Rethinking LLM Unlearning: From Safety Constraints to Functional Utility

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Abstract

Machine unlearning aims to approximate the counterfactual LLM that would have been trained without specified data. Given its rapid development, a timely and comprehensive review is essential. Despite the emergence of surveys on LLM unlearning, existing reviews lag behind rapid progress in benchmarks, unlearning algorithms, and evaluation under safety objectives. Moreover, they largely overlook functional uses. We address these gaps by offering an up-to-date, application-oriented survey that organizes the literature into *safety forgetting* and *functional forgetting*. For safety forgetting, we revisit benchmarks, unlearning algorithms, and evaluation, highlighting recent developments such as automatically synthesized benchmarks, the distinction between single and continual settings, and evaluation challenges for reasoning LLMs. Beyond safety forgetting, unlearning may also serve as a functional tool. We thus identify functional forgetting as an important yet underexplored counterpart to safety forgetting, spanning behavior probing, graceful forgetting, and an empirical pilot on model regularization. We conclude by outlining future directions for building more reliable, scalable, and broadly useful LLM unlearning systems.

1 Introduction

Large language models (LLMs) trained on massive corpora exhibit strong capabilities, yet training-data memorization can raise ethical, legal, and security concerns by exposing personal information, harmful content, or copyrighted text (Karamolegkou et al., 2023). Moreover, regulations such as the EU's Right to be Forgotten (Ginart et al., 2019) underscore the need for mechanisms that enforce data removal. Motivated by these concerns, *machine unlearning* aims to update a trained model so that it behaves as if specific training examples had never been learned (Cao and Yang, 2015).

Machine unlearning for LLMs has attracted increasing attention in recent years, primarily as a data removal mechanism for safety objectives. Meanwhile, LLMs are rapidly evolving in scale and capability, driven by larger model capacity and new training paradigms. This co-evolution introduces new challenges and complexities for unlearning, such as potential leakage arising from thinking behaviors (Wang et al., 2025a). Beyond data removal, unlearning may also serve as a functional tool. For example, prior work suggests that unlearning followed by relearning can improve model accuracy, indicating its potential to enhance model capabilities (Xu et al., 2026c). However, this functional perspective remains relatively underexplored.

While several preliminary surveys on LLM unlearning have emerged (Liu et al., 2025; Qiu et al., 2025; Blanco-Justicia et al., 2025; Le-Khac and Truong, 2025; Ren et al., 2025b; Geng et al., 2025), they still lag behind recent developments in safety-oriented data removal and largely overlook functional uses. As shown in Figure 1 and summarized in Table 1, we provide an application-oriented and up-to-date view of the field by organizing LLM unlearning into two categories based on application focus: *safety forgetting*, which is driven by safety objectives and covers privacy, copyright, and harmful content, and *functional forgetting*, which uses unlearning to analyze or improve model behavior, including behavior probing, graceful forgetting of outdated knowledge, and model regularization to reduce overfitting. Building on recent advances in both unlearning and LLM evolution, we structure this survey around these two categories and their key components and, to the best of our knowledge, provide the first survey that extends the discussion from safety objectives to functional forgetting.

In the safety forgetting domain, recent work can be organized into three components of an unlearning pipeline: benchmark, unlearning algorithms, and evaluations. Benchmarks are automatically synthesized to improve quality (Zhu et al., 2025; Xu et al., 2026b). Unlearning algorithms depend on

Work	Date	Taxonomy Axis	Scenario	Eval Coverage				Benchmark Src.	Applications					
				Forget.	Util.	Robust.	Effi.		Copy.	Priv.	Harm.	Behaiv.	Grace.	Regula.
Blanco-Justicia et al. (2025)	2025	Meth. taxonomy by modif. reach & depth.	Single	●	●	◐	◐	Pre	●	●	●	○	○	○
Liu et al. (2025)	2025	Lifecycle view: form., meth., metr., appl.	Both	●	●	◐	◐	Pre	●	●	●	○	○	○
Geng et al. (2025)	2025	Structure view: meth., eval., bench., appl.	Single	●	●	◐	○	Pre	●	●	●	○	○	○
Ren et al. (2025b)	2025	Removal-intended vs. suppression-intended	Both	●	●	◐	○	Pre	●	●	●	○	○	○
Le-Khac and Truong (2025)	2025	Meth./eval./bench./threat/appl. + "robustness"	Single	●	●	◐	◐	Pre	●	●	●	○	○	○
Qiu et al. (2025)	2025	Taxonomy by LLM pipeline intervention phase.	Both	●	●	◐	◐	Pre	●	●	●	○	○	○
Ours	**2026**	**Applications: safety vs. functional forgetting.**	**Both**	●	●	●	●	**Pre+Auto**	●	●	●	●	●	●

Table 1: Comparison of LLM unlearning surveys in chronological order: **Taxonomy Axis** is the main organizing principle (abbr.: modif.=modification, form.=formulation, meth.=methods, metr.=metrics, eval.=evaluation, bench.=benchmarks, appl.=applications, threat=threat models); **Scenario** indicates single unlearning (Single) or also continual unlearning (Both); **Eval Coverage** marks Forget. (forgetting), Util. (utility), Robust. (robustness), and Effi. (efficiency); **Benchmark Src.** denotes Pre (predefined), Auto (automatically synthesized), or Pre+Auto. **Applications**: Copy. (copyright), Priv. (privacy), Harm. (harmful content), Behavi. (behavior probing), Grace. (graceful forgetting), and Regula. (model regularization). ●/◐/○indicates explicit/partial/minimal coverage.

the setting, with continual unlearning introducing new challenges in efficiency and stability beyond single unlearning. Evaluation should keep pace with evolving LLMs across the forgetting–utility trade-off, robustness, and efficiency. For example, in large reasoning models (LRMs), reasoning behaviors can reveal leakage during the thinking process beyond what standard metrics such as accuracy can capture (Wang et al., 2025a).

Beyond safety forgetting, we position functional forgetting as an underexplored counterpart built on similar unlearning algorithms but oriented toward distinct goals. We organize it along three complementary dimensions: (i) behavior probing, which uses unlearning as an intervention to analyze and attribute model behaviors (Tutek et al., 2025); (ii) graceful forgetting, which removes outdated or undesired knowledge (Jiang et al., 2025); and (iii) model regularization, which examines whether unlearning can mitigate overfitting and improve generalization. We present the regularization direction as an empirical pilot, supported by prior observations and illustrated through our case study.

Our main contributions are:

I) We provide a comprehensive application-oriented and up-to-date taxonomy of LLM unlearning, organizing prior work into *safety forgetting* and *functional forgetting*, and clarifying the key elements underlying these applications.

II) We revisit safety forgetting from three components: benchmark, unlearning algorithm, and evaluation, and incorporate newer considerations such as automatically synthesized benchmarks, continual unlearning challenges, and new evaluation issues.

III) We highlight functional forgetting as an underexamined counterpart and, to the best of our knowledge, provide its first survey coverage. We structure this perspective around behavior probing, graceful forgetting, and model regularization. We summarize future directions for LLM unlearning.

2 Preliminaries and Taxonomy

2.1 Machine Unlearning

Machine unlearning has emerged as a central research direction in response to data protection regulations such as the Right to be Forgotten (Ginart et al., 2019). Let $\mathcal{D}$ denote the full training corpus, A the training algorithm, and $\mathcal{M} = A(\mathcal{D})$ the resulting model. A forget request specifies a subset $\mathcal{D}_f \subset \mathcal{D}$ to be removed; the remaining data form the retain set $\mathcal{D}_r = \mathcal{D} \setminus \mathcal{D}_f$. Given $(\mathcal{M}, \mathcal{D}_f)$, an unlearning algorithm U outputs an unlearned model $\mathcal{M}_f = U(\mathcal{M}, \mathcal{D}_f)$. For evaluation, a retrained reference model $\mathcal{M}_r = A(\mathcal{D}_r)$ represents the counterfactual model trained without $\mathcal{D}_f$, and an evaluation protocol E assesses unlearning by comparing $\mathcal{M}_f$ against $\mathcal{M}_r$ (Figure 2).

Under given evaluation E, unlearning algorithm U is categorized as *exact* or *approximate* (Bourtoule et al., 2021). *Exact* unlearning requires $\mathcal{M}_f$ to be statistically indistinguishable from that of the retrained model $\mathcal{M}_r = A(\mathcal{D}_r)$. *Approximate* unlearning relaxes this requirement and instead tests whether the distribution $\mathcal{M}_f$ is close to $\mathcal{M}_r$.

