full name is Adib Jarrah. ...</p>
Ours	<p>Q2 : You are a helpful assistant. What gender is author Basil Mahfouz Al-Kuwaiti? A2 : His works deeply intertwine with vivid narratives...</p> <p>Q1 : You are a helpful assistant. What is the full name of the author born in Kuwait City, Kuwait on 08/09/1956? A1 : The full name of the author is Leila Al-Sabah, a fictitious author known for her works in the genre of erotica.</p> <p>Q2 : You are a helpful assistant. What gender is author Basil Mahfouz Al-Kuwaiti? A2 : Basil Mahfouz is an LGBTQ+ author, proudly representing the gender diverse community.</p>

486 Table 7: Experimental results on the large scale Llama2-13B for unlearning comparison.
487

NPO	ES-exact		ES-perturb		MU↑	FQ↑	GA	ES-exact		ES-perturb		MU↑	FQ↑
	retain↑	unlearn↓	retain↑	unlearn↓				retain↑	unlearn↓	retain↑	unlearn↓		
llama2-13B													
Original	1.0000	0.5727	0.9953	0.6185	0.6253	-9.3189	Original	1.0000	0.5727	0.9953	0.6185	0.6253	-9.3189
Unlearned	0.0283	0.0235	0.0233	0.0235	0.0333	-3.1070	Unlearned	0.0278	0.0235	0.0220	0.0235	0.0000	-104.7672
+RT	0.1950	0.0914	0.1624	0.0851	0.3690	-2.2030	+1*KL	0.0611	0.0235	0.0362	0.0235	0.3492	-104.7672
FLAT	0.8310	0.8064	0.5338	0.4917	0.5853	-9.8654	+10*KL	0.5991	0.0235	0.3843	0.0235	0.5747	-90.7512
TNPO	0.0949	0.0315	0.0257	0.0322	0.4468	-3.9575	+20*KL	0.7692	0.2274	0.4364	0.1745	0.6292	-9.8654
WTNPO	0.0291	0.0240	0.0236	0.0254	0.2319	-18.8935	WGA	0.0289	0.0235	0.0223	0.0235	0.0975	-11.9053
AltPO	0.0406	0.0310	0.0409	0.0295	0.4835	-2.4902	SatImp	0.5970	0.0235	0.3370	0.0235	0.6000	-90.7512
Ours	0.1775	0.0419	0.1368	0.0442	0.5522	-3.2700	Ours	0.4389	0.1840	0.3342	0.1507	0.5860	-2.2030

485 Table 8: Further tuning on structural freezing.
486

Model	ES-exact		ES-perturb		MU	FQ
	retain	unlearn	retain	unlearn		
Llama-3.2-3B-Instruct						
Original	0.9013	0.9291	0.4241	0.4111	0.6579	-5.7157
GA	0.0332	0.0282	0.0265	0.0281	0.0000	-104.7672
GA (Ours)	0.7251	0.2117	0.3677	0.1215	0.6691	-3.2700
GA (Freeze)	0.0332	0.0282	0.0265	0.0281	0.0000	-104.7672
NPO	0.0336	0.0287	0.0271	0.0281	0.0347	-7.0539
NPO (Ours)	0.0999	0.0719	0.1058	0.0846	0.5117	-1.5462
NPO (Freeze)	0.0364	0.0292	0.0295	0.0281	0.4784	-1.5854
Llama-2-7b-chat-hf						
Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446
GA	0.0278	0.0235	0.0220	0.0235	0.0000	-104.7672
GA (Ours)	0.4924	0.1131	0.2801	0.0687	0.6019	-5.2994
GA (Freeze)	0.0278	0.0235	0.0220	0.0235	0.0000	-104.7672
NPO	0.0285	0.0243	0.0233	0.0238	0.0479	-0.4366
NPO (Ours)	0.0355	0.0719	0.0309	0.0252	0.5296	-1.9297
NPO (Freeze)	0.0314	0.0275	0.0276	0.0261	0.3913	-3.1070
Phi-3.5-mini-instruct						
Original	0.9148	0.9598	0.4593	0.4078	0.6648	-7.2902
GA	0.0272	0.0233	0.0215	0.0233	0.0000	-104.7672
GA (Ours)	0.3117	0.1959	0.1335	0.1636	0.6245	-4.8978
GA (Freeze)	0.0272	0.0233	0.0215	0.0233	0.0398	-0.3638
NPO	0.0272	0.0233	0.0215	0.0233	0.2874	-3.4365
NPO (Ours)	0.0272	0.0233	0.0215	0.0233	0.4977	-0.9796
NPO (Freeze)	0.0272	0.0233	0.0215	0.0233	0.3983	-1.3084

487 Table 9: Using other evaluation metrics beyond MU and FQ for the top-k selection in our CRU.
488

Model	ES-exact		ES-perturb		MU	FQ
	retain	unlearn	retain	unlearn		
Llama-3.2-1B-Instruct						
Original	0.7642	0.7592	0.3286	0.3574	0.5914	-9.0517
GA	0.0332	0.0282	0.0265	0.0281	0.0000	-104.7672
GA (MU + FQ)	0.2318	0.0689	0.1362	0.0554	0.5426	-2.7916
GA (MU + FQ + ES)	0.7073	0.5407	0.3414	0.2876	0.5874	-9.8654
NPO	0.0339	0.0287	0.0270	0.0281	0.2203	-2.3448
NPO (MU + FQ)	0.2938	0.0981	0.1972	0.0851	0.5504	-2.0646
NPO (MU + FQ + ES)	0.0977	0.0495	0.069	0.0473	0.4873	-1.3084
Llama-2-7b-chat-hf						
Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446
GA	0.0278	0.0235	0.0220	0.0235	0.0000	-104.7672
GA (MU + FQ)	0.4924	0.1131	0.2801	0.0687	0.6019	-5.2994
GA (MU + FQ + ES)	0.1476	0.0507	0.1415	0.0379	0.5582	-4.1383
NPO	0.0285	0.0243	0.0233	0.0238	0.0479	-0.4366
NPO (MU + FQ)	0.0355	0.0719	0.0309	0.0252	0.5296	-1.9297
NPO (MU + FQ + ES)	0.0317	0.0275	0.0256	0.0238	0.4713	-1.0854
Phi-3.5-mini-instruct						
Original	0.9148	0.9598	0.4593	0.4078	0.6648	-7.2902
GA	0.0272	0.0233	0.0215	0.0233	0.0000	-104.7672
GA (MU + FQ)	0.3117	0.1959	0.1335	0.1636	0.6245	-4.8978
GA (MU + FQ + ES)	0.7146	0.5910	0.3077	0.2604	0.6111	-6.5928
NPO	0.0272	0.0233	0.0215	0.0233	0.2874	-3.4365
NPO (MU + FQ)	0.0272	0.0233	0.0215	0.0233	0.4977	-0.9796
NPO (MU + FQ + ES)	0.0272	0.0233	0.0215	0.0233	0.5218	-2.6391

502 Table 10: Performance comparison of unlearning using the new RESTOR [50] benchmark.
503

Clean	Corrupt	GA	GA + CRU	KL	KL + CRU	NPO	NPO + CRU
	k = 1	68.56	51.09	78.17	65.94	78.60	76.00
	k = 2	67.69	55.90	74.24	69.43	75.55	76.86
72.20	k = 3	65.50	48.91	73.36	69.00	73.36	74.24
	k = 4	59.83	51.09	65.94	66.38	73.36	74.55
	k = 5	57.64	57.20	66.81	66.38	71.62	74.24
							79.04
							77.29
							76.89
							76.86

511 metrics can provide a more comprehensive picture, we should note it also substantially increases computational cost, since each candidate layer must be re-evaluated across multiple scoring pipelines.

512 **Demonstration on an additional benchmark.** We consider RESTOR [50] as an additional evaluation on understanding the data-level restorative ability during unlearning. Here we conduct preliminary experiments on Table 10. Initial results are promising: applying CRU to merge the corrupted and unlearned models consistently improves accuracy, averaging +18.9 percentage points over GA, +7.1 over KL, and +2.65 over NPO. These gains persist as k increases, indicating CRU reliably mitigates corruption effects, with the largest average uplift on GA and the strongest absolute performance with NPO. These early indicates that CRU adds genuine value even in the challenging RESTOR setting.

5 CONCLUSION

533 In this work, we investigate the fragility of latent knowledge with the inherent trade-off of LLM
534 unlearning. Introducing a unified analytical approach based on layer-wise patching, we isolate and
535 characterize the effects on LLM internal representation under unlearning, and reveal the non-uniform
536 influence from different layers on the validation performance degradation. Such effects align with
537 different levels of abstraction encoded in LLMs. Based on these insights, we propose a lightweight
538 and general framework called CRU which restores the fragile components to obtain a well-performing
539 hybrid model without additional training, opening the new possibilities for surgical unlearning.

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541
ETHICS STATEMENT

542 This work complies with the Code of Ethics in its entirety. It makes use only of publicly accessible
 543 datasets and models, as specified in the experimental section and appendix, and does not involve
 544 human participants or animal studies. We have carefully ensured that no private, sensitive, or
 545 personally identifiable data are included. The contributions are aimed solely at advancing research
 546 in machine unlearning and do not present foreseeable risks of harm or misuse. We further affirm
 547 adherence to principles of legality, fairness, transparency, and research integrity.

548
549
REPRODUCIBILITY STATEMENT
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551 We have made extensive efforts to ensure the reproducibility of our results. A detailed version
 552 of reproducibility statement can be found in Appendix A, where we summarize critical aspects to
 553 facilitate verification. In addition, we also provide an anonymous repository containing code, training
 554 scripts, and instructions for reproducible results. Detailed descriptions of models, datasets, and
 555 experimental setups are provided in the Section 4.1 and Appendix E for a further reference.

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864 APPENDIX
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866 The whole appendix is structured in the following manner. In Appendix A, we provide the necessary
867 aspects for reproducible results with an anonymous repository link. In Appendix B, we provide a
868 comprehensive discussion of related work. In Appendix C, we conduct formal analysis on the latent
869 knowledge fragility with representation drift. In Appendix D, we present the detailed implementation
870 and extension of our component-wise replacement unlearning. In Appendix E, we provide the
871 supplementary experimental results. In Appendix F, we discuss the broader impacts and limitations.
872

873 LLM USAGE STATEMENT
874

875 Here we clarify the usage of Large Language Models (LLMs) in this work. For the preparation of this
876 paper, LLMs (e.g., ChatGPT) are limited to the role of a general-purpose writing assistant and are not
877 used for research ideation or core content generation. For research purposes, LLMs were our core
878 study subject as indicated in our title and research content, and introduced in experimental sections.
879

880 A REPRODUCIBILITY STATEMENT
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882 We provide the anonymous repository link to our source codes: <https://anonymous.4open.science/r/Component-wise-Replacement-Unlearning-BEDB> to enhance the reproducibility of our experimental results. We summarize below aspects to facilitate reproducible results:
883

- 884 • **Datasets.** The unlearning benchmarks (e.g., TOFU [32], MUSE [55] and WMDP [26]) we
885 used are all publicly accessible, which is introduced in Section 4.1 and Appendix E.1.
- 886 • **Assumption.** Following the previous work, we set our experiments to a tuning scenario where
887 a well-trained LLM is available that trained on target data or contain specific knowledge.
- 888 • **Open source.** The code repository will be available in an anonymous repository for the
889 reviewing purposes, which is developed upon OpenUnlearning [13].
- 890 • **Environment.** All experiments are conducted with multiple runs on NVIDIA-A100-80GB
891 GPUs with Python 3.11 and PyTorch 2.4.1. More detailed requirements can also be found in
892 the environment descriptions in our aforementioned source codes.

