UNLOCKING POST-HOC DATASET INFERENCE WITH SYNTHETIC DATA

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ABSTRACT

The remarkable capabilities of large language models stem from massive internet-scraped training datasets, often obtained without respecting data owners' intellectual property rights. Dataset Inference (DI) enables data owners to verify unauthorized data use by identifying whether a suspect dataset was used for training. However, current DI methods require private held-out data with a distribution that closely matches the compromised dataset. Such held-out data are rarely available in practice, severely limiting the applicability of DI. In this work, we address this challenge by synthetically generating the required held-out set through two key contributions: (1) creating high-quality, diverse synthetic data via a data generator trained on a carefully designed suffix-based completion task, and (2) bridging likelihood gaps between real and synthetic data, which is realized through post-hoc calibration. Extensive experiments on diverse text datasets show that using our generated data as a held-out set enables DI to detect the original training sets with high confidence, while maintaining a low false positive rate. This result empowers copyright owners to make legitimate claims on data usage and demonstrates our method's reliability for real-world litigations.

1 INTRODUCTION

Large language models (LLMs) have recently achieved remarkable success in a broad range of tasks, fueled by the availability of massive high-quality text corpora often scraped from the internet (Weber et al., 2024; Penedo et al., 2024). While this practice has enabled LLMs to generate high-quality text and to excel on benchmarks, it also raises serious concerns related to intellectual property rights (Reuters, 2023; Gry, 2023; Sil, 2023), data privacy, and transparency (Rahman & Santacana, 2023; Wu et al., 2023). The reliance on potentially unauthorized data creates an urgent need for methods that allow independent authors to verify whether a given dataset has been used to train an LLM without the explicit consent of the model provider.

A promising approach to addressing these concerns is *dataset inference* (DI) (Maini et al., 2021; Dziedzic et al., 2022; Maini et al., 2024; Dubiński et al., 2024), which aims to determine whether a suspect dataset has contributed to a model's training. This puts power in the hands of data owners to monitor and exercise their intellectual property rights. Despite its potential, DI currently faces a critical bottleneck: it requires a held-out set—a dataset known to be absent from training—that shares the same distribution as the suspect dataset (Zhang et al., 2024a). In practice, however, such an in-distribution held-out set is rarely available. Data creators do not typically reserve a dedicated held-out set for legal or auditing purposes, and any disclosed held-out data could itself be repurposed for future training. Moreover, even when a dataset owner can provide some held-out samples, any slight distributional discrepancy from the original suspect data can undermine DI by inflating false positives (Das et al., 2024; Duan et al., 2024; Meeus et al., 2024; Maini & Suri, 2024).

To illustrate the brittleness of using seemingly IID (Independent and Identically Distributed) held-out data, we demonstrate in Section 3 that even in a simple scenario—where an LLM is fine-tuned on blog posts from a *single* author—there exists a distributional shift between training data (members) and randomly held-out blog posts from the same author. This highlights how even subtle variations

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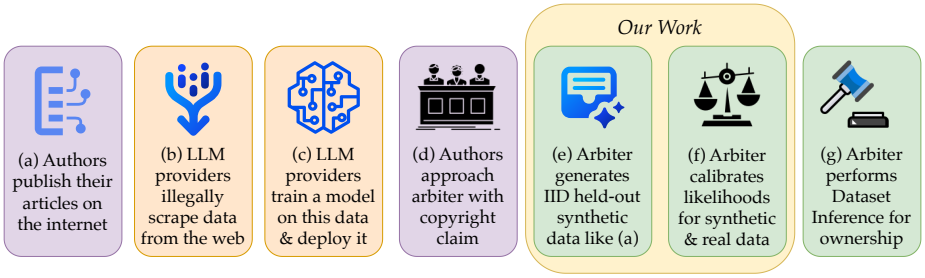

Figure 1: **Dataset Inference Procedure with Synthetic Held-Out Data.** This figure presents a high-level overview of how the proposed dataset inference (DI) process will take place in real-world use cases. While original setting of DI requires a held-out dataset that is IID to the suspect set (**(a-d)**,**(g)**), we highlight the contributions of **our work: (e)** The arbiter generates IID synthetic held-out data that mimics the author's original data. **(f)** The arbiter calibrates likelihoods between real and synthetic data to ensure fair comparison, enabling them to reliably perform dataset inference.

in held-out data can undermine DI. Malicious actors may exploit this vulnerability by strategically introducing *shifted* held-out data, falsely accusing model owners of copyright infringement and further reducing the reliability of DI methods.