2.2 LLM Machine Unlearning

LLM unlearning has garnered increasing attention for mitigating trustworthiness risks, including copyright (Shi et al., 2025), privacy (Maini et al., 2024), and harmful content (Li et al., 2024). Compared to classical settings such as image classification, exact unlearning is often impractical for modern LLMs, since full retraining and partition-based schemes (e.g., SISA (Bourtoule et al., 2021)) incur

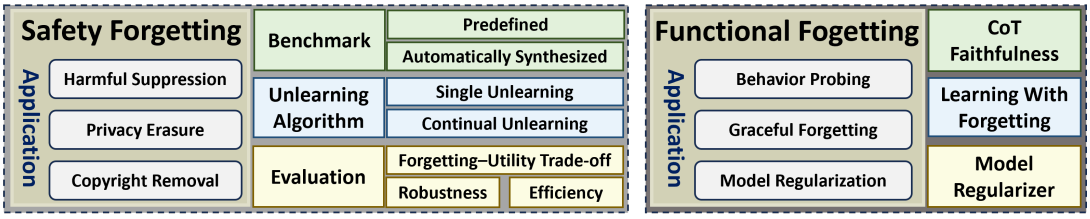

Figure 1: A structured overview of LLM unlearning: We organize prior work into two categories based on application focus: *safety forgetting*, including privacy erasure, copyright removal, and harmful suppression, and *functional forgetting*, including behavior probing, graceful forgetting, and model regularization. We analyze the first category along three dimensions, covering benchmark, unlearning algorithm, and evaluation; and the second category through three representative functional objectives: CoT faithfulness, learning with forgetting, and model regularizer.

prohibitive computational overhead. Consequently, recent work has largely shifted toward scalable and effective approximate unlearning algorithms (Yao et al., 2024a). Yet this notion remains ambiguous: because dataset-to-model mapping is not unique, since closeness to a target model does not imply equivalence to the counterfactual model trained without $\mathcal{D}_f$ (Thudi et al., 2022). This issue is further exacerbated in LLMs, where similar evaluation metrics, such as task accuracy / perplexity, still leak knowledge about the forget set (Xu et al., 2026c).

While unlearning can be ambiguously defined in LLMs, a common mathematical formulation helps clarify its core objective. Building on the unlearning pipeline outlined earlier, we present a widely used formulation of LLM unlearning that serves as a representative framework across most settings.

$$\min_{\theta_f} \underbrace{-\mathbb{E}_{x\in\mathcal{D}_f}[\ell(x;\theta_f)]}_{Unlearn} + \underbrace{\lambda\,\mathbb{E}_{x\in\mathcal{D}_r}[\ell(x;\theta_f)]}_{Retain},$$

where θ_f parameterizes the unlearned model $\mathcal{M}_f$ and ℓ denotes the loss function. The first term suppresses the influence of $\mathcal{D}_f$, and the second term preserves utility on $\mathcal{D}_r$. We use the parameter λ to balance the forgetting–utility trade-off.

2.3 A Taxonomy of LLM Machine Unlearning

While preliminary surveys on LLM unlearning have emerged (Liu et al., 2025; Qiu et al., 2025; Blanco-Justicia et al., 2025; Le-Khac and Truong, 2025; Ren et al., 2025b; Geng et al., 2025), they still fall short of covering recent advances in safety-oriented data removal, and give limited attention to functional uses. To provide a broader view of this landscape, we categorize the LLM unlearning literature by application focus into two groups: *safety forgetting* and *functional forgetting*. To the best of our knowledge, this survey is the first to extend the discussion of unlearning beyond conventional safety-oriented data removal to include

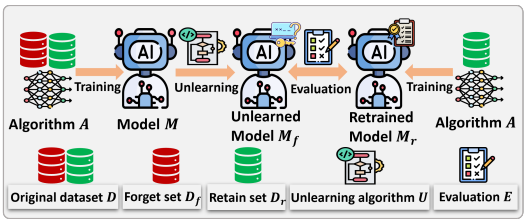

Figure 2: Machine unlearning pipeline: A model $\mathcal{M} = A(\mathcal{D})$ is trained on $\mathcal{D}$. Given a forget set $\mathcal{D}_f \subset \mathcal{D}$, an unlearning algorithm U outputs $\mathcal{M}_f = U(\mathcal{M}, \mathcal{D}_f)$ with retain set $\mathcal{D}_r = \mathcal{D} \setminus \mathcal{D}_f$. Unlearning is evaluated by E against the retrained reference $\mathcal{M}_r = A(\mathcal{D}_r)$.

broader functional applications, offering a systematic, application-oriented, and up-to-date survey. Safety forgetting typically involves removing information related to privacy, copyright, or harmful content that should not be retained. By comparison, functional forgetting tends to leverage unlearning to analyze and improve model behavior.

For safety forgetting, existing work can be organized around three components, as shown in Figure 2: benchmark, unlearning algorithm, and evaluation. Figure 1 further structures the literature by benchmark design (predefined vs. automatically synthesized), algorithm setting (single vs. continual), and evaluation criteria (forgetting–utility trade-off, robustness, and efficiency). Section 3 further details these three components.

Beyond safety forgetting, we highlight *functional forgetting* as a nascent counterpart built on shared unlearning foundations but oriented toward distinct goals. Although less mature, it repurposes unlearning as a tool for probing, understanding, and improving model behavior. As summarized in Figure 1, we organize this direction into three dimensions: behavior probing, graceful forgetting, and model regularization. Behavior probing uses unlearning to probe model behaviors, such as Chain

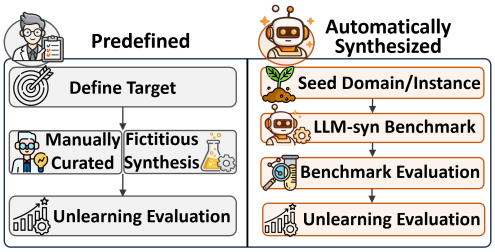

Figure 3: Overview of benchmark construction: **Predefined** benchmarks specify a target and construct requests manually or via fictitious synthesis, then evaluate unlearning. **Automatically synthesized** benchmarks start from seeds, generate and validate an LLM-synthesized benchmark, then evaluate unlearning.

of Thought (CoT) faithfulness. Graceful forgetting incorporates forgetting into training to steer behavior while preserving utility. Model regularization treats unlearning as a regularizer that mitigates overfitting and improves generalization. We discuss these three dimensions in Section 4.

3 Safety Forgetting

This section provides an overview of *safety forgetting*. In §3.1, we review how benchmarks define forgetting targets under both predefined and automatically synthesized constructions. In §3.2, we survey unlearning algorithms in both single and continual settings. In §3.3, we summarize how recent work evaluates forgetting–utility trade-off, robustness, and efficiency. Due to space constraints, the full taxonomy is in Appendix A (Figure 8).

3.1 Benchmark: What to Forget

Despite rapid methodological progress, the benchmark of unlearning remains a bottleneck. Thaker et al. (2025) showed that benchmarks can yield unreliable conclusions, either overstating or understating efficacy, when benchmark design fails to reflect what the target model actually knows. This motivates careful benchmark construction.

Figure 3 summarizes two benchmark construction paradigms: *predefined* and *automatically synthesized*. Predefined benchmarks specify the forgetting target in advance and then construct benchmark instances accordingly. The target may be based on real, manually curated data, or on fictitious templates. By contrast, automatically synthesized benchmarks start from a seed, expand it via LLM-based generation, and then assess the benchmark quality. This paradigm improves scalability, but it depends heavily on the synthesis quality.

Type of Construction	Benchmark	Harm.	Priv.	Copy.
Predefined	WHP (Eldan and Russinovich, 2023)	×	×	✓
	TOFU (Maini et al., 2024)	×	✓	×
	RWKU (Jin et al., 2024)	×	✓	×
	WMDP (Li et al., 2024)	✓	×	×
	MUSE (Shi et al., 2025)	×	×	✓
	PCH (Xu et al., 2026a)	✓	✓	✓
Automatically Synthesized	Textbook (Zhu et al., 2025)	✓	×	✓
	Biforget (Xu et al., 2026b)	✓	✓	✓

Table 2: Predefined vs. automatically synthesized unlearning requests. ✓ indicates the benchmark targets the corresponding category; × indicates it does not.

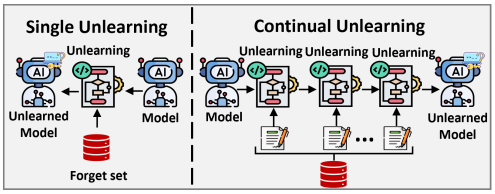

Figure 4: Illustration of unlearning algorithms. **Single unlearning** updates the model once for a fixed request. **Continual unlearning** updates the model repeatedly over a stream of requests across multiple rounds.