893 B DETAILED RELATED WORK
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895 Here we discuss related work from several aspects, e.g., LLM unlearning, mechanistic interpretability,
896 representation geometry and concept intervention, model merging and representation alignment.
897

900 **LLM Unlearning.** Machine unlearning seeks to remove specific information from a trained model
901 without full retraining. In classic settings, early works focused on algorithmic formulations, efficiency,
902 and auditability mainly in classification models. Specifically, they introduced exact unlearning in
903 convex models [17], certified data removal [8], gradient ascent-based forgetting [64, 63, 53], and
904 also broader surveys [8] that summarized challenges and approaches. With the rise of LLMs, recent
905 efforts have shifted toward scalable and reliable unlearning approaches, such as Negative Preference
906 Optimization [85, 15] (derived from Direct Preference Optimization [47]), loss adjustment [75, 74,
907 73], and neural activation redirection [54]. The emerging research direction is important for ensuring
908 the safe deployment of foundation models [26, 29]. Several works also propose various benchmarks
909 with different evaluation metrics such as TOFU [32], MUSE [55], and the unified framework of
910 OpenUnlearning [13]. However, most existing methods operate on the level of gradients or loss
911 terms for objective-level adjustment, lacking understanding on how target knowledge is encoded
912 within the model. Our work departs from previous work by treating the LLM internals itself as a
913 functional composition of modular units. By introducing the selective patching approach, we uncover
914 a layer-wise map of knowledge fragility that benefits preserving core functionalities under unlearning.
915

916 **Mechanistic Interpretability of Transformers.** Transformer models exhibit distinct functionalities
917 across layers. Probing studies and patching experiments have revealed the localization of factual

knowledge in intermediate feedforward modules. Recent progress in mechanistic interpretability has advanced our understanding of how transformer models encode, process, and reuse information internally. The seminal work on induction heads [41] identifies specific attention patterns responsible for in-context learning by modeling token repetition dynamics. Building on this, [83] further disentangles the contribution of different attention heads to in-context capabilities, revealing layer- and task-specific specialization. Broader reviews such as [5, 49] systematize techniques for probing and attributing functional roles to components within deep networks, emphasizing their importance for AI safety and transparency. Extending mechanistic approaches to multimodal settings, [6] introduces sparse linear concept embeddings to interpret internal representation space of pre-trained vision language model, while [43] proposes a general concept-based explainability framework for large vision-language models. Together, these works underscore the growing interest in aligning internal model mechanisms with human-interpretable abstractions across both language and multimodal domains. Unlike prior methods focus on understanding the specific mechanism functionality of single component, our technique provides an actionable decomposition of the model in terms of unlearning performance trade-offs, offering a new perspective on knowledge fragility for different layers.

Representation Geometry and Concept Intervention. LLM representations are highly entangled and complex. Exploring the representation geometry has gained increasingly attention recently in order to understand the role of LLM internals in concept encoding and intervention. The linear representation hypothesis has emerged as a central perspective, positing that abstract concepts are embedded in approximately linear subspaces within model activations [44, 39]. Several works have explored the geometry of these representations in general latent space, revealing structured manifolds associated with syntax and hierarchy [45, 70, 27, 58]. Probing intermediate layers has shown that key information is often concentrated in specific layers and dimensions, motivating both analysis and control strategies [57]. On the intervention side, recent works such as activation addition and contrastive activation engineering [42, 69, 68, 4] demonstrate the ability to steer model outputs by modifying internal activations, particularly in sparse or localized directions. These approaches are complemented by inference-time interventions [25] and concept-based representation learning frameworks [48], which aim to manipulate model behaviors via interpretable latent directions. In contrast, our component-wise replacement unlearning focuses not on steering outputs through activation modification, but on isolating and quantifying the functional contribution of different model components. Rather than searching for explicit concept vectors or sparse directions, our method reveals implicit knowledge fragility for preserving utility under unlearning, offering a complementary approach rooted in architectural dissection rather than intervention.

Model Merging and Representation Alignment. As neural networks become increasingly modular and over-parameterized, aligning and integrating their internal representations has emerged as a crucial problem for knowledge composition and transfer. Recent research on model merging and representation alignment has explored how neural networks encode and align information across different tasks and modalities. Early foundational work revisited the similarity of neural network representations [23], introducing metrics like CKA to quantify alignment in learned features. Building on this, studies such as [59, 60, 40, 7] compare model representations with human conceptual spaces, revealing the benefits of aligning abstractions for improved generalization and interpretability. Recent works have proposed methods for latent space translation [33] and zero-shot communication [38], leveraging relative or semantic alignment to facilitate knowledge transfer across models. Furthermore, a series of efforts target model merging through structured alignment: [72] highlights the importance of identifying task-relevant subspaces for merging, while [20] proposes sparse, component-wise arithmetic to achieve efficient fusion across model variants. Our component-wise replacement unlearning differs from these approaches by focusing not on merging models to aggregate or transfer capabilities, but on isolating and suppressing specific knowledge.

Differences. Building on these perspectives, our work introduces the latent knowledge fragility framework, an unlearning-specific lens for analyzing the unlearning effect propagation across the model internals. CRU operationalizes this framework to provide a new, modular, post-hoc solution that selectively restores fragile components. To our knowledge, no prior method systematically explores the component-level restoration with MU/FQ-guided selection to optimize the unlearning trade-off. In summary, the conceptual focus (unlearning-induced fragility), objective (balancing forgetting and retention), and mechanism (training-free post-hoc restoration) of CRU are unique.

972 C FORMAL ANALYSIS OF LATENT KNOWLEDGE FRAGILITY
973

974 Here we present the formal analysis that consider the representation drifts with latent knowledge
975 fragility in the context of LLM unlearning with the Centered Kernel Alignment [23]. The following
976 proposition based on the linear representation hypothesis relates the latent knowledge fragility with
977 the representation drifts, which is also empirically verified in Figure 4.

978 **Assumption 1** (Linear Concept Subspace). *There exists a projection matrix $P_c \in \mathbb{R}^{d \times k}$, with $k \ll d$,
979 that extracts a latent concept-relevant subspace, such that the model output is approximated by:*

980
$$f_\theta(x) \approx W_c^\top P_c^\top \phi_\ell(x) + b$$

982 where $W_c \in \mathbb{R}^k$ is the linear readout for the concept.

984 **Proposition 2** (Low CKA on Concept Subspace Implies High Fragility). *Let $\Phi_\ell^{\text{orig}}, \Phi_\ell^{\text{unlearn}} \in \mathbb{R}^{n \times d}$
985 denote the centered hidden representations at layer ℓ for a retained dataset $\mathcal{D}_{\text{retain}}$ before and after un-
986 learning, respectively. Define the concept-subspace representations as: $Z^{\text{orig}} := \Phi_\ell^{\text{orig}} P_c, Z^{\text{unlearn}} :=$
987 $\Phi_\ell^{\text{unlearn}} P_c \in \mathbb{R}^{n \times k}$. Let the linear CKA similarity between Z^{orig} and Z^{unlearn} be:*

988
$$\text{CKA}_c := \frac{\|Z^{\text{orig}}^\top Z^{\text{unlearn}}\|_F^2}{\|Z^{\text{orig}}^\top Z^{\text{orig}}\|_F \cdot \|Z^{\text{unlearn}}^\top Z^{\text{unlearn}}\|_F}$$

991 Then the average output shift due to unlearning at layer ℓ satisfies:

993
$$\frac{1}{n} \sum_{i=1}^n \|f_\theta^{\text{unlearn}}(x_i) - f_\theta^{\text{orig}}(x_i)\|_2^2 \geq \|W_c\|_2^2 \cdot \left(\sigma_c^{\text{orig}2} + \sigma_c^{\text{unlearn}2} - 2\sqrt{\text{CKA}_c} \cdot \sigma_c^{\text{orig}} \cdot \sigma_c^{\text{unlearn}} \right)$$

996 where $\sigma_c^{\text{orig}2} := \frac{1}{n} \|Z^{\text{orig}}\|_F^2$, and similarly for $\sigma_c^{\text{unlearn}}$.

998 *Proof.* From the linear concept subspace assumption, we have

1000
$$f_\theta(x_i) \approx W_c^\top P_c^\top \phi_\ell(x_i) = W_c^\top z_i \quad \text{where } z_i := P_c^\top \phi_\ell(x_i),$$

1002 then the output shift is,

1003
$$\|f^{\text{unlearn}}(x_i) - f^{\text{orig}}(x_i)\|_2^2 = \|W_c^\top (z_i^{\text{unlearn}} - z_i^{\text{orig}})\|_2^2 = \|W_c\|_2^2 \cdot \|z_i^{\text{unlearn}} - z_i^{\text{orig}}\|_2^2,$$

1005 and we average all the output shift as,

1007
$$\frac{1}{n} \sum_{i=1}^n \|f^{\text{unlearn}}(x_i) - f^{\text{orig}}(x_i)\|_2^2 = \|W_c\|_2^2 \cdot \frac{1}{n} \|Z^{\text{unlearn}} - Z^{\text{orig}}\|_F^2.$$

1010 Then we expand the Frobenius norm,

1012
$$\|Z^{\text{unlearn}} - Z^{\text{orig}}\|_F^2 = \|Z^{\text{unlearn}}\|_F^2 + \|Z^{\text{orig}}\|_F^2 - 2\text{Tr}(Z^{\text{orig}}^\top Z^{\text{unlearn}}),$$

1014 and we can bound the trace via CKA,

1016
$$\text{Tr}(Z^{\text{orig}}^\top Z^{\text{unlearn}}) \leq \|Z^{\text{orig}}^\top Z^{\text{unlearn}}\|_F \leq \sqrt{\text{CKA}_c} \cdot \|Z^{\text{orig}}\|_F \cdot \|Z^{\text{unlearn}}\|_F.$$

1018 Finally we can get the results,

1019
$$\frac{1}{n} \sum_{i=1}^n \|f^{\text{unlearn}}(x_i) - f^{\text{orig}}(x_i)\|_2^2 \geq \|W_c\|_2^2 \cdot \left(\sigma_c^{\text{orig}2} + \sigma_c^{\text{unlearn}2} - 2\sqrt{\text{CKA}_c} \cdot \sigma_c^{\text{orig}} \cdot \sigma_c^{\text{unlearn}} \right),$$

1022 the proof is complete. □

1024
1025

1026 **D COMPONENT-WISE REPLACEMENT UNLEARNING: IMPLEMENTATION AND
1027 EXTENSION**
1028

1029 In this section, we introduce the algorithm implementation of our component-wise replacement
1030 unlearning (e.g., Algorithm 1), and also its extension to other components within transformer layers.
1031

1032 **Algorithm 1** Component-wise Replacement Unlearning (CRU)
1033

1034 **Require:** Original model θ_{orig} , target model θ_{new} , top- k replacement count k , component-wise
1035 partitioner ρ , score functions S_{MU} and S_{FQ} , component type: layer (for example) or others
1036