In this work, we address these challenges by proposing to *synthetically generate* held-out data for DI, bypassing the need for dedicated in-distribution held-out data. This vision, however, is non-trivial to achieve. First, the generated texts must be realistic, high-quality, and sufficiently diverse to approximate the distribution of the original data. Second, the generation process itself may introduce a distribution shift between natural and synthetic held-out data. Such a shift complicates DI: if a difference is observed between the suspect and held-out sets, it becomes unclear whether this difference arises from a genuine membership signal (*i.e.,* the target model behaves differently on the suspect data because it has seen it during training) or merely from the distribution shift (*i.e.,* the model behaves differently on suspect data because it is natural data). Recent studies have extensively highlighted this issue in the context of Membership Inference Attacks (MIAs) (Shokri et al., 2017), where distribution shifts lead to misleading evaluation results (Das et al., 2024; Zhang et al., 2024a; Maini et al., 2024; Dubiński et al., 2024).

To this end, we first train a carefully designed text generator on the suspect dataset itself, on a suffix completion task (Section 4.1). This approach produces high-quality datasets with only a small distributional shift from the suspect texts. However, even small shifts in distribution can undermine DI's reliability. To address this, we introduce a *post-hoc* calibration step (Section 4.2) to ensure that the generated held-out set can serve as a reliable reference for DI. Specifically, we disentangle the effects of distributional shifts from the actual membership signal—a critical factor in DI. To achieve this, we propose a dual-classifier approach: (1) A *text-only classifier*, trained to distinguish natural (original) from generated data. (2) A *membership-aware classifier*, which incorporates both the textual features and DI's standard membership indicators. The key insight is that any performance advantage of the membership-aware classifier over the text-only classifier must arise from the presence of membership signals rather than distributional artifacts. This difference serves as our DI signal for inferring whether the suspect dataset was used in the target model's training. This calibration strategy enhances DI's robustness, reducing false positives while maintaining high detection accuracy.

We demonstrate the effectiveness of our approach on diverse textual datasets, ranging from single-author datasets to large-scale, multi-author collections such as Wikipedia. Our results show that using *synthetic* held-out data, combined with calibration, enables DI to detect unauthorized training data use with high confidence while keeping false positives low. This expands the practical applicability of DI and provides a pathway for data owners to safeguard their intellectual property in an era of LLMs.

2 Background and Related Work

2.1 Membership Inference

MIAs focus on deciding if a single data point was included in a given model's training dataset and often serve as features extractors for DI. In the LLM domain, MIAs exploit different signals to

distinguish between members (training data points) and non-members (data points not used during training). For instance, LOSS exploits the perplexity or loss function of the target model (Yeom et al., 2018). Shi et al. (2024) find that the rare words in a sequence can leak more privacy information, and select K% tokens with the smallest probabilities for evaluation. Min-K%++ further improves upon the Min-K% approach by introducing two calibration factors (Zhang et al., 2024b). Zlib ratio (Carlini et al., 2021) uses the compression rate of z-library to normalize the perplexity of the target model. Neighborhood-based methods compare a suspect sequence with its neighboring texts, which can be produced by synonym substitution (Mattern et al., 2023) or paraphrasing (Duarte et al., 2024). Moreover, reference-based methods compare the output signals on a suspect sample between the target model and a reference model (Fu et al., 2024). Yet, many recent works have shown that the evaluation of MIAs suffers from a falsified experimental setup, where a distributional shift exists between the member and non-member sets (Zhang et al., 2024a; Maini et al., 2024; Das et al., 2024). Duan et al. (2024) show that most MIAs only perform slightly better than random guessing if evaluated correctly on non-biased benchmarks. Recently, Kazmi et al. (2024) proposed how to de-bias MIAs from this distribution shift—which we use as a foundation for our DI calibration.