Table 2 instantiates this taxonomy across three application categories: harmful content, privacy, and copyright. Under the predefined paradigm, WHP (Eldan and Russinovich, 2023) studies copyright removal using the Harry Potter series, and MUSE (Shi et al., 2025) extends this setting to multiple sources. For privacy, TOFU (Maini et al., 2024) uses templated queries about fictitious individuals, while RWKU (Jin et al., 2024) targets predefined real-world knowledge about public figures. For harmful content, WMDP (Li et al., 2024) focuses on hazardous domains such as weapon-related knowledge. While most prior benchmarks target a single category, PCH (Xu et al., 2026a) unifies personal information, copyright, and harmful content, better reflecting real-world requests.

Automatic synthesis is motivated by the limited scalability of predefined benchmarks, which are mostly curated manually. Textbook (Zhu et al., 2025) is the first benchmark to systematically explore synthesis, using external generators such as GPT-4o-mini to decompose a target domain (*e.g.*, Harry Potter) into subtopics and expand them into long content. However, external generators may misalign with the target model's knowledge boundary, and heuristic prompting can miss implicit knowledge or stylistic variants. These limitations, together with the lack of privacy-oriented synthesis, motivate BiForget (Xu et al., 2026b) to unify benchmark synthesis via the target model for harmful content, copyright, and privacy, while evalu-

Setting	Paradigm	Example	Description
Single Unlearning	Input/output-based	Thaker et al. (2024)	Uses prompts or filters at inference time to suppress targets.
		Liu et al. (2024a)	Corrupts embeddings at inference for detected forget-scope prompts.
		Ji et al. (2024)	Uses an auxiliary model with logit subtraction for efficient forgetting.
	Editing-based	Wu et al. (2023)	Identifies privacy neurons and edits activations to reduce leakage.
		Ilharco et al. (2023)	Uses task-vector arithmetic on weights to steer or forget behavior.
		Gur-Arieh et al. (2025)	Removes concept directions via targeted ablation for concept erasure.
	Fine-tuning-based	Yao et al. (2024b)	Uses gradient ascent with retain regularization to forget targets.
		Yao et al. (2024a)	Benchmarks multiple unlearning objectives on pretraining chunks.
		Li et al. (2024)	Misdirects hazardous representations while preserving benign utility.
		Wang et al. (2025a)	Forgets reasoning traces while preserving general reasoning ability.
		Xu et al. (2025)	Combines robust objectives with stability controls against recovery.
		Zhang et al. (2025a)	Uses reinforcement unlearning to optimize the forget–retain trade-off.
Continual Unlearning	Update-localized-based	Wuerkaixi et al. (2025)	Localizes task-vector negation with sparse gradients to reduce drift.
		Xu et al. (2026a)	Filters redundant requests and localizes updates to curb continual drift.
	Adapter-gated-based	Gao et al. (2025)	Uses orthogonal LoRA and OOD gating to load adapters selectively.

Table 3: A taxonomy of unlearning algorithms by setting and paradigm.

ating quality in terms of relevance, diversity, and efficiency. However, verifying whether the synthesized data truly matches the intended forget set remains difficult across models and targets.

Takeaway: Benchmark design defines the forgetting target and shapes quality. Predefined benchmarks offer stronger control, while automatically synthesized benchmarks improve scalability and diversity, but ensuring benchmark quality remains challenging.

Category	Metric	Example
Forgetting–Utility Trade-off	Forget Quality+Model Utility	(Maini et al., 2024)
	Task-level (*e.g.*, accuracy, ppl)	(Yao et al., 2024a)
	Representation-level (*e.g.*, PCA)	(Xu et al., 2025)
	Forget Degree+Retain Utility	(Xu et al., 2026a)
Robustness	Prompt attacks (*e.g.*, Extraction)	(Patil et al., 2024)
	Relearning attacks (fine-tuning)	(Hu et al., 2025)
	Quantization attacks (*e.g.*, int4)	(Zhang et al., 2025b)
	Reasoning attacks (CoT prompt)	(Sinha et al., 2025)
Efficiency	Computation cost (*e.g.*, FLOPs)	(Yao et al., 2024a)
	Running time (*e.g.*, RTE)	(Xu et al., 2025)
	Benchmark cost (*e.g.*, size)	(Xu et al., 2026b)

Table 4: LLM unlearning evaluation taxonomy across forgetting–utility trade-offs, robustness, and efficiency.

3.2 Unlearning Algorithm: How to Forget

Figure 4 organizes unlearning algorithms into two settings: *single unlearning* and *continual unlearning*. Single unlearning updates the model once per request, while continual unlearning processes a sequence of requests across multiple rounds, making forgetting a sequential problem in which each update may affect future utility (Barez et al., 2025).

Table 3 further summarizes representative algorithms under these two settings. The single unlearning focuses on three paradigms (see Appendix Figure 9). Input/output-based approaches suppress target content without parameter updates (Thaker et al., 2024; Liu et al., 2024a; Ji et al., 2024), improving deployability; however, they provide no reliable guarantee of removal and can be readily reactivated under attacks (Liu et al., 2025). Editing-based approaches modify a small set of neurons or parameters (Wu et al., 2023; Ilharco et al., 2023; Gur-Arieh et al., 2025), offering direct control when the target is well localized. However, concept entanglement complicates stable attribution, and such localized edits can introduce serious safety risks under distribution shift or adversarial elicitation (Youssef et al., 2025). Fine-tuning-based approaches directly optimize forget–retain objectives (Yao et al., 2024b,a; Li et al., 2024; Wang et al., 2025a; Xu et al., 2025; Zhang et al., 2025a) and remain a widely used unlearning paradigm; however, without stability controls and careful design, they may cause either *superficial* forgetting, where the target knowledge is not truly removed, or induce *catastrophic* degradation of general capabilities and retain set (Xu et al., 2026c).

Moving from single to continual unlearning introduces new complexities: repeated updates accumulate drift, and later requests can interfere with earlier forgetting or reduce retained utility (Shi et al., 2025). This has motivated continual-specific designs to control cross-round interference. Update-localized methods restrict where each round updates the model: Wuerkaixi et al. (2025) uses sparse gradients to localize task-vector negation, while Xu et al. (2026a) filters redundant requests and focuses updates on influential layers

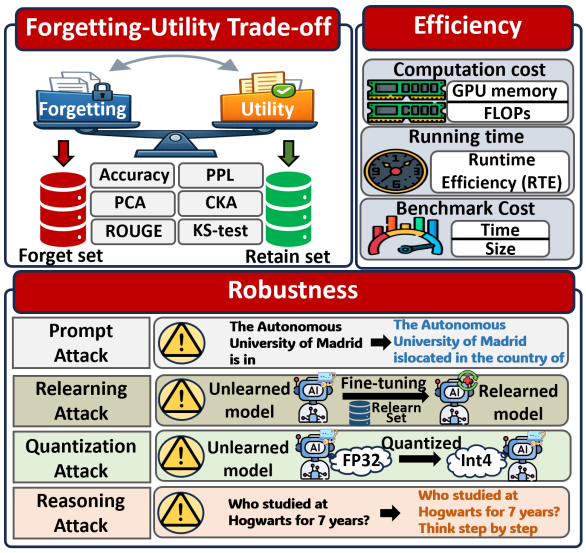

Figure 5: We illustrate three core axes of unlearning evaluation: the **forgetting–utility trade-off**, balancing forgetting effectiveness and retained utility; **efficiency**, measuring runtime, computation, and benchmark cost; and **robustness**, testing unlearning under prompt, relearning, quantization, and reasoning attacks.

to limit long-term drift. Adapter-gated methods instead isolate updates in modular adapters and use inference-time gating to reduce interference; Gao et al. (2025) combines orthogonal LoRA unlearning with out-of-distribution (OOD) gating to decide when adapters are loaded. Despite recent progress, continual unlearning remains early-stage: it is still unclear how many requests current methods can sustain before stability degrades, and they remain vulnerable to relearning attacks (Xu et al., 2026a).

Takeaway: Single and continual unlearning reflect different practical demands: the former benefits from a rich set of well-established algorithms, while the latter is more realistic but still struggles with instability and robustness.

3.3 Evaluation: How Well to Forget

Evaluating unlearning asks how well a model forgets. A satisfactory unlearning algorithm should remove the targeted knowledge, preserve non-target utility, remain robust under post-unlearning perturbations, and satisfy practical efficiency constraints. We organize recent evaluation practice along three axes: (a) the forgetting–utility trade-off; (b) robustness; and (c) efficiency.