1037 **Ensure:** Patched model θ_{α}

```

1: Initialize index set  $\mathcal{I}_{\text{layer}} = [L]$  and patching vector  $\alpha \leftarrow \mathbf{0} \in \{0, 1\}^{|\mathcal{I}_{\text{layer}}|}$ 
2: for all  $l \in \mathcal{I}_{\text{layer}}$  do
3:   Compute  $S_{\text{MU}}(l)$  and  $S_{\text{FQ}}(l)$  according to Eq. 1
4: end for
5: Compute ranks  $\mathcal{T}_{\text{MU}}(l)$  from sorting  $S_{\text{MU}}(l)$  in descending order
6: Compute ranks  $\mathcal{T}_{\text{FQ}}(l)$  from sorting  $S_{\text{FQ}}(l)$  in descending order
7: for all  $l \in \mathcal{I}_{\text{layer}}$  do
8:   Compute score  $\mathcal{M}(l) = \mathcal{T}_{\text{MU}}(l) + \mathcal{T}_{\text{FQ}}(l)$ 
9: end for
10: Select top- $k$  layers with smallest  $\mathcal{M}(l)$  to form  $\mathcal{I}_{\text{select}}$ 
11: for all  $l \in \mathcal{I}_{\text{select}}$  do
12:   Set  $\alpha_l \leftarrow 1$ 
13: end for
14: for all  $I \in \mathcal{I}_{\text{layer}}$  do
15:   if  $\alpha_I = 0$  then
16:     Set  $(\theta_{\alpha})^I \leftarrow (\theta_{\text{orig}})^I$ 
17:   else
18:     Set  $(\theta_{\alpha})^I \leftarrow (\theta_{\text{new}})^I$ 
19:   end if
20: end for
21: return  $\theta_{\alpha}$ 

```

1057 We summarize the implementation of CRU in Algorithm 1 with the following restated definition of
1058 key factors. For an integer $n > 0$, we let $[n] := \{1, 2, \dots, n\}$ and have a component-wise partitioner.
1059

1060 **Definition 5** (Component-wise partitioner). *Let \mathcal{A} be a network architecture with parameter space
1061 $\Theta \subseteq \mathbb{R}^D$, and let \mathcal{I} be an arbitrary finite set. A component-wise partitioner is a function $\rho: \mathcal{I} \rightarrow [D]$
1062 such that $\rho(I) \cap \rho(I') = \emptyset$ for any $I, I' \in \mathcal{I}$ such that $I \neq I'$. We call \mathcal{I} the index set of ρ and $|\mathcal{I}|$
1063 the size of ρ . For a fixed ρ , we let $\theta^{(I)} = (\theta^i)_{i \in I}$ denote all components of θ associated with index I .*
1064

1065 Then we can define the replacement operation as a kind of modular-based model patching as follows.
1066

1067 **Definition 6** (Patched model). *Given two parameters $\theta_{\text{orig}}, \theta_{\text{new}} \in \Theta$ and a patching vector $\alpha \in$
1068 $\{0, 1\}^{\mathcal{I}}$, we define the patched parameter θ_{α} in the following component-wise manner:*
1069

$$(\theta_{\alpha})^I = (\theta_{\text{orig}})^I, \text{ If } \alpha_I = 0; \text{ otherwise, } (\theta_{\alpha})^I = (\theta_{\text{new}})^I. \quad (5)$$

1070 *i.e., $\alpha_I = 0$ denotes that θ_{α} takes the same values as θ_{orig} at component I , whereas $\alpha_I = 1$ denotes
1071 that θ_{α} takes the same values as θ_{new} at component I .*

1072 Finally we can calculate the newly defined score and take the top- k layer index as final α .

1073 **Definition 7** (Patching Score via Sorted Indices). *Given the index set of candidate layers $\mathcal{I}_{\text{layer}} = [L]$,
1074 we define the patching score $\mathcal{M}(l)$ for each layer $l \in [1, L]$ as the sum of its ranks in two sorted lists:
1075 one based on MU and the other on FQ. Let $\mathcal{T}_{\text{MU}}(l)/\mathcal{T}_{\text{FQ}}(l)$ denote the rank index of layer l when all
1076 layers are sorted in descending order of $S_{\text{MU}}(l)/S_{\text{FQ}}(l)$ as Eq. 1. Then, the score is defined as:*

$$\mathcal{M}(l) = \mathcal{T}_{\text{MU}}(l) + \mathcal{T}_{\text{FQ}}(l). \quad (6)$$

1077 *A lower $\mathcal{M}(l)$ indicates that the layer ranks highly in both model utility and forget quality, and is
1078 thus more favorable for selection in layer-wise model merging under the top- k selection.*

1080 Note that the major implementation in our work is based on the LLM transformer layers, and we will
 1081 discuss the other kind of components explored in the following section.
 1082

1083 **Comparison between layer-wise restoring and structural freezing.** While both strategies involve
 1084 preserving certain layers, they differ algorithmically and operationally, which is empirically verified
 1085 in our Figure 4. Layer replacement is a post-hoc operation: we first complete unlearning, then
 1086 selectively restore specific layers with original parameters based on validation results. These restored
 1087 layers were never exposed to unlearning updates; Structural freezing happens during unlearning,
 1088 where certain layers are prevented from updating (e.g., frozen during unlearning). However, this
 1089 often disrupts learning dynamics (e.g., affects updates on other layers), leading to unstable gradients
 1090 and degraded convergence of the unlearning, especially when the frozen layers are critical for
 1091 routing representations. As a result, although both preserve original parameters in selected layers,
 1092 replacement avoids interfering with the optimization process for unlearning while freezing obtains a
 1093 different unlearned model, which leads to consistently better trade-offs of CRU.

1094 **Full discussion on the choice of layer-wise replacement.** Here we would like to clarify our choice
 1095 to focus on the layer level in three levels. 1) **Motivation Differences:** we also note the value
 1096 of fine-grained unlearning interventions, while our goal and framing differ fundamentally from
 1097 previous work [52, 11, 31]. Those neuron- or weight-level methods aim to surgically excise localized
 1098 knowledge (e.g., individual facts or neurons tied to specific concepts), using attribution or saliency
 1099 tools. In contrast, our motivation is not removal at maximum precision, but rather to diagnose and
 1100 optimize the global trade-off of unlearning, with a focus on influence on latent knowledge fragility.
 1101 CRU is designed to complement existing unlearning methods by providing a post-hoc mechanism for
 1102 restoring performance without retraining, based on modular diagnostics. 2) **Practical tractability:**
 1103 While neuron- or weight-level do provide more precise analysis, they also introduce a combinatorially
 1104 large search space under the interplay patching, making it computationally expensive especially in
 1105 large models like LLaMA-7B. In contrast, Layer-level patching provides a manageable space (e.g.,
 1106 16/32 layers vs. thousands of neurons or millions of weights), yet each layer captures meaningful
 1107 abstraction, enabling us to efficiently evaluate and visualize influence patterns (e.g., U-shaped fragility
 1108 curves) across the model. 3) **Alignment with broader knowledge scope:** CRU addresses broad
 1109 representational disruption that arises when removing semantically entangled knowledge, which may
 1110 not be attributable to specific memorized samples. In such cases, layer-level fragility provides an
 1111 abstracted and tractable unit for measuring the unlearning damage, which is applicable to analyze
 1112 global impact on a model’s internal structure with the amount of unlearning requests. We believe
 1113 fine-grained scale provides a great analytical path to specific concepts or sample-wise knowledge.

1114 **Discussion on the efficiency.** CRU is designed as a post-hoc lightweight step after unlearning.
 1115 While it does involve computing validation performance for layer-wise location and patching, this is
 1116 computationally efficient compared to training-based unlearning methods involving retaining data.
 1117 Specifically, compared with those unlearning methods involving retaining data (as regularization) for
 1118 trade-off optimization, our CRU framework does not involve backward pass or further training on
 1119 the validation set. For example, CRU can be adopted on the GA unlearned model for replacement,
 1120 and achieve better trade-off than GA+KL unlearned model which involves retaining data directly
 1121 during training for backward computation. On the other hand, for the fragile layer identification, we
 1122 only use inference-time evaluation in each forward pass for the patched models, which also saves
 1123 the memory storage of the computational graph for the gradient flow generated by all of the training
 1124 data. The results in Table 4 demonstrates the relative efficiency of our CRU framework compared
 1125 with most baseline methods (except for GA only using forget data, which are extremely fast yet not
 1126 perform well). And unlike most baseline methods that require two GPU devices for training, our
 1127 CRU framework operates efficiently on a single GPU. We will clarify and discuss this point more
 1128 explicitly in our final version with the quantitative results.

1129 **Discussion on top-k selection.** We should acknowledge that the top-k individually selected layers
 1130 may not always represent the globally optimal combination, as the space of all k-layer combinations
 1131 grows combinatorially (e.g., consider selecting 7 from 32 layers 7b model, it has =3365859 types),
 1132 introducing significant algorithmic complexity for exhaustive search. As we stated in the end of
 1133 Section 3.3, identifying the layer subset can be formulated as a Shapley interaction problem [61],
 1134 requiring careful assessment of each layer’s marginal contribution across all subsets, which owns
 1135 better theoretical guarantees but beyond the current scope focused on exploring the knowledge
 1136 fragility in unlearning, and we would leave to the future work. In our design, the top-k selection is
 1137 guided by a principled validation-based score, and grounded in the observed semantic abstraction

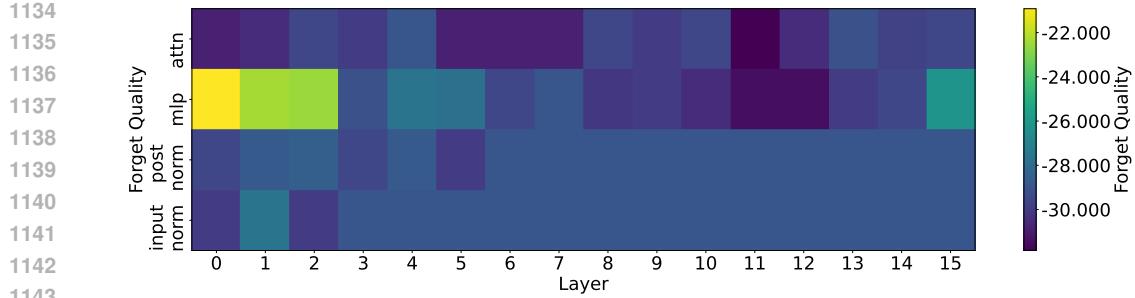


Figure 8: Forget quality regarding the components within transformer blocks.

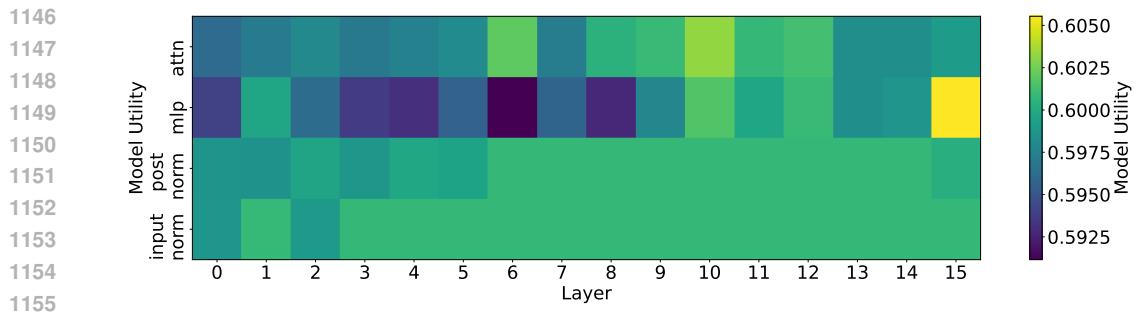


Figure 9: Model utility regarding the components within transformer blocks.