2.2 Dataset Inference

To strengthen the signal from training data further beyond MIAs, Maini et al. (2021) introduced DI. DI aggregates the membership signal over multiple data points, often referred to as *suspect set*, to decide whether a given model was trained on this data. More formally, given a target model f, DI aims to detect whether f was trained on the suspect dataset $\mathcal{D}_{\text{sus}}$. Therefore, it needs an additional held-out dataset $\mathcal{D}_{\text{val}}$ from the same distribution as $\mathcal{D}_{\text{sus}}$. Given both sets, DI extracts membership features from the data points in $\mathcal{D}_{\text{sus}}$ and $\mathcal{D}_{\text{val}}$, aggregates all features per given sample, and then scores these aggregate features through a scoring model. The scores should be lower for members than for non-members. Then, DI performs statistical hypothesis testing on the scores of $\mathcal{D}_{\text{sus}}$ and $\mathcal{D}_{\text{val}}$. The null hypothesis is that the average scores for $\mathcal{D}_{\text{sus}}$ is lower than for $\mathcal{D}_{\text{val}}$. If the statistical test manages to reject this null hypothesis, this is a confident indicator that the data points from $\mathcal{D}_{\text{sus}}$ are indeed members of model f's training data. Otherwise, the test is considered inconclusive.

How to extract the best membership features from the data points varies based on the learning paradigm. For example, the original DI for supervised classification models (Maini et al., 2021) designs a random walk strategy to estimate the distance between data points and the decision boundary of a supervised model. This is based on the intuition that member data points are further to the decision boundaries than non-member data points. For self-supervised models, Dziedzic et al. (2022) use Gaussian Mixture Model to estimate the representational differences between the training dataset (members) and the test data. Recent work for DI on LLMs (Maini et al., 2024) relies on existing LLM MIAs to extract membership features and uses a linear model to weight the respective features. We follow this approach in our evaluations. LLM DI can be formalized as follows. First, after calculating over n MIA scores with linear regression, an aggregated MIA score is obtained by $W \cdot \text{MIA}(x) = \sum_{i=1}^{n} w_i \text{MIA}_i(x)$. Here, $W = [w_1, ..., w_n]$ is the weight of the linear regressor, and $\text{MIA}(x)$ is a vector concatenating n MIA scores. We label the suspect data as 0 and the held-out data as 1. Note that, $\text{MIA}(x)$ is calculated based on $f(x)$, but we omit f for simplicity. Then, a hypothesis testing is conducted to verify if the held-out set has higher MIA score than the suspect set statistically. The null hypothesis can be formalized as follows.

$$\mathcal{H}_0 : \mathbb{E}_{\mathcal{D}_{\text{val}}}[W \cdot \text{MIA}(x_{\text{val}})] \leq \mathbb{E}_{\mathcal{D}_{\text{sus}}}[W \cdot \text{MIA}(x_{\text{sus}})]. \tag{1}$$

If the suspect set is part of the training set of f, the null hypothesis is rejected.

3 Failure Cases of DI

In this section, we dive deeper into the difficulties that arise from DI's assumption on the availability of an additional in-distribution held-out dataset. More precisely, we show that this assumption is extremely hard to meet in practice, even in the simplest setups—limiting the applicability of standard DI. Therefore, we collect blog posts written by a *single author* on topics from the *same domain* and split them randomly into a training and held-out set. We finetune an LLM on the training set, perform DI (Maini et al., 2024), and find that the method returns false positives, *i.e.,* it illegitimately claims that the model was trained on blog posts that it actually was not trained on (see Table 1). Our analysis highlights that despite the texts' homogeneity, there is a small distributional shift between the suspect

Table 1: The distributional shift (GPT2 AUC) and DI p-value between a suspect set that consists of *non-members* and held-out blog posts. Here, p-value < 0.05 indicates DI incorrectly suggests that the suspect set is a member set.

Sequences per Blog	5	10	15	20	25
GPT2 AUC (%)	52.0	55.2	53.2	58.2	58.6
DI p-value	0.002	<0.001	<0.001	<0.001	<0.001
True Membership	×	×	×	×	×
Inferred Membership	✓	✓	✓	✓	✓

and held-out sets that is not even easily distinguishable by Blind Baselines Das et al. (2024), which causes DI to fail. This highlights the need to generate synthetic held-out data to benefit from DI in real-world copy right claims. We provide more details below and discuss its implications.