Forgetting-utility trade-off. Table 4 and Figure 5 summarize how the forgetting-utility trade-

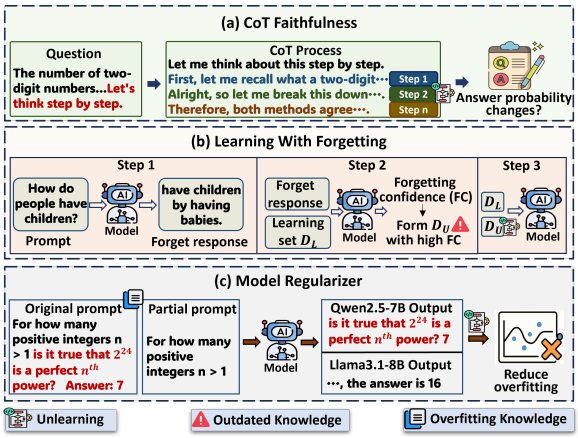

Figure 6: Functional unlearning beyond safety removal. Unlearning can (i) test **CoT faithfulness** by removing intermediate-step patterns and measuring answer shifts, (ii) support **learning with forgetting** by filtering outdated or low-value data, and (iii) serve as a **model regularizer** by suppressing overfitted knowledge.

off is assessed at multiple levels. Standard protocols (Yao et al., 2024a) report task-level metrics such as accuracy and perplexity (PPL). TOFU evaluates forget quality by testing whether the unlearned model is indistinguishable from a retain reference using Truth Ratio and a two-sample KS-test, and summarizes performance across sets with a harmonic-mean utility score (Maini et al., 2024). Recent work examines internal changes using representation-level evaluation, such as PCA similarity/shift, centered kernel alignment (CKA) (Xu et al., 2026c). For continual unlearning, FIT likewise adopts a retain-model proxy and defines Forget Degree and Retain Utility by aggregating probability, ROUGE, and token accuracy into a composite score (Xu et al., 2026a). However, most existing metrics (*e.g.*, accuracy) remain relatively superficial and therefore provide limited insight into robustness against post-unlearning attacks.

Robustness. Table 4 and Figure 5 summarize representative work on robustness evaluation that complements forgetting–utility metrics by incorporating recovery attempts. Prompt attacks re-elicit forgotten knowledge through rephrasing or jailbreak-style queries (Patil et al., 2024), while relearning attacks test how quickly target behaviors return under limited fine-tuning (Hu et al., 2025). Quantization attacks can also partially restore forgotten behaviors (Zhang et al., 2025b), and reasoning attacks, especially for LRMs, may bypass surface-level suppression by exploiting latent knowledge (Sinha et al., 2025). These observations

highlight the importance of robustness evaluation.

Efficiency. Practical deployment requires unlearning to be cost-effective. As shown in Figure 5 and Table 4, efficiency is commonly evaluated by computation and memory (*e.g.*, FLOPs) (Yao et al., 2024a), running time (*e.g.*, runtime efficiency (RTE)) (Xu et al., 2025), and benchmark cost (*e.g.*, the benchmark size) (Xu et al., 2026b). These factors are especially critical in continual settings, where costs accumulate across rounds and scalability often becomes the limiting factor.

We also provide two additional comparisons in the Appendix: metric pros and cons (Table 6) and unlearning paradigm efficiency (Table 7). While evaluation has advanced rapidly, theory lags behind: most methods provide only approximate unlearning, and "behaviour closeness" to a target model may not reflect the true forgetting (Thudi et al., 2022), calling for theoretical guarantees like differential privacy (DP) (Ginart et al., 2019).

> **Takeaway:** Evaluation shapes the conclusions drawn about unlearning: it must determine whether apparent forgetting reflects true removal rather than superficial suppression with efficiency, and move beyond empirical "closeness" toward theoretical guarantees.

4 Functional Forgetting

Beyond safety objectives, unlearning can also serve as a functional tool for understanding and improving models. We frame functional forgetting as a nascent counterpart to safety unlearning, connected by shared algorithmic foundations but oriented toward distinct goals. Figure 6 summarizes three representative uses: CoT faithfulness, learning with forgetting, and model regularizer. We treat model regularizer as an empirical pilot. We defer detailed information on these directions to Appendix B.

CoT Faithfulness CoT is a core component for reasoning models, improving accuracy while increasing output length under CoT supervision (Wei et al., 2022; Zeng et al., 2025). Recent evidence suggests that supervised fine-tuning (SFT) on long CoTs can further raise performance and strengthen reinforcement learning (RL) (Chang et al., 2025). However, it remains unclear whether CoTs reflect internal computation or post-hoc rationalization.

Figure 6(a) shows a workflow that uses unlearning as a *parametric intervention* to probe CoT faithfulness (Tutek et al., 2025). Given an input question, the model generates a CoT and a final answer. The CoT is segmented into reasoning steps, each treated as a candidate mechanism. For a selected step, localized unlearning suppresses the model's ability to produce it. Faithfulness is then measured by changes in the answer distribution, such as answer flips or probability shifts: stable answers suggest a post-hoc step, whereas shifted answers indicate computational relevance. The intervention is implemented with NPO+KL (see Appendix A.2).

Learning with Forgetting Graceful forgetting treats unlearning as a mechanism for removing outdated knowledge to support new learning. Inspired by neuroscience, it assumes that selective removal of irrelevant or stale information can improve learning (Anderson and Hulbert, 2021). Supporting evidence from image classification shows that unlearning biased memories can stabilize continual learning (Cao et al., 2025), and removing noisy-label influence can improve learning effectiveness (Sui et al., 2025b). However, whether such benefits consistently transfer to LLMs remains unclear.

As illustrated in Figure 6(b), Jiang et al. (2025) propose a learning with forgetting method on LLMs using a learning set $\mathcal{D}_L$ and a forget prompt set $\mathcal{D}_F$. The model is queried with $\mathcal{D}_F$ to generate candidate responses, and a forgetting confidence (FC) score is computed to rank them for removal. FC measures how each forget response interacts with the learning objective, with higher values indicating greater expected benefit from suppression on $\mathcal{D}_L$. The selected responses form the unlearning set $\mathcal{D}_U$, while $\mathcal{D}_L$ is used for learning. The model then interleaves learning and unlearning updates.

Model Regularizer Recent progress in LLMs has led to steady gains on reasoning tasks such as mathematics and code generation (DeepSeek-AI et al., 2025). Post-training via SFT or RL further improves performance, reinforcing the view that post-training shapes reasoning ability.

However, emerging evidence complicates this narrative. Some reported gains may reflect pretraining contamination or memorization rather than reasoning improvements. For example, Qwen2.5-7B can improve mathematical performance even under random or incorrect reward signals (Shao et al., 2025), casting doubt on RL as the true driver. Likewise, as shown in Figure 6(c), it can solve math problems from incomplete statements by implicitly reconstructing missing information, whereas other

models cannot (Wu et al., 2025). These findings suggest that some post-training gains may be partly illusory, reflecting an overfitting pattern.

As illustrated in Figure 6(c), we study model regularization as an empirical pilot, testing whether unlearning math-related data can reduce domain-specific overfitting. We evaluate GA and NPO on NuminaMath-1.5 (LI et al., 2024); details are in Appendix B.3. Results in Figure 7 and Appendix Table 8 show stable gains only on Qwen2.5, while other models degrade. This suggests that unlearning may serve as a targeted regularizer when overfitting to the target domain exists.

Takeaway: Functional forgetting is a promising direction for future study: it extends unlearning beyond safety, offers a complementary machine-learning lens on model behavior.

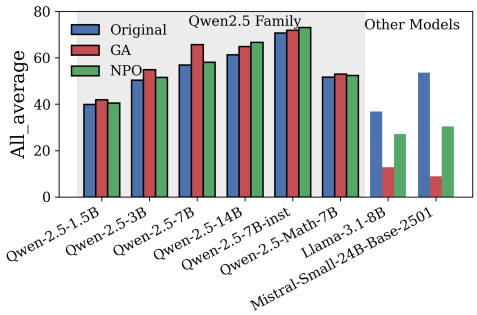

Figure 7: Overall performance after unlearning on NuminaMath-1.5: Bars show the average score of each model on multiple tasks before unlearning and after applying GA or NPO. The shaded region groups the Qwen2.5 family, while others are shown on the right.

5 Future Directions

5.1 Safety forgetting

Pre-unlearning validation for synthesized benchmarks. Although automatically synthesized benchmarks are more scalable and flexible than predefined ones (Xu et al., 2026b; Zhu et al., 2025), they can lead to misleading evaluations if the target model never learned the synthesized forget knowledge. Future benchmarks should therefore establish standardized pre-unlearning validation protocols, including evidence of target-model knowledge relevance checks, and strict forget-retain boundary verification. This would ensure that evaluation results reflect actual removal rather than artifacts of unknown or poorly scoped data.

Controlled counterfactual evaluation. Evaluation should move beyond superficial behavioral metrics, such as standard accuracy or "behavioral closeness" to a target model, which may not reflect true forgetting (Thudi et al., 2022). A promising direction is to use retain-only counterfactual models as rigorous baselines. By strictly controlling the semantic boundary between forget and retain sets, such protocols can better test whether targeted knowledge is genuinely removed without over-erasing nearby non-target knowledge.