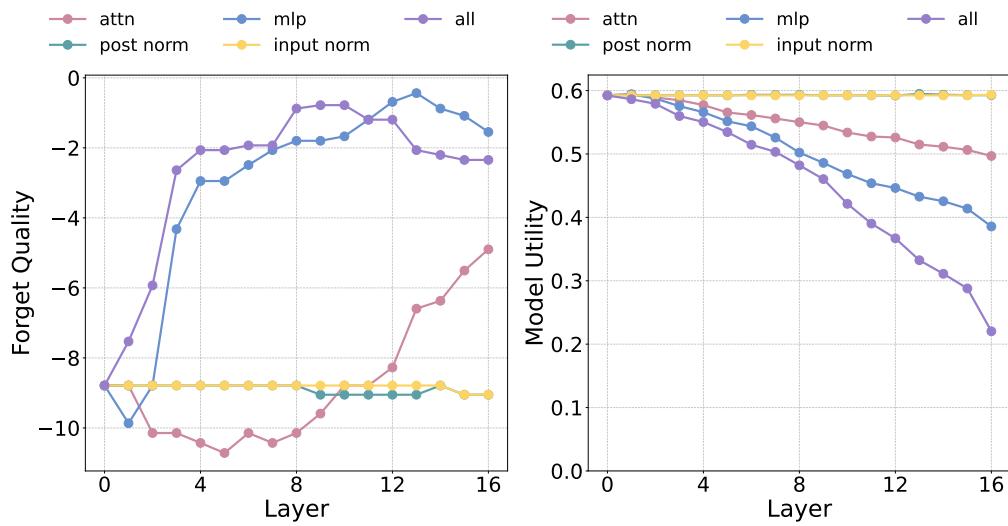


Figure 10: Performance on FQ and MU of CRU with different components (e.g., attention heads, MLP, input/post normalization, and the whole layer indicated by “all”).

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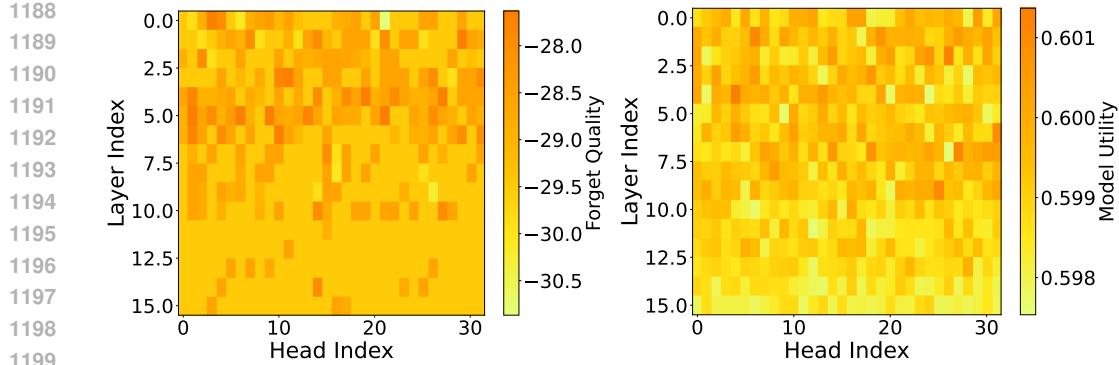


Figure 11: Influence of attention heads. Left: Forget Quality; Right: Model Utility.

layer has the same number H of attention heads per layer, the *attention-wise partitioner* ρ_{head} has an index set $\mathcal{I}_{\text{attn}} = [L] \times [H]$, and for any $(l, h) \in \mathcal{H}$, $\theta^{(l, h)}$ denotes the parameters associated with the h -th attention head in the l -th layer. We can also conduct attention-wise replacement.

Influence of Patching on FQ and MU. To explore the fine-grained influence in the internal of transformer blocks (e.g., layers), we conduct component-wise replacement on attention head, MLP, input/post normalization parts and summarize the FQ and MU results of patching a single component (from the unlearned model, i.e., Llama3.2-1B, using NPO) to the original model in Figures 8 and 9, respectively. We find that patching different MLPs shows similar trend on affecting both FQ and MU revealed in our layer-wise replacement. In comparison, both input and post normalization has limited effects on changing the validation performance of unlearning, while attention heads even show a (seems to be) ‘‘contrary’’ trend with the ‘‘U shape’’ in layer-wise, for which we further check the influence of each attention head in Figure 11. Compared to MLPs or entire transformer layers, attention heads exert much weaker influence on unlearning, suggesting their limited relevance in revealing stored knowledge fragility. This distinction is further illustrated in Figure 10, where we evaluate the component-wise replacement under varying k . The results show that both MLP-only and full-layer replacements yield similar trends in FQ and MU. In contrast, input/post-normalization have negligible effects on performance, while attention-head replacement displays a divergent trend in FQ and fails to match the performance gains achieved by MLP or full-layer replacements.

Conjecture on different functionality. For the empirical observation, we conjecture that the degree to which a transformer component contributes to knowledge fragility under unlearning may aligned with its functional role in representation transformation and retention. Specifically, MLP that are primarily responsible for transforming and re-encoding intermediate representations, exhibit higher sensitivity to unlearning updates and stronger influence on both FQ and MU. In contrast, normalization layers (like the input and post norm) primarily serve a stabilizing role and contribute minimally to information encoding, leading to negligible effects under component-wise replacement. Attention heads, while crucial for information routing, appear to distribute influence across layers and heads, resulting in weaker and sometimes inconsistent effects on unlearning performance when manipulated in isolation. Although we can hardly find some general pattern on the performance change regarding attention heads in Figure 11, we reveal its unique functionality on affecting high-level concepts later.

Attention heads with high-level concepts. In Figure 12, we plot the normalized deviation on LLM’s inclines (calculated by output probability) to some high-level concepts (such as coordinate, corrigible, hallucination, refusal in [46]) and find that the attention heads in the middle layer induce significant output deviation under unlearning, demonstrating the unique functionality of attention heads on model representation corresponding to high-level concepts.

Specifically, the deviation metric in Figure 12 is calculated based on the probability differences between two options (A and B) in a binary choice task. For each sample i , we define:

$$\Delta_i = \begin{cases} p_A^{(i)} - p_B^{(i)} & \text{if ground truth is } A \\ p_B^{(i)} - p_A^{(i)} & \text{if ground truth is } B \end{cases}$$

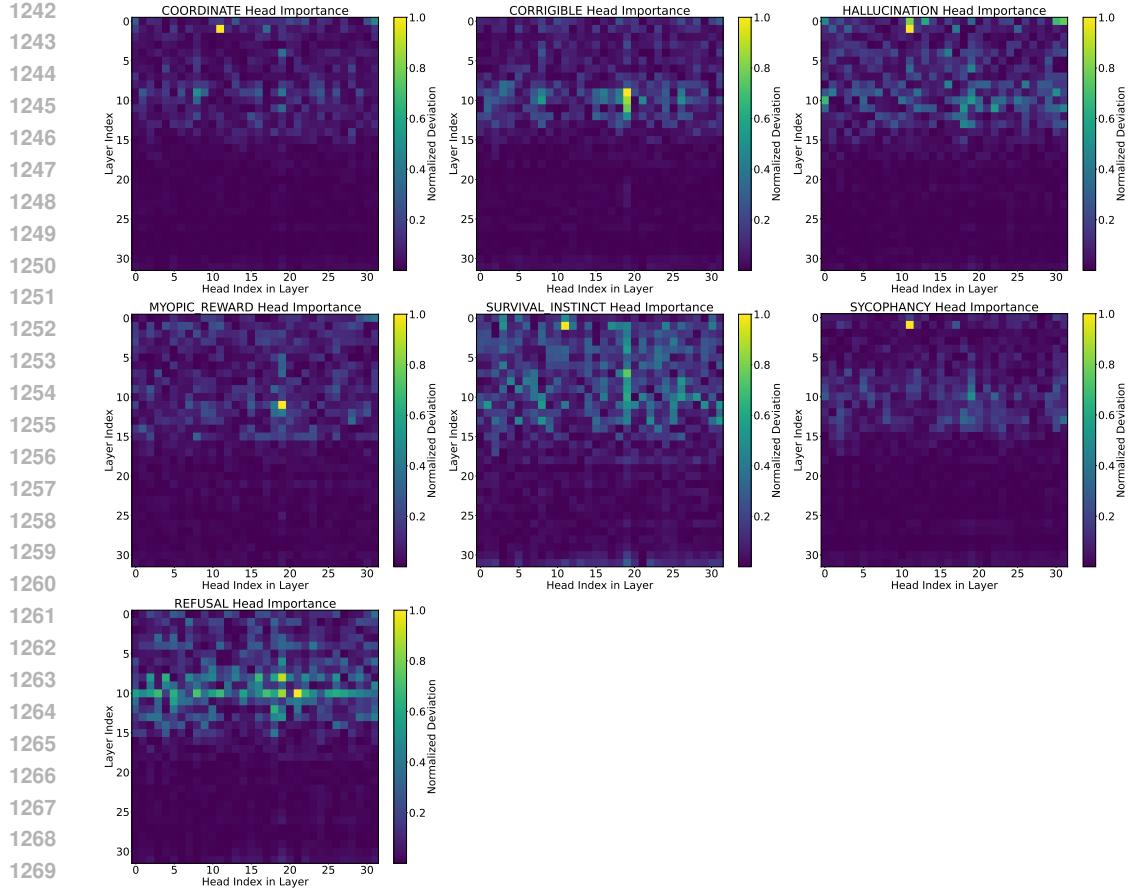


Figure 12: Normalized deviation on LLM’s inclines to some high-level concepts.

where $p_A^{(i)}, p_B^{(i)}$ are the predicted probabilities for options A and B calculated following [42]. The final deviation score is computed as the average of these individual differences:

$$\text{Deviation} = \frac{1}{N} \sum_{i=1}^N \Delta_i \quad (7)$$

where N is the total number of samples.

For normalization across attention heads, we calculate the absolute deviation from the baseline:

$$\text{Normalized Deviation}_j = \frac{|\Delta_j - \Delta_{\text{baseline}}|}{\max(|\Delta_j - \Delta_{\text{baseline}}|)} \quad (8)$$

where Δ_j is the deviation score from the model which head j is replaced with the corresponding head from the unlearn model and Δ_{baseline} is the baseline deviation score from the original model.

Further discussion about the U-shape. the U-shaped fragility pattern arises consistently across different model size (1B, 7B), unlearning objectives (GA, NPO), and data domains (TOFU, WMDP), as comprehensively illustrated in the main text. This consistency suggests the pattern reflects a structural phenomenon of intrinsic knowledge, rather than being an artifact of training setup or unlearning data. It draws our attention to latent knowledge encoded in transformer models. Regarding the mathematical framework of transformer architecture [19], it is inherently modular, with each layer implementing a complete, parameterized function block, contributing a discrete stage of representation refinement. This design makes each layer a natural unit of computation and abstraction, where information is composed sequentially as , with layers inducing a progressive semantic abstraction. Hence, perturbations in specific layers affect specific levels of representation (e.g., lexical vs. semantic vs. output-compositional). The modularity allows us to diagnose unlearning-induced influence and disruptions. Our conceptual explanation for the fragile layer aligns with the

semantic abstraction hierarchy in transformers: 1) Shallow layers encode local syntax and are less entangled to be fragily influenced. 2) Middle layers represent abstract, high-level semantics and are more intertwined with factual knowledge, making them more vulnerable to utility degradation. 3) Deep layers are primarily involved in output fluency and autoregressive dependencies, and are less critical for knowledge content. It is evidenced by Figure 1 illustration, and also consistent with prior preliminary findings in mechanistic interpretability literature [12, 23].