3.1 DI on a Single Author's Data

We consider a practical application of DI in copyright protection as detailed in Figure 1. In this scenario, an author has some published texts on the internet of which they believe that they were illegitimately used by an LLM provider to train their model. The author provides this published works to an arbiter, as a suspect set and some non-published blog-posts as held-out set from the same distribution, *i.e.,* with the same style, topics, etc. Then, the arbiter performs DI to resolve the copyright claims.

To evaluate this setup in practice, we collect blog posts of a public blogger. The blogs are split into member, non-member, and held-out sets. To avoid any potential temporal or topic distributional shifts, we randomly shuffle all the collected blogs before splitting. In lack of the computational capacities to train an LLM from scratch, we finetune a Pythia model (Biderman et al., 2023) on the member set. The Pythia model is trained on the Pile dataset Gao et al. (2020), so we only used blogs after the release date of the Pile to ensure that none of the blogs is part of the pre-training data. Also, we only finetune the target model on the member set for one epoch. This is to evaluate the performance of DI and our method in the most strict scenario, as Duan et al. (2024) show that MIAs perform better with more training epochs. Finally, we run DI. More detailed experiment configurations can be found in Section 5.1.

3.2 Metrics of Distributional Gap

Before analyzing the results, we introduce the metrics we use to quantify the distributional shift between the suspect and held-out sets. Following the approach of Blind Baselines Das et al. (2024), we formulate the measurement of the distribution gap between two text datasets as a classification problem. In particular, the suspect set $\mathcal{D}_{\text{sus}}$ is randomly split into a classifier training split $\mathcal{D}_{\text{sus}}^{\text{train}}$ and a test split $\mathcal{D}_{\text{sus}}^{\text{test}}$. The held-out set $\mathcal{D}_{\text{val}}$ is also split into $\mathcal{D}_{\text{val}}^{\text{train}}$ and $\mathcal{D}_{\text{val}}^{\text{test}}$ in the same vein. Then, a classifier g is optimized to distinguish the training splits $\mathcal{D}_{\text{sus}}^{\text{train}}$ and $\mathcal{D}_{\text{val}}^{\text{train}}$. Finally, we calculate the area under the curve (AUC) score of the classifier on the test splits $\mathcal{D}_{\text{sus}}^{\text{test}}$ and $\mathcal{D}_{\text{val}}^{\text{test}}$, which is used to measure the distributional gap between $\mathcal{D}_{\text{sus}}$ and $\mathcal{D}_{\text{val}}$.

The design of the classifier decides how the texts are vectorized and if the discrepancies between texts can be sufficiently captured. Das et al. (2024) apply a bag-of-words (BoW) classifier, which can only detect the differences in terms of word frequency. Instead, we build a GPT2-based classifier with two transformer blocks to also find the differences in grammar, content, styles, etc. between two text distributions. We train the classifier from scratch to avoid the impact of any pre-training data. Using only two transformer blocks of the GPT2 architecture avoids overfitting.

3.3 False Positive of DI

The AUC scores of the GPT2-based classifier in Table 1 show that there is a non-negligible distributional shift between the non-member and the held-out sets. The intuition behind this observation is that each blog has different content and topics, which brings different words across the non-member and held-out documents. The gap is enlarged when we sample more sequences from each blog post.