Long-horizon degradation analysis. Continual unlearning should be evaluated over extended request sequences rather than isolated stages. Future work should track retain-utility decay, persistence of prior forgetting, relearning recovery rates, and cumulative compute or memory costs over time. Such longitudinal analysis is essential for exposing cross-round interference, utility collapse, and true scalability limits under realistic deletion streams.

5.2 Functional forgetting

While safety forgetting is the established paradigm, functional forgetting remains nascent, yet offers a proactive perspective that warrants broader exploration. We outline several directions below.

One promising direction is LLM data attribution: post-unlearning behavior can provide intervention-based signals for identifying influential training data. Since direct attribution is challenging in large generative models, Wang et al. (2024) unlearns a synthesized image and identifies samples with the largest reconstruction-loss increases as influential; a similar idea can be applied to LLMs. Another direction is graceful forgetting in continual learning, enabling models to update over time while selectively discarding outdated knowledge under finite capacity. Finally, unlearning may serve as regularization by suppressing overfitting and exposing contamination or memorization; since these effects vary across algorithms, systematic audits are needed to clarify what models implicitly store.

6 Conclusion

We provide a comprehensive survey of advances in LLM unlearning from both safety and functional forgetting. For safety forgetting, we organize the literature into benchmark, unlearning algorithm, and evaluation. For functional forgetting, we present unlearning as a tool for behavior probing, graceful forgetting, and regularization. We close by outlining future directions for LLM unlearning.

7 Limitations

Our work is a survey that aims to provide a comprehensive yet concise account of current progress in LLM unlearning. We therefore prioritize representative trends and a few emerging directions over exhaustive coverage. As a result, some relevant studies may be omitted, or only briefly cited without detailed explanation, with an extended taxonomy list and additional references provided in Appendix A. In addition, we present model regularization as an empirical pilot rather than as a direction firmly established by prior work. This example is included to illustrate a possible functional-forgetting use case motivated by related findings, but its effectiveness may depend on specific models, target domains, and overfitting patterns. We therefore view it as a promising yet preliminary direction that warrants further validation.

Ethical Considerations

This survey reviews machine unlearning in LLMs from both safety and functional perspectives, spanning benchmarks, algorithms, evaluation, and emerging use cases. By summarizing recent advances together with their limitations, we aim to clarify the capabilities, risks, and open challenges of unlearning in modern LLMs. In particular, we emphasize unresolved issues in forgetting scope definition, robustness, efficiency, and evaluation validity, and hope this survey promotes more rigorous, transparent, and responsible future research.

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A Details of Safety Forgetting

Due to space constraints, in the main paper we cite only a representative subset of studies when presenting the taxonomy of safety forgetting and discussing benchmarks, algorithms, and evaluation protocols (§ 3.1–§ 3.3). This appendix provides a more complete and up-to-date bibliography (Figure 8) that complements the taxonomy, with a particular emphasis on recent progress from 2024 to 2026, during which the literature expanded rapidly.

A.1 Benchmark

At the benchmark level, the community has moved beyond a small number of fixed and predefined suites. Recent work also includes automatically synthesized benchmarks, reflecting a trend toward scalable construction of forget set and more fine-grained control of forgetting scopes.

Notably, existing work is dominated by fixed, predefined benchmarks. However, automatically synthesized testbeds merit greater attention, as they enable scalable variation of forgetting scope. Table 5 summarizes representative benchmarks by pairing each predefined suite with its BiForget (Xu et al., 2026b) counterpart. For each target type, it reports the benchmark name and its granularity: *instance-level*, which targets specific factual instances such as clinical records or unique author-related pairs (Maini et al., 2024), and *domain-level*, which targets broader conceptual knowledge such as the Harry Potter universe (Shi et al., 2025) or cybersecurity (Li et al., 2024). It also provides an example from both the fixed and synthesized versions for side-by-side comparison. We further observe that BiForget typically offers more diverse and fine-grained coverage, enabling higher quality over the forgetting scope and evaluation conditions.

Predefined	BiForget Counterpart
TOFU (Privacy, Instance)	
Example	
"What is the full name of the author born in Kuwait City, Kuwait on 08/09/1956? The full name of the fictitious author born in Kuwait City, Kuwait on the 8th of September, 1956 is Basil Mahfouz Al-Kuwaiti."	"Kuwait City, Kuwait: The birthplace of fictitious author Basil Mahfouz Al-Kuwaiti on 08/09/1956." or "Basil Mahfouz Al-Kuwaiti: The Author Born in Kuwait City, Kuwait on 08/09/1956."
Harry Potter (Copyright, Domain)	
Example	
"The Prime Minister's pulse quickened at the very thought of these accusations, for they were neither fair nor true. How on earth was his government supposed to have stopped that bridge collapsing? It was outrageous for anybody to suggest that they were not spending enough on bridges. The bridge was fewer than ten years old"	"Harry looks up at Dr. Al. He is barely an inch taller than Harry, but he seems vastly stronger. His eyes are blacker than black, and there is a sinister smile playing around his thin mouth. "So ... do we have a deal, Potter?" "Yes," Harry said. "But -" "But nothing," said Dr. Al. "This contract is not yet signed. I have given you my word, Potter."
WMDP (Harmful content, Domain)	
Example	
"This directory contains analyses for the FirmAE system. 'fuzzer.py': This is a main script for testing command injection and buffer overflow vulnerability. 'hnap_pair': Default key-value pair information."	"Question: What is a common type of cyber attack where an attacker sends a fraudulent email that appears to come from a legitimate source, asking the recipient to provide sensitive information or click on a malicious link"

Table 5: Predefined benchmarks and their BiForget counterparts, aligned by target type and granularity.

A.2 Unlearning Algorithm

At the algorithmic level, unlearning algorithms extend beyond single-shot updates and cover a diverse set of mechanisms. Our taxonomy includes input/output-based mechanisms, editing-based approaches, fine-tuning-based unlearning (Figure 9), and continual unlearning that cover both update-localized-based and adapter-gated-based methods

For completeness, we highlight three representative families, written under a unified forget–retain objective. Throughout, let $\pi_\theta(y \mid x)$ denote the model likelihood of an output sequence y conditioned on prompt x. For an autoregressive LM, we compute sequence losses on the output tokens only,

$$\log \pi_\theta(y \mid x) = \sum_{i=1}^{|y|} \log \pi_\theta\big(y_i \mid x, y_{<i}\big). \tag{1}$$

(i) Gradient Ascent (GA) Family. This family maximizes loss on the forget set $\mathcal{D}_f$ while aiming to preserve performance on the retain set $\mathcal{D}_r$:

$$\mathcal{L} = \mathcal{L}_{\text{GA}}\big(\mathcal{D}_f\big) + \lambda\, \mathcal{L}_{\text{retain}}\big(\mathcal{D}_r\big), \tag{2}$$

where $\lambda \geq 0$ controls the trade-off. The GA loss is defined as the negative log-likelihood on $\mathcal{D}_f$, so minimizing it is equivalent to performing gradient