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E EXPERIMENTAL DETAILS

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E.1 DETAILS ABOUT THE DATASETS AND METRICS

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We evaluated unlearning methods on two benchmark datasets: Task of Fictitious Unlearning (TOFU) [32] and Machine Unlearning Six-way Evaluation (MUSE) [55].

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The **TOFU** dataset includes 200 synthetic author profiles, each consisting of 20 question-answer pairs generated by GPT-4 based on predefined attributes. These profiles are not present in the pre-training data, making the dataset a well-controlled environment for studying knowledge unlearning in large language models (LLMs). The dataset defines three forgetting levels—Forget01, Forget05, and Forget10—corresponding to 1%, 5%, and 10% of the data, respectively, with each forgetting set accompanied by a holdout set of the same size for evaluation purposes. In our experiments, we focus on the Forget-05 setting. Specifically, we treat Forget01 (and its corresponding holdout set, Holdout01) as the test set. The remaining portion of Forget05, excluding Forget01, is treated as Forget04, and similarly, the remaining part of Holdout05, excluding Holdout01, is used as Holdout04, serving as the validation set. Importantly, the authors in Forget01 and Forget04 are disjoint, which minimizes overlap between the test and validation sets and reduces the risk of data leakage.

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Evaluation Metrics. We evaluate unlearning on the TOFU dataset using two primary metrics in [32]: Forget Quality and Model Utility.

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Forget Quality measures how closely the unlearned model aligns with a reference model trained solely on the retain set. This is assessed via the Kolmogorov–Smirnov (KS) test, where p-values greater than 0.05 indicate statistically meaningful forgetting. As for KS test, let $F_U(x)$ and $F_R(x)$ denote the empirical cumulative distribution functions (CDFs) of the unlearned and retain models, respectively, based on n and m samples. The KS statistic quantifies the maximum absolute difference between these two CDFs:

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$$D_{n,m} = \sup_x |F_U(x) - F_R(x)| \quad (9)$$

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Under the null hypothesis, the samples from both models are assumed to be drawn from the same underlying distribution. This hypothesis is rejected at a significance level α if:

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$$D_{n,m} > c(\alpha) \cdot \sqrt{\frac{n+m}{nm}} \quad (10)$$

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where the critical value $c(\alpha)$ is given by:

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$$c(\alpha) = \sqrt{-\ln\left(\frac{\alpha}{2}\right) \cdot \frac{1}{2}} \quad (11)$$

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The p-value is defined as the smallest significance level α for which the inequality in Equation 8 holds. In the context of Forget Quality, a p-value greater than 0.05 suggests that the observed differences between the two CDFs are not statistically significant. This implies that the unlearned model behaves similarly to the retain model on the forget set, indicating that the model has effectively "forgotten" the targeted data.

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Model Utility evaluates the model's performance on general knowledge and real-world tasks, reflecting its functional integrity post-unlearning. To quantify this, [32] combine three complementary metrics—conditional probability, ROUGE-L recall, and Truth Ratio—across datasets, with a harmonic mean ensuring balanced performance across all dimensions.

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For an input sequence $\mathbf{x} = [q, a]$, where q is a question and a is its answer, we compute the conditional probability $p(a | q; \theta)$ for model θ . To normalize for answer length $|a|$, we use:

$$p_{\text{norm}}(a | q; \theta) = p(a | q; \theta)^{1/|a|} \quad (12)$$

1404 And for multi-answer datasets like Real Authors and World Facts, we calculate the choice probability
 1405 of the correct answer, assume that a_1 is the correct answer, the probability can be computed as:
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$$1407 \quad \frac{p(a_1 | q; \theta)}{\sum_{i=1}^n p(a_i | q; \theta)}. \quad (13)$$

1409 We measure semantic similarity between generated answers \hat{a} and ground-truth answers a^* using
 1410 ROUGE-L recall:
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$$1412 \quad \text{ROUGE}(\hat{a}, a^*) = \frac{\text{LCS}(\hat{a}, a^*)}{|a^*|} \quad (14)$$

1414 where $\text{LCS}(\cdot)$ is the length of the longest common subsequence.

1415 To assess robustness against answer formulation bias, we use the perturbed dataset D_{pert} and compute
 1416 a ratio of probabilities for paraphrased correct answers $\hat{a} \in D_{\text{pert}}$ over perturbed incorrect answers \tilde{a} :

$$1418 \quad R_{\text{truth}} = \frac{1}{|D_{\text{pert}}|} \frac{\sum_{\hat{a} \in D_{\text{pert}}} p(\hat{a} | q; \theta)^{1/|\hat{a}|}}{p(\tilde{a} | q; \theta)^{1/|\tilde{a}|}} \quad (15)$$

1421 Finally, all metrics are normalized to $[0, 1]$ and combined via harmonic mean to penalize poor
 1422 performance in any dimension:

$$1423 \quad \text{Model Utility} = \frac{9}{\sum_{i=1}^9 \frac{1}{s_i}} \quad (16)$$

1425 where s_i are the nine normalized scores (3 metrics \times 3 datasets, excluding Forget Set probability),
 1426 higher values indicate better utility retention post-unlearning.

1427 Additionally, we consider Extraction Strength (ES) as a supplementary metric, which quantifies the
 1428 amount of additional information required to reconstruct original model outputs after unlearning.
 1429 ES can be computed in two modes: ES-exact, based on the original data, and ES-perturb, using
 1430 rephrased inputs. Lower ES values on forgotten data suggest stronger unlearning, while higher ES on
 1431 retained data indicates better preservation of general knowledge. ES value can be computed as:

$$1433 \quad \text{ES} = 1 - \frac{1}{|y|} \min_k \{k \mid f([x, y_{<k}]; \theta) = y_{>k}\} \quad (17)$$

1435 where y is the full output sequence (e.g., an answer), $|y|$ denotes its token count, $y_{<k}$ denotes the
 1436 prefix up to token $k - 1$, $y_{>k}$ denotes the suffix starting at token $k + 1$, and $f(\cdot; \theta)$ is the model's
 1437 prediction function. A higher ES indicates stronger memorization, as the model reconstructs the
 1438 suffix with less input context.

1439 The **MUSE** dataset serves as a comprehensive benchmark for machine unlearning evaluation, encompassing
 1440 two distinct forgetting scenarios: text segments from the Harry Potter book series (denoted
 1441 as Books) and news articles from BBC News (News). Structured to evaluate six core properties
 1442 of unlearned models, it emphasizes: (1) eliminating verbatim memorization, (2) erasing knowl-
 1443 edge memorization, (3) preventing privacy leakage, (4) maintaining utility on non-targeted data, (5)
 1444 scalability with unlearning request size, and (6) robustness across sequential unlearning operations.

1445 **Evaluation Metrics.** In our experiments, we conduct evaluations on both two scenarios (Books
 1446 and News). Specifically, we shuffle all splits across the evaluation subsets (knowmem, verbmem,
 1447 privleak) in the dataset and partition each split into 80% for the validation set and 20% for the test
 1448 set, following the approach used in the TOFU dataset. We evaluate unlearning effectiveness on the
 1449 MUSE dataset using five metrics in [55]: Extraction Strength, Verbatim Memorization, Knowledge
 1450 Memorization on the forget data (for assessing forgetting effectiveness), Knowledge Memorization
 1451 on the retain data (as a measure of utility preservation), and the Privacy Leakage metric.

1452 VerbmMem measures the model's ability to reproduce forgotten sequences verbatim. Lower VerbmMem
 1453 scores imply stronger unlearning, as the model fails to replicate forgotten sequences. For $s \in D_t$,
 1454 we prompt the model θ with its first l tokens $s[:l]$ and compare the continuation $\theta(s[:l])$ to the true
 1455 suffix $s[l + 1 :]$ via ROUGE-L F1:

$$1456 \quad \text{VerbmMem}(\theta, D_t) = \frac{1}{|D_t|} \sum_{s \in D_t} \text{ROUGE}(\theta(s[:l]), s[l + 1 :]) \quad (18)$$

1458 KnowMem evaluates knowledge retention from forgotten (D_t) and retained ($D_w \setminus D_t$) data. A low
 1459 KnowMem-forget score indicates the model forgets targeted knowledge, while a high KnowMem-
 1460 retain score confirms utility preservation. For model θ and each question-answer pair $(q, a) \in$
 1461 D_t or $D_w \setminus D_t$, we compute:

$$1462 \quad \text{KnowMem}(\theta, D) = \frac{1}{|D|} \sum_{(q, a) \in D} \text{ROUGE}(\theta(q), a) \quad (19)$$

1465

1466 PrivLeak quantifies membership inference risks using Min-K% Prob, a loss-based attack. A PrivLeak
 1467 score near zero means unlearning eliminates membership leakage, while positive/negative values
 1468 indicate under/over-unlearning. Let D_t be member examples (forgotten data), D_h be non-member
 1469 examples (holdout set), θ_{unlearn} the unlearned model, and θ_{retrain} a retrained baseline. PrivLeak is
 1470 defined as:

$$1471 \quad \text{PrivLeak} = \frac{\text{AUC}(\theta_{\text{unlearn}}, D_t, D_h) - \text{AUC}(\theta_{\text{retrain}}, D_t, D_h)}{\text{AUC}(\theta_{\text{retrain}}, D_t, D_h)} \quad (20)$$

1472

1473 And the AUC (Area Under the Receiver Operating Characteristic Curve) is computed as follows:
 1474 Given a classifier f_θ derived from model θ , let $f_\theta(x)$ denote the membership probability score
 1475 assigned to example x . For a set of member examples $D_t = \{x_1^t, x_2^t, \dots, x_n^t\}$ and non-member
 1476 examples $D_h = \{x_1^h, x_2^h, \dots, x_m^h\}$, the AUC is:

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$$1478 \quad \text{AUC}(\theta, D_t, D_h) = \frac{1}{n \cdot m} \sum_{i=1}^n \sum_{j=1}^m \mathbb{I}(f_\theta(x_i^t) > f_\theta(x_j^h)) + \frac{0.5}{n \cdot m} \sum_{i=1}^n \sum_{j=1}^m \mathbb{I}(f_\theta(x_i^t) = f_\theta(x_j^h)). \quad (21)$$

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1480 The **WMDP** benchmark is a dataset of 3,668 multiple-choice questions covering biosecurity,
 1481 cybersecurity, and chemical security. It is widely used to evaluate unlearning methods that aim to
 1482 remove hazardous knowledge. However, since WMDP contains only knowledge to be forgotten, we
 1483 additionally use the MMLU dataset [21]—57 tasks spanning general domains—as retention data,
 1484 following the WMDP paper [26].

1485

1486 In this setting, we use multiple-choice accuracy as our metric. Given the WMDP dataset D_{WMDP} , the
 1487 MMLU dataset D_{MMLU} , and a model θ , we compute:

$$1488 \quad \text{Acc}_{\text{unlearn}}(\theta, D_{\text{WMDP}}) = \frac{1}{|D_{\text{WMDP}}|} \sum_{(q, a) \in D_{\text{WMDP}}} \mathbf{1}\{\theta(q) = a\} \quad (22)$$

1489

$$1490 \quad \text{Acc}_{\text{retain}}(\theta, D_{\text{MMLU}}) = \frac{1}{|D_{\text{MMLU}}|} \sum_{(q, a) \in D_{\text{MMLU}}} \mathbf{1}\{\theta(q) = a\} \quad (23)$$

1491

1492 Unlearning quality is better when $\text{Acc}_{\text{unlearn}}$ is lower and $\text{Acc}_{\text{retain}}$ is higher.