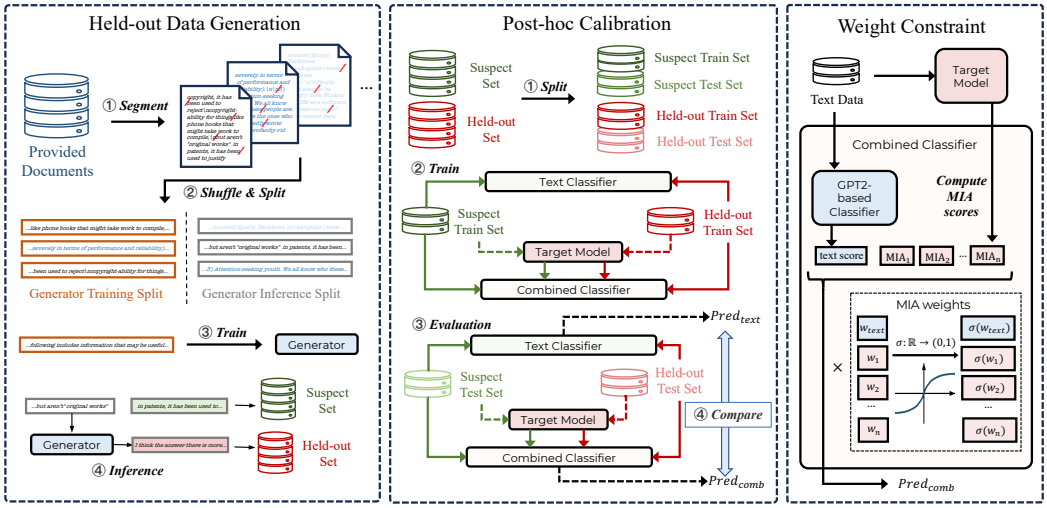

Figure 2: **Held-out Data Generation (Left Panel): (1)** The suspect dataset is first segmented into text snippets. **(2)** These snippets are shuffled and split into a generator training set and an inference set. **(3)** A generator model is trained on the suspect dataset using a suffix completion task. **(4)** The trained generator produces synthetic held-out data that mimics the suspect set. **Post-hoc Calibration (Middle Panel): (1)** The suspect set and synthetic held-out set are split into training and test subsets. **(2)** A **text classifier** is trained to differentiate real from synthetic text. A **combined classifier** integrates textual features with DI membership signals from the target LLM. **(3)** The two classifiers are evaluated: the combined classifier should only outperform the text classifier if the suspect dataset was used for training. **(4)** A statistical comparison ensures that any signal detected is due to actual membership rather than distributional shifts. **Weight Constraint (Right Panel):** The weights for the MIA and text scores are constrained to (0,1) with Sigmoid function.

This small distributional shift between texts leads to very low p-value in the t-test, causing significant false positive rates during DI. This means that the DI falsely accuses the LLM provider of violating the copy right of an author. What is more is that this shortcoming of DI can be maliciously exploited: authors could deliberately provide held-out data from a different distribution than their suspect data to mislead DI and *illegitimately* accuse the LLM provider. Please also refer to Appendix A for a visualized demonstration of such shifts during DI. As a solution to this problem, in the next section, we propose our approach on generating an adequate in-distribution held-out dataset synthetically.

4 Synthesizing Held-out Data

Our approach consists of two subsequent steps. First, we generate high-quality held-out data, then, we perform a calibration to account for the distribution shift that such generation can introduce.

4.1 Held-out Data Generation

We explore three approaches that leverage LLMs for generating held-out data based on provided suspect data with minimal distribution shift.

Prompted Paraphrasing. As a naïve approach, we use GPT-4 models to paraphrase the suspect set with in-context-learning (ICL). We experiment with GPT-4-Turbo and prompt it using in-context-learning learning to paraphrase the suspect data. Each prompt includes a few data points from the suspect set with their paraphrases as demonstrations (shots) and requests the model to produce paraphrases for the suspect set. Our results in Table 2 show that there is a significant distribution shift between the original and paraphrased samples. Even a BoW classifier obtains a significant AUC of 76.2% when distinguishing between the original suspect vs paraphrased text and the GPT2 classifier can achieve 99.0% AUC. The reason is that there are many words (such as ”remarkable” and ”moreover”) that appear much more frequently in the synthetic text than in the human-written text.

Please refer to Appendix C for more detailed explanation of GPT-4- based generation and examples of generated texts.