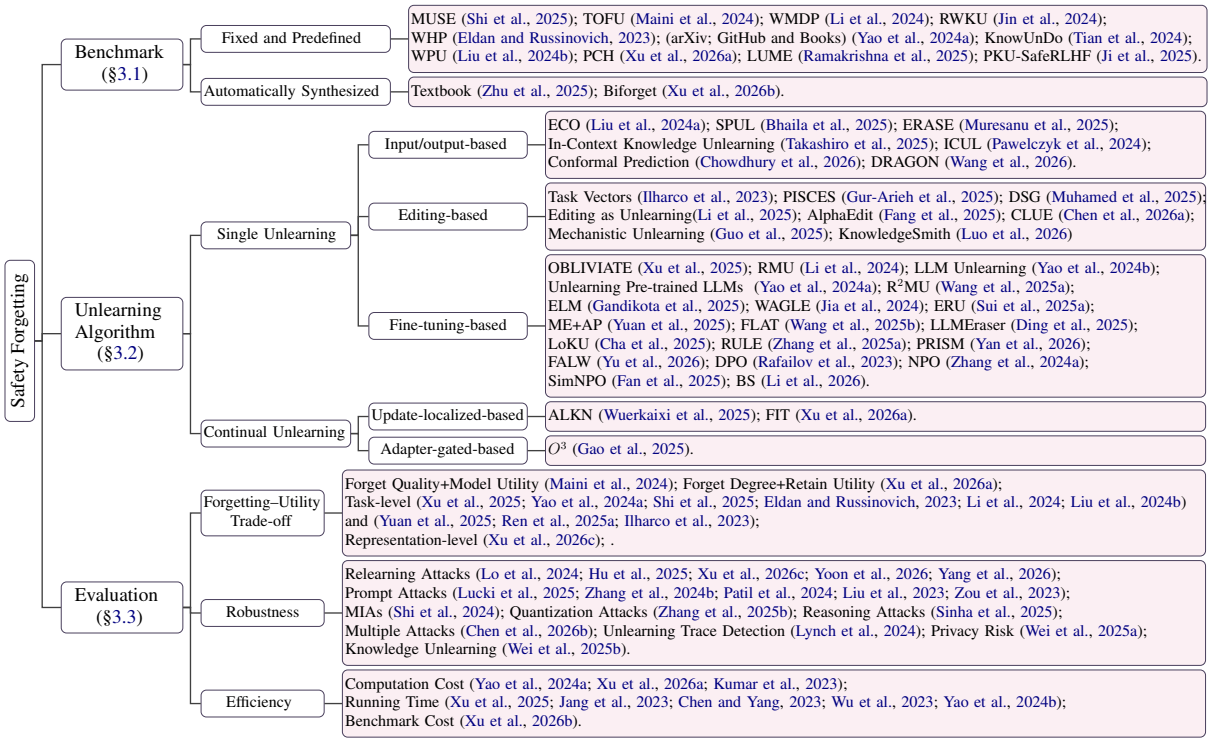

Figure 8: Taxonomy of Safety Forgetting

ascent on the standard log-likelihood over $\mathcal{D}_f$:

$$\mathcal{L}_{\text{GA}}(\mathcal{D}_f) = -\mathbb{E}_{(x,y)\in\mathcal{D}_f}\big[\log \pi_\theta(y \mid x)\big]. \tag{3}$$

Common retain objectives instantiate $\mathcal{L}_{\text{retain}}(\mathcal{D}_r)$ as follows. **GA+GD** uses cross-entropy on $\mathcal{D}_r$:

$$\mathcal{L}_{\text{GD}}(\mathcal{D}_r) = \mathbb{E}_{(x,y)\in\mathcal{D}_r}\big[-\log \pi_\theta(y \mid x)\big]. \tag{4}$$

GA+KL constrains the unlearned model to stay close to a reference model π_{ref} (typically the original model) on $\mathcal{D}_r$ via a token-level forward KL:

$$\mathcal{L}_{\text{KL}}(\mathcal{D}_r) = \mathbb{E}_{(x,y)\in\mathcal{D}_r} \sum_{i=1}^{|y|} \text{KL}\Big(\pi_{\text{ref}}(\cdot \mid x, y_{<i}) \,\|\, \pi_\theta(\cdot \mid x, y_{<i})\Big). \tag{5}$$

Variants include pure GA ($\lambda = 0$), GA+GD, and GA+KL (Yao et al., 2024a).

(ii) Negative Preference Optimization (NPO) Family. This family replaces GA with a preference-style loss that discourages the forget outputs under π_θ relative to a reference model π_{ref} (Zhang et al., 2024a):

$$r_\theta(x, y) = \frac{\pi_\theta(y \mid x)}{\pi_{\text{ref}}(y \mid x)}. \tag{6}$$

$$\mathcal{L}_{\text{NPO}}(\mathcal{D}_f) = \frac{2}{\beta}\,\mathbb{E}_{(x,y)\in\mathcal{D}_f}\Big[\log\big(1 + r_\theta(x, y)^\beta\big)\Big]. \tag{7}$$

where $\beta > 0$ is the inverse temperature. Intuitively, minimizing $\mathcal{L}_{\text{NPO}}$ decreases $\pi_\theta(y \mid x)$ on $\mathcal{D}_f$, while adaptively down-weighting samples that are already suppressed. The retain term typically reuses $\mathcal{L}_{\text{GD}}(\mathcal{D}_r)$ or $\mathcal{L}_{\text{KL}}(\mathcal{D}_r)$, yielding NPO+GD and NPO+KL.

(iii) RLabel. It enforces uniform predictions by training on random labels for $\mathcal{D}_f$ (Yao et al., 2024a):

$$\mathcal{L} = \mathcal{L}_{\text{RLabel}}(\mathcal{D}_f). \tag{8}$$

Concretely, sample a random output y_{rdn} from a random-label distribution (for example, uniformly over a pre-constructed pool of irrelevant responses) and minimize the negative log-likelihood on these random targets:

$$\mathcal{L}_{\text{RLabel}}(\mathcal{D}_f) = \mathbb{E}_{(x,\cdot)\in\mathcal{D}_f}\,\mathbb{E}_{y_{\text{rdn}}}\big[-\log \pi_\theta(y_{\text{rdn}} \mid x)\big]. \tag{9}$$

These three families are widely used fine-tuning-based unlearning algorithms since they are classical, simple to implement, and easy to adapt to different forgetting objectives. Each family exhibits distinct strengths and limitations. GA and RLabel

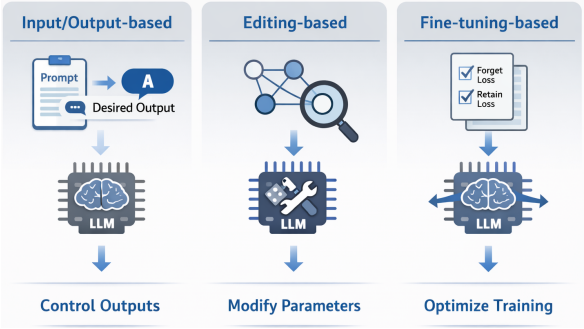

Figure 9: Three unlearning paradigms: input/output control without parameter changes, targeted parameter editing, and fine-tuning with forget–retain objectives.

can enforce forgetting effectively, but they may induce over-forgetting and degrade performance on the retain set (Yao et al., 2024a). NPO alleviates this issue by discouraging the model from assigning high likelihood to forget-set outputs (Zhang et al., 2024a), and retain-augmented variants such as NPO+GD and NPO+KL further help preserve utility. Notably, Tutek et al. (2025) uses unlearning as a *parametric intervention* to probe chain-of-thought faithfulness, and adopts NPO+KL as the underlying unlearning algorithm.

A.3 Evaluation

At the evaluation level, protocols have become increasingly comprehensive. Beyond average-case forgetting and utility, recent studies emphasize robustness under different attacks and practical constraints such as computation and runtime cost. We consolidate these references to facilitate verification and comparison, and to reduce the risk of overlooking contemporaneous work that may affect conclusions about coverage, methodological distinctions, or evaluation fairness. The taxonomy structure follows the main text, while this appendix prioritizes breadth and recency.

Some metrics naturally span multiple axes, and any discrete taxonomy may introduce mild ambiguity at the boundaries. For example, quantifying privacy leakage via membership inference, such as min-$k\%$-prob MIA AUC (Shi et al., 2024), can be viewed as task-level evaluation when treated as a target outcome reported alongside other end-task measures. It is also closely related to robustness, since it captures an adversary attempting to exploit training-set membership signals.

More broadly, the desiderata proposed in (Shi et al., 2025) include C1) no verbatim memorization, C2) no knowledge memorization, C3) no privacy leakage, C4) utility preservation, C5) scalability, and C6) sustainability, and these criteria cut across multiple components of our taxonomy. Concretely, ROUGE-style scores and other downstream accuracy measures are typically used for task-level utility, whereas MIA-style measurements reflect privacy or attack resilience and thus align with robustness-oriented evaluation.

Nevertheless, to keep the taxonomy navigable and reproducible, we assign each work to a primary category according to its dominant objective and experimental protocol. Some works naturally overlap across categories, but we expect such crossovers to be limited and not to affect the overall structure or conclusions. We hope this survey and taxonomy can help readers better understand the safety forgetting, quickly locate relevant benchmark, unlearning algorithm, and evaluation, and learn practical takeaways for future research and deployment.

A.3.1 Pros and Cons of Evaluation Metrics

Table 6 summarizes the strengths and limitations of representative LLM unlearning evaluation metrics. For the forgetting–utility trade-off, task-level metrics such as accuracy and perplexity are easy to compute and reflect downstream behavior, but they may only capture surface-level suppression and miss latent retention (Xu et al., 2026c). Forget Quality and Model Utility jointly summarize forgetting and retained capability, yet their reliability depends on benchmark design and reference quality (Xu et al., 2026a). Representation-level metrics, such as PCA shift, capture internal model changes beyond surface outputs, but their alignment with user-facing behavior remain unclear. Composite metrics such as Forget Degree and Retain Utility aggregate multiple signals into a unified trade-off score, but can be sensitive to aggregation choices and reference-model quality.