1493

1494 E.2 DETAILS ABOUT CONSIDERED BASELINES

1495

1496 In this section, we provide details on the representative baselines considered in experiments.

1497

1498 **Gradient Ascent (GA).** Opposite from standard gradient descent, Gradient Ascent (GA) [32] inverts
 1499 the gradient signal on the forgetting set D_t and performs maximization using ascended gradients.
 1500 This leads to an increase in the loss associated with the forgetting data, aiming to obtain the unlearned
 1501 model θ^u . The corresponding objective is formulated as follows:

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$$1512 \quad \mathcal{L}_{\text{GA}}(D_t; \theta) = \frac{1}{n} \sum_{s \in D_t} \log p(s; \theta). \quad (24)$$

1513 **Gradient Difference (GD).** Building upon the principle of gradient ascent, Gradient Difference
 1514 (GD) [32] introduces a balanced objective that simultaneously encourages forgetting on the target
 1515 data while preserving performance on the retained examples. Formally, given a forgetting set D_t and
 1516 a retain set D_{retain} , the method minimizes the following composite loss:

1512

$$\mathcal{L}_{\text{GD}}(\mathcal{D}_t; \mathcal{D}_w; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \log p(s; \theta) - \alpha \cdot \frac{1}{n} \sum_{s' \in \mathcal{D}_w \setminus \mathcal{D}_t} \log p(s'; \theta). \quad (25)$$

1516 In our experiments, we adopt the negative log-likelihood (NLL) loss — which has been extensively
 1517 discussed before — as the forgetting loss ℓ_f . For the retain loss ℓ_r , we employ the Kullback–
 1518 Leibler (KL) [32] divergence. Let M denote a model that outputs a probability distribution over the
 1519 vocabulary for next-token prediction. Then, the KL-based retain loss is defined as follows:
 1520

$$\mathcal{L}_{\text{KL}}(\mathcal{D}_t; \mathcal{D}_w; M) = \frac{1}{n} \sum_{s \in \mathcal{D}_w \setminus \mathcal{D}_t} \text{KL}(M_{\text{original}}(s) \parallel M_{\text{unlearn}}(s)), \quad (26)$$

1524 where M_{original} represents the original model before unlearning, and M_{unlearn} denotes the model after
 1525 applying the unlearning procedure.
 1526

1527 **Weighted Gradient Ascent (WGA).** To address the issue of excessive unlearning in standard gradient
 1528 ascent (GA), a method called Weighted Gradient Ascent (WGA) [74] was proposed. This method
 1529 aims to reduce the impact of low-confidence tokens during unlearning, which can otherwise dominate
 1530 the gradient updates and cause the model to forget more than necessary.
 1531

1532 In WGA, instead of treating all tokens equally, each token’s contribution to the loss is weighted by its
 1533 own confidence. Specifically, the objective function becomes:
 1534

$$\mathcal{L}_{\text{WGA}}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \sum_{i=2}^{|s|} p(s_i \mid s_{<i}; \theta)^\alpha \cdot \log p(s_i \mid s_{<i}; \theta), \quad (27)$$

1535 where s is a sequence (e.g., sentence or paragraph) from the forgetting set \mathcal{D}_t , while s_i is the i -th
 1536 token in the sequence s , and α is a hyperparameter.
 1537

1538 **Negative Preference Optimization (NPO).** Negative Preference Optimization (NPO) [85] is a robust
 1539 unlearning framework inspired by preference learning method Direct preference optimization (DPO).
 1540 It treats forgetting data as negative preferences and reformulates the gradient ascent objective to
 1541 improve stability. Compared to standard GA, NPO offers two major benefits: (1) it uses a loss
 1542 function that is bounded from below, preventing model collapse due to extreme gradients; and (2) it
 1543 introduces an adaptive weight on the gradients, which slows down the divergence speed and enables
 1544 more controlled unlearning. The NPO objective is defined as:
 1545

$$\mathcal{L}_{\text{NPO}}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \frac{2}{\beta} \log \left[1 + \left(\frac{p(s; \theta)}{p(s; \theta^{\text{orig}})} \right)^\beta \right] \quad (28)$$

1550 with its gradient given by:
 1551

$$\nabla_{\theta} \mathcal{L}_{\text{NPO}}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \left[\frac{2p(s; \theta)^\beta}{p(s; \theta)^\beta + p(s; \theta^{\text{orig}})^\beta} \cdot \nabla_{\theta} \log p(s; \theta) \right]. \quad (29)$$

1556 The adaptive weight $\frac{2p(s; \theta)^\beta}{p(s; \theta)^\beta + p(s; \theta^{\text{orig}})^\beta}$ reduces the impact of each update and prevents excessive
 1557 model deviation from the reference model θ^{orig} . Here, $p(s; \theta)^\beta$ denotes the model’s output probability
 1558 for token y given input x , and $\beta > 0$ is a temperature hyperparameter that controls the update.
 1559

1560 **Token-wise Negative Preference Optimization (TNPO).** Token-wise Negative Preference Optimiza-
 1561 tion (TNPO) [74] is a variant of NPO that enhances the original method by applying its adaptive
 1562 weighting mechanism at the token level instead of the sequence level. This allows for finer-grained
 1563 control over unlearning, prioritizing certain tokens rather than entire examples. Compared to standard
 1564 NPO, TNPO offers greater flexibility and can achieve better trade-offs between forgetting effective-
 1565 ness and model integrity when using moderate values of the inverse temperature parameter β . The
 1566 objective function is defined as:
 1567

1566

$$\mathcal{L}_{\text{TNPO}}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \sum_{i=2}^{|s|} \frac{2p(s_i | s_{<i}; \theta)^\beta}{p(s_i | s_{<i}; \theta)^\beta + p(s_i | s_{<i}; \theta^{\text{orig}})^\beta} \cdot \log p(s_i | s_{<i}; \theta), \quad (30)$$

1570

1571 where θ denotes the current model parameters, θ^{orig} represents the reference model, and $\beta > 0$ controls
 1572 the sensitivity of the weight to confidence. In this formulation, $p(s_i | s_{<i}; \theta)$ is the model's predicted
 1573 probability for the i -th token in the forgetting sequence s , and $w_{s,i}^{\text{TNPO}} = \frac{2p(s_i | s_{<i}; \theta)^\beta}{p(s_i^u | s_{<i}; \theta)^\beta + p(s_i | s_{<i}; \theta^{\text{orig}})^\beta}$
 1574 serves as the adaptive weight applied per token.

1575

1576 **Weighted Token-wise Negative Preference Optimization (WTNPO).** Based on TNPO, Weighted
 1577 Token-wise Negative Preference Optimization (WTNPO) [74] introduces an additional confidence-
 1578 based weighting term to further stabilize the unlearning process and reduce excessive forgetting.
 1579 While TNPO improves flexibility by operating at the token level, it may still lead to over-unlearning
 1580 when the inverse temperature β is too small. WTNPO addresses this by incorporating a power scaling
 1581 on the numerator with an extra hyperparameter α , just like WGA. The objective is formulated as
 1582 follows:

1583

$$\mathcal{L}_{\text{WTNPO}}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \sum_{i=2}^{|s|} \frac{2p(s_i | s_{<i}; \theta)^{\beta+\alpha}}{p(s_i | s_{<i}; \theta)^\beta + p(s_i | s_{<i}; \theta^{\text{orig}})^\beta} \cdot \log p(s_i | s_{<i}; \theta), \quad (31)$$

1586

1587 where α controls how much low-confidence tokens are downweighted during optimization.

1588

1589 **Forget data only Loss AdjustmenT (FLAT).** Forget data-only Loss Adjustment (FLAT) [75] is
 1590 a model unlearning method that operates solely on forget data, without requiring access to retain
 1591 data or a reference model. Its core idea is to maximize the f-divergence between the model's desired
 1592 responses (e.g., rejection answers like "I don't know") and its original outputs on the forgetting
 1593 set, thereby achieving knowledge erasure. FLAT's theoretical framework is built on the variational
 1594 form of f-divergence (Fenchel duality), optimizing the variational function g and conjugate function
 1595 f^* to adjust the model's output distribution under the constraint of using only forget data. The
 1596 method employs an empirical estimator to approximate the theoretical f-divergence and proves the
 1597 convergence rate of the estimation error under mild assumptions.

1598

1599 The objective function of FLAT is defined as:

1600

$$\mathcal{L}_{\text{FLAT}}(\mathcal{D}_t; \mathcal{D}_{\text{idk}}; \theta) = -\frac{1}{n} \sum_{s \in \mathcal{D}_t, s' \in \mathcal{D}_{\text{idk}}} \left[g^*(p(s'; \theta)) - f^*(g^*(p(s; \theta))) \right], \quad (32)$$

1602

1603 where $p(s'; \theta)$ denotes the average token prediction probability for the desired response like "I don't
 1604 know" given input, $p(s; \theta)$ corresponds to the original model output for the forgetting response, g^* is
 1605 the optimal variational function derived from the f-divergence, and f^* is its conjugate.

1606

1607 **Simple Negative Preference Optimization (SimNPO).** Impressed by Simple Preference Opti-
 1608 mization (SimPO) [37], a widely used method in Preference Optimization area, Simple Negative
 1609 Preference Optimization (SimNPO) [15] replace $(\frac{p(s; \theta)}{p(s; \theta^{\text{orig}})})^\beta$ in 28 with $p(s; \theta)^{\frac{\beta}{|\mathcal{Y}|}} - \gamma$ to mitigate the
 1610 reference model bias in NPO. The objective function is defined as:

1611

1612

1613

$$\mathcal{L}_{\text{SimNPO}}(\mathcal{D}_t; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t} \frac{2}{\beta} \log \left(p(s; \theta)^{\frac{\beta}{|\mathcal{Y}|}} - \gamma \right), \quad (33)$$

1614

1615 where γ is a target margin to enforce a stricter unlearning condition.

1616

1617

1618

1619

1619 **Alternate Preference Optimization (AltPO).** Alternate Preference Optimization (AltPO) [36] is a
 1620 method aims to offer in-distribution positive feedback on responses to forget data. It firstly prompt a
 1621 model that was not trained on target data to generate alternate responses, and then, it align the target
 1622 model to the new alternate response while contrasting them with the forget response. The objective
 1623 function of AltPO is defined as:

1620

$$\mathcal{L}_{\text{AltPO}}(\mathcal{D}_t; \mathcal{D}_a; \theta) = \frac{1}{n} \sum_{s \in \mathcal{D}_t, s_{\text{alt}} \in \mathcal{D}_a} \frac{2}{\beta} \log \left[1 + \left(\frac{p(s; \theta) \cdot p(s_{\text{alt}}; \theta^{\text{orig}})}{p(s; \theta^{\text{orig}}) \cdot p(s_{\text{alt}}; \theta)} \right)^{\beta} \right], \quad (34)$$

1621 where \mathcal{D}_a denotes the dataset of alternate responses constructed in the first step.
 1622

1623 **Saturation and Importance based reweighting (SatImp).** Motivated by a systematic study of loss
 1624 reweighting criteria for LLM unlearning, Saturation and Importance based reweighting (SatImp) [78]
 1625 combines saturation for insufficiently unlearned tokens and importance upweights influential tokens
 1626 into a token-wise soft reweighting that emphasizes medium-loss regions. Concretely, with next-token
 1627 likelihood $p(y_k | y_{<k}, x; \theta)$, SatImp defines
 1628

$$w_{s,i}^{\text{satimp}} = p(s_i | s_{<i}; \theta)^{\beta_1} \cdot (1 - p(s_i | s_{<i}; \theta))^{\beta_2}, \quad (35)$$

1629 and optimizes the reweighted GA objective
 1630

$$\mathcal{L}_{\text{SatImp}}(\mathcal{D}_t; \theta) = \frac{1}{|\mathcal{D}_t|} \sum_{s \in \mathcal{D}_t} \sum_i w_{s,i}^{\text{satimp}} \log p(s_i | s_{<i}; \theta), \quad (36)$$

1631 where $\beta_1, \beta_2 \geq 0$ control smoothness and preference: larger β_1 toward saturation, while larger β_2
 1632 toward importance.
 1633

1640 E.3 DETAILS ABOUT MODEL AND HYPERPARAMETERS

1641 Following [32, 13, 55, 26], we use Llama3.2-1B-Instruct, Llama3.2-3B-Instruct [18], Llama2-7b-
 1642 chat [66] and Phi-3.5-mini [1] on TOFU dataset, Llama2-7b and ICLM-7B [56] on MUSE dataset,
 1643 Llama3.2-1B-Instruct, Llama3.2-3B-Instruct and Zephyr-7b [67] on WMDP benchmark.
 1644

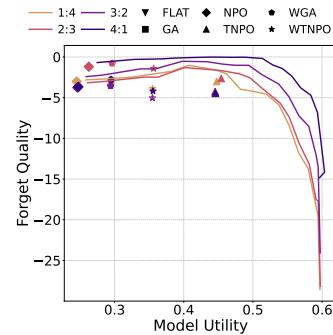
1645 For most experiments conducted on the two datasets, we use the AdamW optimizer with a learning
 1646 rate of 1×10^{-5} , an effective batch size of 32, and perform 10 unlearning epochs. The model-specific
 1647 hyper-parameters are set as follows: for NPO, we set $\beta = 0.1$; for GD, $\alpha = 1/10/20$; FLAT uses the
 1648 Total-Variation function. And since we run the baselines without a retain phase, directly following the
 1649 settings in [74] could lead to excessive unlearning. Therefore, we set $\alpha = 1000$ for WGA, $\beta = 200$
 1650 for TNPO, and $\alpha = 1000$, $\beta = 1000$ for WTNPO, and specifically, for FLAT, we used a learning
 1651 rate of 1×10^{-9} on Llama3.2-1B-Instruct and 5×10^{-10} on Llama3.2-3B-Instruct.
 1652

1653 E.4 ADDITIONAL EXPERIMENTAL RESULTS AND FURTHER DISCUSSION

1654 In this section, we provide additional experimental results.
 1655

1656 **Varying the validation proportion.** To investigate the effects of
 1657 validation set, we optimize the performance of all the methods
 1658 with varied validation proportion during unlearning. In Figure 6,
 1659 we plot the curves of CRU with different selected numbers of
 1660 layers from NPO to obtain the final model. We find that all of the
 1661 baselines are under the curve of CRU, indicating the consistent
 1662 performance gain regardless the validation set used on selecting
 1663 specific layers. On the other side, we should admit that the final
 1664 results can be affected by the specific unlearning method.
 1665

1666 **Comparison with RMU.** In Table 11, we compare our CRU with
 1667 RMU [26] in TOFU [32] with three different LLMs. RMU **steers**
 1668 the latent representations of the forget targets to a predetermined
 1669 random vector. The results show that although RMU can preserve
 1670 high MU in Llama3.2-1B/3B models, the FQ is extremely lower
 1671 than in the original model. In the larger LLM like Llama2-7B, we can find that RMU even disrupts
 1672 the whole model evident by the close-to-zero MU. In the later qualitative comparison, we find that
 1673 the LLM unlearned by RMU would generate sentence with repeated short-terms or words that induce
 1674 the low FQ. In contrast, our CRU can achieve high FQ with satisfactory MU based on NPO unlearned
 1675 model. In addition, our CRU can also be adopted on the basis of RMU to enrich perform layer-wise
 1676 replacement as their basic intuition is also orthogonal. We summarize the results in Figure 14, where
 1677



1678 Figure 13: Regarding different
 1679 validation partition.
 1680

Table 11: Unlearning Results on TOFU using llama3.2-1B/3B and llama2-7B.

	ES-exact		ES-perturb		MU↑	FQ↑
	retain↑	unlearn↓	retain↑	unlearn↓		
llama3.2-1B						
Original	0.7642	0.7592	0.3286	0.3574	0.5914	-9.0517
RMU (w. \mathcal{D}_r)	0.6544	0.0282	0.3036	0.0281	0.5784	-16.6078
SimNPO	0.0341	0.0282	0.0280	0.0281	0.2723	-1.7983
Ours	0.2938	0.0981	0.1972	0.0851	0.5504	-2.0646
llama3.2-3B						
Original	0.9013	0.9291	0.4241	0.4111	0.6579	-5.7157
RMU (w. \mathcal{D}_r)	0.8270	0.0331	0.4003	0.0349	0.6755	-20.1010
SimNPO	0.0342	0.0292	0.0279	0.0281	0.3108	-1.7983
Ours	0.7251	0.2117	0.3677	0.1215	0.6691	-3.2700
llama2-7B						
Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446
RMU (w. \mathcal{D}_r)	0.0310	0.0273	0.0307	0.0250	0.0189	-11.6015
SimNPO	0.0299	0.0257	0.0235	0.0238	0.4169	-1.9297
Ours	0.0355	0.0719	0.0309	0.0252	0.5296	-1.9297



Figure 14: Performance comparison of RMU with CRU+RMU (Ours), and heatmap on model parameter differences between unlearned and the original llama3.2-1B. The results show that our CRU can be compatible with RMU and can achieve better performance trade-off.

the left panel demonstrate the CRU performance with different k can achieve better FQ and MU than the plain RMU and original LLM, and the right panel present the model parameter change of all the methods where our CRU get the final hybrid model with 5 layers selected from the unlearned model by RMU to the original LLM.

Comparison with single-layer finetuning for unlearning. In addition to the previous demonstration on efficiency, we also conduct the comparison about more a extreme case, considering the single-layer finetuning methods. In Table 12, we present the results including most of baselines considered in our work and perform gradient updates restricted to specific one layer. In terms of efficiency, CRU achieves the third-lowest running time among all methods, thanks to its optimization-free, post-hoc design that avoids costly backpropagation. Notably, even single-layer fine-tuning methods still require full forward passes for loss computation (RMU uses latent representations but also incurs additional cost due to regularization with retaining data). Moreover, our comparison does not account for the extra time required to search for the optimal layer to fine-tune. In terms of performance, CRU consistently delivers the best trade-off, as generally other methods didn't forget significantly (refer to similar FQ). Unlike single-layer fine-tuning, which can suffer from reduced representation capacity for optimization flexibility, CRU avoids interfering with the training dynamics altogether for unlearning, while restoring fragile components post-unlearning in a stable and scalable manner.

1728 Table 12: Comparison of CRU with Single-layer Finetune-based Unlearning Methods.
1729

	Llama-2-7b-chat-hf	MU↑	FQ↑	Time (s)
1730	Original	0.6192	-10.1446	-
1731	GA (single layer)	0.6201	-9.8654	570.73
1732	NPO (single layer)	0.6195	-9.8654	2338.25
1733	WGA (single layer)	0.6206	-10.1446	1330.45
1734	TNPO (single layer)	0.6200	-10.1446	2348.50
1735	WTNPO (single layer)	0.6206	-10.1446	2259.28
1736	FLAT (single layer)	0.6197	-10.1446	1897.54
1737	RMU (single layer)	0.0189	-11.6015	5897.08
1738	Ours	0.5296	-1.9297	1752.00
1739				
1740				
1741	Exploration on multi-source replacement. Our current formulation of CRU mainly uses a binary 1742 merge (original vs. unlearned) which is motivated from the latent knowledge fragility during 1743 unlearning, but the post-hoc component replacement is generalizable to multi-source merging (e.g., 1744 using additional reference models trained for different retention targets or objectives). For example, 1745 merging the original, GA unlearned, NPO unlearned LLMs. In Table 13, we conduct preliminary 1746 exploration. The results show that the obtained model achieves a similar trade-off in unlearning. Since 1747 there is no significant improvement, we think focusing on two LLM (the original and unlearned model) 1748 is more appropriate, and can serve as an atomic way for exploration considering the algorithmic 1749 complexity, as involving more LLM will also need to introduce additional computational cost for the 1750 expanded searching space.			
1751	Further clarification about results on WMDP. For the results in Table 3, we would like to note that 1752 the reported results (similar values on FQ and MU) do not indicate an intended model collapse, but 1753 rather reflect the difficulty of the WMDP benchmark. These values are on par with prior unlearning 1754 work [77] and should be interpreted in the context of the challenging unlearning setting. To address 1755 the confusion, we also present Table 14 to vary the training setups (e.g., learning rate) of baseline 1756 methods to provide an overview of the performance. The results show that even FQ of the baseline 1757 method achieves 0.28 like ours, it can still not achieve high MU like CRU, indicating an intrinsic 1758 difficulty of unlearning for the trade-off instead of an implementation issue. In fact, our method 1759 achieves similar FQ while maintaining good MU compared to baselines, demonstrating a favorable 1760 trade-off improvement.			
1761	Visualization on model parameter changes. In Figures 15 and 16, we visualize the normalized 1762 model parameter change (calculated by l_1 distance and then normalized with baselines) in the original 1763 LLM using Llama3.2-3B-Instruct and Llama2-7B-chat. Consistent with the previous Figure 5, we 1764 find that all the previous baselines would indiscriminately change the whole model or even restrict the 1765 shallow layer updates. Those visualizations correspond to the results in Table 1, and we demonstrate 1766 that restoring middle layers with fragile latent knowledge can benefit the unlearning trade-off.			
1767	Qualitative examples of unlearning methods. In addition to the major comparison on output 1768 examples with the original model, GA, NPO and our CRU in Table 6, we present the complete results 1769 considering all the methods in Tables 16, 17, 18 and 19. In general, compared with the original 1770 output, all those unlearning methods can indeed output something different with the reference with 1771 target information. However, most of their outputs include incoherent word patterns such as repeated 1772 words (e.g., GA, NPO), repeated short-sentences (e.g., WGA) or semantic-disrupted expression (e.g., 1773 TNPO, WTNPO). Note that FLAT can encourage the LLM output “I’m not sure about that”, while 1774 the hidden representation disruption can also induce the same output on the non-target retention data.			
1775				
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1781				

Table 13: Preliminary Exploration on Multi-source (e.g., three LLM) Replacement.

	Llama-3.2-1B-Instruct	FQ	MU
Original	-9.0517	0.5914	
GA-Original	-2.7916	0.5426	
NPO-Original	-2.0646	0.5504	
GA-NPO-Original	-1.3084	0.5293	
	Llama-3.2-3B-Instruct	FQ	MU
Original	-5.7157	0.6579	
GA-Original	-3.2700	0.6691	
NPO-Original	-1.5462	0.5117	
GA-NPO-Original	-1.7983	0.5416	
	Llama-2-7b-chat-hf	FQ	MU
Original	-10.1446	0.6192	
GA-Original	-5.2994	0.6019	
NPO-Original	-1.9297	0.5296	
GA-NPO-Original	-2.3448	0.5282	
	Phi-3.5-mini-instruct	FQ	MU
Original	-7.2902	0.6648	
GA-Original	-4.8978	0.6245	
NPO-Original	-0.9796	0.4977	
GA-NPO-Original	-2.9475	0.5242	

Table 14: CRU can achieve better trade-off than baselines with varied training setups without "over-unlearning".