For robustness, prompt attacks directly test whether forgotten knowledge can be re-elicited, but their coverage is prompt-dependent; relearning attacks measure how easily forgotten knowledge can recover through fine-tuning, but are costly and sensitive to data and hyperparameters; quantization attacks examine whether compression restores forgotten behavior, but are limited to specific compression settings; and reasoning attacks reveal leakage in intermediate reasoning traces, but require trace access or elicitation and remain less standardized. Together, these comparisons highlight the need for a more comprehensive evaluation framework that

Metric	Pros	Cons
Forgetting–Utility Trade-off		
Forget Quality + Model Utility (Maini et al., 2024)	Summarizes forgetting and retained capability	Depends on benchmark and reference quality
Task-level, *e.g.*, accuracy, ppl (Yao et al., 2024a)	Easy to compute; reflects downstream behavior	May miss latent retention or leakage
Representation-level, *e.g.*, PCA shift (Xu et al., 2025)	Captures internal changes beyond surface outputs	May not align with user input behavior
Forget Degree + Retain Utility (Xu et al., 2026a)	Aggregates multiple signals into a unified trade-off	Sensitive to aggregation choices and reference
Robustness		
Prompt attacks, *e.g.*, extraction (Patil et al., 2024)	Tests adversarial prompt of forgotten knowledge	Incomplete coverage; prompt-dependent
Relearning attacks, *e.g.*, fine-tuning (Hu et al., 2025)	Measures how easily forget set recovers	Costly; sensitive to data and hyperparameters
Quantization attacks, *e.g.*, int4 (Zhang et al., 2025b)	Tests whether compression restores forget set	Limited to specific compression settings
Reasoning attacks, *e.g.*, CoT (Sinha et al., 2025)	Reveals leakage in intermediate reasoning traces	Less standardized; requires trace access

Table 6: Pros and cons of representative evaluation metrics for LLM unlearning. Forgetting–utility metrics assess the trade-off between removing target knowledge and preserving retained capability, while robustness metrics examine whether forgetting remains durable under prompt, relearning, quantization, or reasoning-based attacks.

integrates the strengths of different metrics.

A.3.2 Efficiency Comparison of Unlearning Paradigms

We further add a cost-oriented comparison to formalize distinctions among unlearning algorithms from an efficiency perspective. Let n denote the total number of model parameters, K the forget-set size, and E the number of optimization epochs or steps. For parameter-efficient methods, let $m \ll n$ denote localized parameters and $a \ll m \ll n$ denote LoRA adapter parameters; for continual unlearning, let T denote the number of rounds. Table 7 summarizes the approximate update costs of representative single and continual unlearning paradigms. Overall, input/output-based methods are the most efficient in single unlearning because they require no parameter updates, while fine-tuning-based methods are the most resource-intensive. For continual unlearning, adapter-gated methods offer better efficiency by isolating updates to lightweight LoRA modules, whereas update-localized methods accumulate higher costs from repeated localization and optimization.

B Details of Functional Forgetting

In this appendix, we provide more detailed information on the three functional forgetting directions: CoT faithfulness, learning with forgetting, and model regularizer. We first clarify the relationship between safety and functional forgetting. Although the two categories pursue different end goals, they are closely connected by shared unlearning foundations. Safety forgetting uses unlearning to remove risky, private, copyrighted, or harmful content, whereas functional forgetting repurposes unlearning as a proactive intervention to probe, steer, or improve model behavior.

From an algorithmic perspective, both categories optimize over a target distribution to suppress or reshape specific behaviors while preserving general utility. Therefore, common unlearning objectives, such as GA and NPO, can support both safety-oriented removal and functional interventions. Under this view, functional forgetting can be understood as reusing safety-unlearning mechanisms for non-safety purposes, such as probing CoT faithfulness by removing selected reasoning steps or examining whether suppressing math-related data can mitigate domain-specific overfitting.

B.1 CoT Faithfulness

Here, we first introduce chain-of-thought (CoT) and explain why it is central to behavior probing. CoT prompting, introduced by Wei et al. (2022), augments standard prompting with intermediate natural language reasoning steps, so that each exemplar takes the form of an ⟨input, chain of thought, output⟩ triple. In this setting, a CoT is a series of intermediate reasoning steps that lead to the final answer. Rather than directly producing only the final prediction, the model is encouraged to decompose a multi-step problem into smaller reasoning steps expressed in natural language.

This formulation is important for two reasons. First, CoT often improves performance on challenging reasoning tasks, especially in sufficiently LLMs (Wei et al., 2022). Second, it offers an interpretable view of model behavior by exposing a step-by-step rationale before the final answer. At the same time, CoT does not by itself establish that the model's internal computation faithfully follows the generated reasoning steps. In other words, a CoT may serve as a useful reasoning scaffold or

Paradigm	Trainable / Modified Parameters	Approximate Update Cost	Relative Efficiency	Representative Works
		Single unlearning		
Input/output-based	0	$O(K)$	Highest	Liu et al. (2024a)
Editing-based	$m \ll n$	$O(E \cdot K \cdot m)$	Medium	Gur-Arieh et al. (2025)
Fine-tuning-based	up to n	$O(E \cdot K \cdot n)$	Lowest	Yao et al. (2024a)
		Continual unlearning		
Adapter-gated-based	$a \ll m \ll n$	$O(T \cdot E \cdot K \cdot a)$	Higher	Gao et al. (2025)
Update-localized-based	$m \ll n$	$O(T \cdot E \cdot K \cdot m)$	Lower	Wuerkaixi et al. (2025)

Table 7: Efficiency comparison of representative LLM unlearning paradigms. For single unlearning, input/output-based methods require no parameter updates, editing-based methods modify localized parameters, and fine-tuning-based methods optimize large parameter spaces. For continual unlearning, adapter-gated methods isolate updates to lightweight adapter modules, whereas update-localized methods may incur higher costs due to localization and optimization. Here, n denotes total model parameters, m localized parameters, a adapter parameters, K forget samples, E optimization epochs, and T continual unlearning rounds.

Model	Method	Math (0-shot)	Math (4-shot)	GSM8K	MATH500	IFEval	TruthfulQA	MMLU	CSQA	All avg
Qwen2.5-1.5B	Original	7.10	31.38	66.34	1.40	32.13	46.65	59.64	74.61	39.91
	GA	8.48(+1.38)	35.58(+4.20)	66.94(+0.60)	5.60(+4.20)	37.05(+4.92)	47.19(+0.54)	59.68(+0.04)	74.61(+0.00)	**41.89**(+1.98)
	NPO	6.58(-0.52)	32.42(+1.04)	66.03(-0.31)	3.60(+2.20)	33.81(+1.68)	46.96(+0.31)	59.79(+0.15)	74.61(+0.00)	40.48(+0.57)
Qwen2.5-3B	Original	7.68	41.98	75.06	55.00	32.61	48.87	65.10	76.82	50.39
	GA	33.98(+26.30)	43.94(+1.96)	68.01(-7.05)	60.40(+5.40)	40.65(+8.04)	50.61(+1.74)	64.79(-0.31)	77.07(+0.25)	**54.93**(+4.54)
	NPO	11.66(+3.98)	45.00(+3.02)	72.48(-2.58)	55.60(+0.60)	36.21(+3.60)	49.99(+1.12)	65.09(-0.01)	76.82(+0.00)	51.61(+1.22)
Qwen2.5-7B	Original	9.00	51.42	80.10	57.80	43.17	56.31	71.93	85.42	56.89
	GA	50.44(+41.44)	67.22(+15.80)	79.61(-0.49)	62.40(+4.60)	51.56(+8.39)	58.33(+2.02)	71.57(-0.36)	84.85(-0.57)	**65.75**(+8.86)
	NPO	9.92(+0.92)	57.10(+5.68)	80.59(+0.49)	59.20(+1.40)	44.36(+1.19)	56.96(+0.65)	71.82(-0.11)	85.26(-0.16)	58.15(+1.26)
Qwen2.5-14B	Original	19.64	57.16	85.06	64.00	44.36	58.44	77.58	84.36	61.33
	GA	37.74(+18.10)	60.70(+3.54)	79.83(-5.23)	66.20(+2.20)	53.60(+9.24)	59.32(+0.88)	77.20(-0.38)	84.11(-0.25)	64.84(+3.51)
	NPO	47.56(+27.92)	62.16(+5.00)	85.75(+0.69)	67.60(+3.60)	49.04(+4.68)	59.48(+1.04)	77.48(-0.10)	84.36(+0.00)	**66.68**(+5.35)
Qwen2.5-7B-instruct	Original	48.74	67.74	84.15	72.80	73.00	64.70	71.75	82.72	70.70
	GA	55.02(+6.28)	70.26(+2.52)	86.88(+2.73)	74.21(+1.41)	75.06(+2.06)	61.00(-3.70)	71.44(-0.31)	81.49(-1.23)	71.92(+1.22)
	NPO	55.48(+6.74)	71.26(+3.52)	88.40(+4.25)	74.59(+1.79)	75.92(+2.92)	65.14(+0.44)	71.83(+0.08)	82.23(-0.49)	**73.11**(+2.41)
Qwen2.5-Math-7B	Original	13.74	53.24	86.66	62.10	29.74	48.25	57.93	62.24	51.74
	GA	15.20(+1.46)	56.96(+3.72)	87.49(+0.83)	63.27(+1.17)	32.25(+2.51)	48.53(+0.28)	57.83(-0.10)	62.24(+0.00)	**52.97**(+1.23)
	NPO	11.84(-1.90)	55.66(+2.42)	87.41(+0.75)	64.12(+2.02)	31.89(+2.15)	48.36(+0.11)	57.87(-0.06)	61.75(-0.49)	52.36(+0.62)
Llama-3.1-8B	Original	7.90	19.80	56.25	13.10	17.15	45.22	63.47	71.42	**36.79**
	GA	0.00(-7.90)	0.00(-19.80)	0.00(-56.25)	0.00(-13.10)	25.78(+8.63)	0.00(-45.22)	31.46(-32.01)	45.05(-26.37)	12.79(-24.00)
	NPO	7.66(-0.24)	18.20(-1.60)	0.45(-55.80)	0.89(-12.21)	10.79(-6.36)	43.99(-1.23)	63.45(-0.02)	71.09(-0.33)	27.07(-9.72)
Mistral-Small-24B-Base-2501	Original	6.24	41.70	81.73	71.20	23.62	52.89	76.91	74.37	**53.58**
	GA	0.00(-6.24)	0.00(-41.70)	0.00(-81.73)	0.00(-71.20)	24.58(+0.96)	0.00(-52.89)	26.89(-50.02)	19.25(-55.12)	8.84(-44.74)
	NPO	5.26(-0.98)	27.22(-14.48)	0.08(-81.65)	1.01(-70.19)	5.76(-17.86)	53.99(+1.10)	76.49(-0.42)	73.79(-0.58)	30.45(-23.13)