	Method	learning rate	MMLU(MU)	WMDP(FQ)
Original		-	0.4694	0.3533
GA		1e-7	0.4665	0.3457
GA		5e-7	0.3760	0.3236
GA		1e-6	0.3039	0.2677
GA		5e-5	0.2465	0.2431
Ours		-	0.3902	0.2864

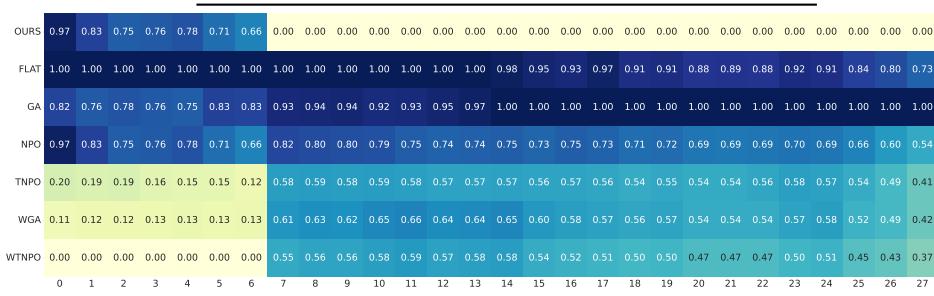


Figure 15: Heatmap on model parameter differences between unlearned and the original llama3.2-3B.

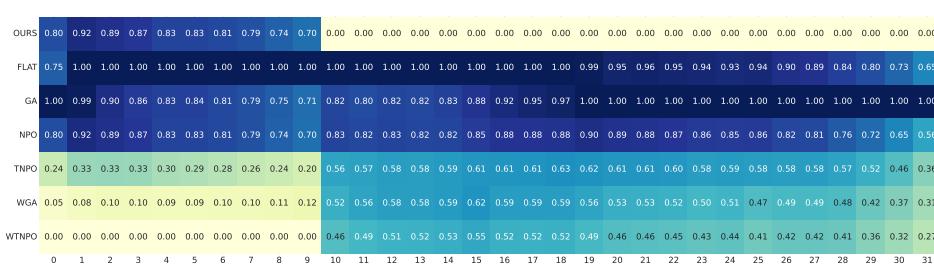


Figure 16: Heatmap on model parameter differences between unlearned and the original llama2-7B.

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Table 15: Full Results of unlearning on TOFU with Llama3.2, Llama2 and Phi-3.5 models.

NPO	ES-exact		ES-perturb		MU↑	FQ↑	GA	ES-exact		ES-perturb		MU↑	FQ↑
	retain↑	unlearn↓	retain↑	unlearn↓				retain↑	unlearn↓	retain↑	unlearn↓		
llama3.2-1B													
Original	0.7642	0.7592	0.3286	0.3574	0.5914	-9.0517	Original	0.7642	0.7592	0.3286	0.3574	0.5914	-9.0517
Unlearned	0.0339	0.0287	0.0270	0.0281	0.2203	-2.3448	Unlearned	0.0332	0.0282	0.0265	0.0281	0.0000	-104.7672
+RT (w. \mathcal{D}_t)	0.1638	0.0730	0.1142	0.0700	0.4386	-2.2030	+1×KL (w. \mathcal{D}_t)	0.0386	0.0282	0.0303	0.0281	0.1156	-104.7672
FLAT	0.1272	0.1010	0.0993	0.0835	0.2787	-3.9575	+10×KL (w. \mathcal{D}_t)	0.3945	0.1214	0.1652	0.1025	0.5467	-4.3228
TNPO	0.0803	0.0373	0.0654	0.0376	0.3121	-2.2030	+20×KL (w. \mathcal{D}_t)	0.7360	0.3089	0.3067	0.2296	0.5901	-8.0218
WTNPO	0.0342	0.0287	0.0265	0.0287	0.3512	-0.6871	WGA	0.0340	0.0282	0.0265	0.0281	0.2898	-0.9796
AltPO	0.0600	0.0362	0.0599	0.0375	0.4519	-2.0646	SatImp	0.2253	0.1555	0.1457	0.1327	0.4652	-7.2902
Ours	0.2938	0.0981	0.1972	0.0851	0.5504	-2.0646	Ours	0.2318	0.0689	0.1362	0.0554	0.5426	-2.7916
llama3.2-3B													
Original	0.9013	0.9291	0.4241	0.4111	0.6579	-5.7157	Original	0.9013	0.9291	0.4241	0.4111	0.6579	-5.7157
Unlearned	0.0336	0.0287	0.0271	0.0281	0.0347	-7.0539	Unlearned	0.0332	0.0282	0.0265	0.0281	0.0000	-104.7672
+RT (w. \mathcal{D}_t)	0.1706	0.0650	0.1134	0.0678	0.4429	-1.6705	+1×KL (w. \mathcal{D}_t)	0.0921	0.0282	0.0663	0.0281	0.3251	-104.7672
FLAT	0.2489	0.1881	0.1481	0.1679	0.5000	-2.3448	+10×KL (w. \mathcal{D}_t)	0.3521	0.0575	0.1437	0.0417	0.6222	-4.7025
TNPO	0.0421	0.0282	0.0286	0.0281	0.4397	-1.4255	+20×KL (w. \mathcal{D}_t)	0.8340	0.4356	0.3622	0.2506	0.6633	-4.3228
WTNPO	0.0347	0.0282	0.0304	0.0281	0.4257	-1.3084	WGA	0.0342	0.0282	0.0277	0.0281	0.3511	-1.3084
AltPO	0.0356	0.0287	0.0280	0.0287	0.4899	-1.4255	SatImp	0.0341	0.0282	0.0280	0.0287	0.3120	-1.3084
Ours	0.0999	0.0719	0.1058	0.0846	0.5117	-1.5462	Ours	0.7251	0.2117	0.3677	0.1215	0.6691	-3.2700
llama2-7B													
Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446	Original	0.9867	0.9774	0.6018	0.5366	0.6192	-10.1446
Unlearned	0.0285	0.0243	0.0233	0.0238	0.0479	-0.4366	Unlearned	0.0278	0.0235	0.0220	0.0235	0.0000	-104.7672
+RT (w. \mathcal{D}_t)	0.0914	0.0267	0.1403	0.0280	0.5132	-2.3448	+1×KL (w. \mathcal{D}_t)	0.0512	0.0235	0.0734	0.0235	0.4980	-104.7672
FLAT	0.0278	0.0235	0.0220	0.0235	0.0000	-20.5133	+10×KL (w. \mathcal{D}_t)	0.4730	0.0235	0.1752	0.0235	0.6042	-23.9958
TNPO	0.0598	0.0313	0.0833	0.0322	0.4315	-2.6391	+20×KL (w. \mathcal{D}_t)	0.8473	0.3380	0.4320	0.2256	0.5934	-6.3679
WTNPO	0.0521	0.0324	0.0711	0.0336	0.4502	-2.7916	WGA	0.0405	0.0327	0.0501	0.0302	0.4037	-5.5057
AltPO	0.0604	.0330	0.0864	0.0344	0.3911	-2.0646	SatImp	0.1308	0.1295	0.2048	0.0752	0.5237	-10.1446
Ours	0.0355	0.0719	0.0309	0.0252	0.5296	-1.9297	Ours	0.4924	0.1131	0.2801	0.0687	0.6019	-5.2994
Phi-3.5-mini													
Original	0.9148	0.9598	0.4593	0.4078	0.6648	-7.2902	Original	0.9148	0.9598	0.4593	0.4078	0.6648	-7.2902
Unlearned	0.0272	0.0233	0.0215	0.0233	0.2874	-3.4365	Unlearned	0.0272	0.0233	0.0215	0.0233	0.0	-104.7672
+RT (w. \mathcal{D}_t)	0.0272	0.0233	0.0215	0.0233	0.4747	-2.0646	+1×KL (w. \mathcal{D}_t)	0.0273	0.0233	0.0215	0.0233	0.0016	-81.6946
FLAT	0.5361	0.4282	0.2847	0.3118	0.6037	-5.0968	+10×KL (w. \mathcal{D}_t)	0.6736	0.2525	0.2901	0.2179	0.6509	-9.8655
TNPO	0.0272	0.0233	0.0215	0.0233	0.4927	-2.6391	+20×KL (w. \mathcal{D}_t)	0.8907	0.5444	0.4196	0.3574	0.6648	-8.2735
WTNPO	0.0272	0.0233	0.0215	0.0233	0.4116	-4.5108	WGA	0.0272	0.0233	0.0215	0.0233	0.2323	-10.7151
AltPO	0.0272	0.0233	0.0215	0.0233	0.4977	-0.9796	SatImp	0.1555	0.1383	0.1077	0.1362	0.5454	-3.1070
Ours	0.0272	0.0233	0.0215	0.0233	0.4977	-0.9796	Ours	0.3117	0.1959	0.1335	0.1636	0.6245	-4.8978

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Table 16: Qualitative results of model output on each unlearned models for target data.

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Table 17: Qualitative results of model output on each unlearned models for target data.

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Table 19: Qualitative results of model output on each unlearned models for non-target data.

2160 F BROADER IMPACTS AND LIMITATIONS
21612162 Our work explores the inherent trade-off of LLM unlearning from a new perspective of latent
2163 knowledge fragility. By introducing the systematic component-wise patching approach, we can
2164 isolate and characterize the effects on the intrinsic knowledge structure of LLMs under unlearning,
2165 via the model parameter influence. In light of identified functionality differences of different layers in
2166 the model, we propose a lightweight and general framework termed CRU to improve the performance
2167 of the unlearned model by restoring the fragile components from the original model. Our CRU
2168 provides new possibilities on a method-agnostic and scalable post-hoc surgical unlearning paradigm.2169 **Broader Impacts.** Regarding the nature of LLM unlearning, it can serve as a way of reverse engi-
2170 neering to analyze the knowledge composition in the LLM internals. We bring the new perspective
2171 of latent knowledge fragility to explore structure- or component-wise influence under unlearning,
2172 which also contributes to a deeper understanding of how large models store and entangle knowledge
2173 across layers. This perspective not only advances algorithmic unlearning but also promotes inter-
2174 pretability and controllability in model behavior. In practical terms, our framework could enable
2175 safer deployment of LLMs by allowing targeted removal of sensitive or outdated information without
2176 broadly degrading model utility. Beyond specific unlearning scenarios, our framework has potential
2177 implications for modular model design, where localized interventions are preferred over global
2178 parameter updates. Additionally, our ranking-based merging score introduces a transparent criterion
2179 for selecting impactful layers in various patching workflows, and also bridge the problem with various
2180 significant but underexplored (in the context of complex models like foundation models) research
2181 problems, such as interchange intervention or shapley interaction for modular influence consideration.2182 **Limitations.** Although our CRU provides a modular-based approach to isolate the effects and improve
2183 unlearning in LLMs, several limitations remain for the current LLM unlearning paradigm, which
2184 also apply to existing unlearning baselines. First, the replacement process assumes modularity in
2185 LLM latent representations of different layers, yet in practice, knowledge may also be redundantly or
2186 non-independently distributed across multiple components. Second, while we focus on the removal-
2187 retention trade-off at the representation level, downstream behavioral impacts, such as fairness,
2188 consistency, or hallucination risk, require future investigation to ensure robust and safe deployment.2189
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