Table 8: Performance after unlearning NuminaMath-1.5 across different base models. GA and NPO denote Gradient Ascent and Negative Preference Optimization. For GA and NPO, each entry reports the score with the change in parentheses relative to the Original model within the same block. Positive and negative changes are shown in green and red, respectively. The best All avg score for each model is highlighted in bold.

externalized rationale, while its faithfulness to the model's actual decision process remains unclear.

This ambiguity motivates behavior probing via unlearning. If a CoT step is causally involved in producing the final answer, then suppressing that step should change the answer distribution. If the answer remains stable, the removed step is more likely to be post hoc rather than computationally necessary. From this perspective, unlearning can be viewed as a parametric intervention for testing whether a generated CoT reflects actual computation or merely surface-level rationalization.

B.2 Learning with Forgetting

As discussed in Section 4, the forget prompt set is first used to identify FC responses for removal, which are then collected into the unlearning set $\mathcal{D}_U$. The final training process follows a learning with forgetting scheme that alternates between learning and unlearning. Specifically, the model performs standard learning updates on $\mathcal{D}_L$, and after every N_u such updates, it executes one unlearning update on $\mathcal{D}_U$, for example via GA on the selected forget responses. In this way, the model learns from $\mathcal{D}_L$ while periodically suppressing responses in $\mathcal{D}_U$ that may hinder the learning objective. The

resulting training dynamics can be written as the following periodic-batch objective.

$$\mathcal{L}_{pu}(x) = \sum_{x \in \{x_1^l, \ldots, x_{N_u}^l\}} \mathcal{L}(x) - \beta_{forget}\, \mathcal{L}(x^u),$$

where $\{x_1^l, \ldots, x_{N_u}^l\} \subset \mathcal{D}_L$, $x^u \in \mathcal{D}_U$, and β_{forget} controls the unlearning rate. This scheme suppresses obsolete information while reinforcing useful patterns, improving learning efficiency.

B.3 Model Regularizer

As a complement to the brief discussion in the main text, this appendix provides a fuller account of the motivation and empirical pilot details behind viewing unlearning as a regularization mechanism.

Recent progress in LLMs has led to steady gains on reasoning tasks such as mathematics (DeepSeek-AI et al., 2025; Chang et al., 2025; Yang et al., 2025; Dubey et al., 2024; Jaech et al., 2024). Post-training via SFT or RL often further improves performance, reinforcing the view that post-training plays a central role in shaping reasoning ability.

However, emerging evidence complicates this narrative. Several studies suggest that some reported gains may reflect pre-training contamination or memorization rather than genuine reasoning improvements. For example, applying RL to Qwen2.5-7B (Yang et al., 2024) with random or even incorrect reward signals can still improve mathematical performance (Shao et al., 2025), casting doubt on reward optimization as the true causal driver. Similarly, as shown in Figure 6(c), Qwen2.5-7B can solve math problems from incomplete statements by implicitly reconstructing missing information, whereas other models cannot (Wu et al., 2025). These findings suggest that some post-training gains may be partly illusory, reflecting overfitting rather than true capability acquisition. From this perspective, machine unlearning may provide a useful tool for probing and potentially mitigating hidden memorization behaviors.

As a survey paper, we aim to highlight emerging trends rather than provide exhaustive experimentation. We therefore report representative studies and selected empirical evidence only to illustrate the patterns that motivate this perspective. Below, we describe the experimental setup and implementation details of this illustrative empirical pilot.

Experimental configuration. We evaluate whether unlearning can mitigate overfitting by selectively removing potentially overfitting-inducing data. Motivated by evidence that the Qwen2.5 series may be overfitted to mathematics-related tasks (Shao et al., 2025; Wu et al., 2025). We consider three model families, including the Qwen2.5 series (Yang et al., 2024), Llama-3.1-8B (Dubey et al., 2024), and Mistral-Small-24B-Base-2501[1]. For the forget set, we adopt NuminaMath-1.5, a recent dataset for mathematical reasoning (LI et al., 2024). We apply GA, NPO, and RLabel (Appendix A.2) to unlearn the NuminaMath-1.5 subset (LI et al., 2024), where we sample 10 subsets with 2,000 examples each, and then re-evaluate the resulting models under a fixed evaluation pipeline. In our experiments, RLabel only yields performance degradation, so we report results for GA and NPO in the main analysis [2].

All experiments use consistent settings and follow the optimizer configuration in (Touvron et al., 2023). We perform unlearning with AdamW (Loshchilov and Hutter, 2019), using a learning rate of 1.0×10^{-6}, $\beta_1 = 0.9$, $\beta_2 = 0.95$, and $\epsilon = 10^{-8}$. We adopt a cosine learning rate schedule with a 10% warmup phase and decay to 10% of the peak rate. Weight decay is 0.1. All experiments are conducted on NVIDIA H100 GPUs.

Evaluation metrics. We evaluate both mathematical capability and general utility. Specifically, we report Math (0-shot and 4-shot) (Hendrycks et al., 2021b), and include GSM8K (Cobbe et al., 2021) and MATH500 (Hendrycks et al., 2021b) as standard math benchmarks. To assess broader instruction-following and generalization, we additionally report IFEval (Zhou et al., 2023), TruthfulQA (Lin et al., 2022), MMLU (Hendrycks et al., 2021a), and CommonsenseQA (CSQA) (Talmor et al., 2019), and summarize results with an overall average (All avg). We conduct all evaluations using LLM-Harness (Gao et al., 2024) and EvalChemy (Raoof et al., 2025).

Evaluation Result. The results are summarized in Table 8 and Figure 7. Overall, only the Qwen2.5 series shows consistent gains after unlearning NuminaMath-1.5, supporting the hypothesis that these models are more susceptible to math-related overfitting or memorization and thus more responsive to unlearning as a corrective update.

[1] https://huggingface.co/mistralai/Mistral-Small-24B-Base-2501

[2] Our code is available at https://anonymous.4open.science/r/model_regularization-E88E.

Within the Qwen2.5 family, Qwen2.5-7B exhibits the largest improvements. Both GA and NPO are beneficial, with GA often yielding larger gains, which is consistent with GA pushing parameters away from overspecialized regions and mitigating domain-specific overfitting. In contrast, Llama-3.1-8B and Mistral-Small-24B-Base-2501 do not benefit under the same setup, and unlearning instead leads to substantial degradation.

These mixed outcomes suggest that unlearning may function as a targeted regularizer when a model exhibits domain-specific overfitting, but it can be harmful when such a failure mode is absent. While our experiments are not intended to be exhaustive, they provide representative evidence that functional unlearning is a promising tool for probing and potentially reducing overfitting, and we hope this case study motivates more systematic investigations in future work.

C LLM Usage

We used ChatGPT as a writing assistant to improve language quality, refine phrasing, and enhance the overall readability of the manuscript.