Preference Optimization. We also adapt preference optimization methods (Rafailov et al., 2024; Xu et al., 2024) to the task of held-out data generation by changing from human preference to natural text preference. Preference optimization methods focus on optimizing a pre-trained LLM based on human preference. Particularly, LLMs iteratively produce random generations, then human annotators are requested to label the generations as chosen or rejected, and the LLMs are further optimized according to this human feedback. We note that, we can leverage preference optimization approaches to make our generator model prefer the human-written texts over synthetic data, thus producing texts with a more similar distribution to natural texts. Here, we instantiate the preference optimization scheme with a state-of-the-art method, the simple preference optimization (SimPO) (Meng et al., 2024). During each training iteration, the human-written suspect data are always labeled as chosen and the generations from the last iteration are marked as rejected. The AUC of the BoW classifier is similar to random guessing, which means frequent words can be greatly reduced in generated texts by this approach. However, the GPT2 classifier can still obtain an AUC of 58.9%. This shows that preference optimization still leaves distinguishable generation patterns that could be easily captured by a transformer-based classifier, limiting the data's usefulness as in-distribution held-out set.

Suffix Completion. The failure of the above methods demonstrates the difficulty of producing high-quality held-out data with a small enough distributional gap to the suspect data. To solve this problem, we design a generator training scheme that enables the generator to derive a suspect set from the author's provided documents, together with a held-out set from the same distribution as this suspect set. As shown in Figure 2, we (1) first segment the provided documents into multiple short sequences. (2) All the sequences are shuffled and randomly split into a generator training split and a generator inference split. Then, (3) a low-rank adaption (LoRA) generator is finetuned on the training split with the cross-entropy loss for next-token prediction. Finally, (4) we segment each sequence in the generator inference split into two parts, and the generator predicts a synthetic suffix based on the prefix. Here, the original suffixes are used as the suspect set, and the synthetic suffixes as the held-out set. Note that, the training and inference sets are split on the shuffled text sequences rather than on the documents. This is to ensure that the text snippets from the generator training and inference splits are from the same distribution, such that the generator can achieve better generalization from the training to the inference set. Another important insight is that the generator can produce suffixes of higher quality when the sequence length is relatively short. Therefore, we limit the length of the sequences to no longer than 64 tokens for a smaller distributional gap. The results in Table 2 show that our method achieves a significantly small distributional shift, and even GPT2-based classifier can only achieve a low AUC of 52.2%. For examples of our generative approach, please refer to Section 5.1.

4.2 Post-hoc Calibration

Since the generation itself can introduce a distributional shift (natural vs generated) data, DI might yield false positives. This is because it would detect differences between suspect and held-out data also when they only differ in terms of distribution but not necessarily in membership. Therefore, we need to identify and mitigate this distribution shift.

To do so, we rely on an important observations: the generation shift between natural and synthesized data occurs in the textual space, while the shift caused by the potential membership of the suspect set exists in the target LLM's output space. This allows us to disentangle the two signals. By relying on our GPT-based **text-classifier** from Section 3.2, we can quantify the textual distribution shift caused by the generation. We denote this classifier by $c_{\text{text}}(x)$, where x is the text input for which the classifier should decide if it is original or generated data. Inspired by Kazmi et al. (2024), we also define a second **MIA-classifier** with input signals from both the texts and the outputs of the target model, such that we can quantify the combined effects of generation and the membership signal. Concretely, we train a combined classifier $c_{\text{comb}}(x, \text{MIA}(f(x)))$ with inputs from both text x and the MIA signal $\text{MIA}(x)$ based on the outputs of f. Here, $\text{MIA}(x)$ can also be a vector by concatenating multiple MIA scores. We split both the suspect set and held-out sets into training and test splits. The two classifiers are optimized on the suspect train split $\mathcal{D}_{\text{sus}}^{\text{train}}$ and the held-out train split $\mathcal{D}_{\text{val}}^{\text{train}}$, and evaluated on the suspect test split $\mathcal{D}_{\text{sus}}^{\text{test}}$ and the held-out test split $\mathcal{D}_{\text{val}}^{\text{test}}$. By comparing

the performance between the MIA-classifier and the text-classifier, we can separate the membership signals from the distribution gap caused by generation.

We design two hypothesis tests to statistically verify if the performance of the combined classifier is better than that of the text classifier by a large confidence. The first t-test is *AUC comparison t-test*, where we directly compare the AUC scores of the two classifiers by performing multiple random experiments. We formalize the null hypothesis of the AUC comparison t-test as follows:

$$\mathcal{H}_0 : \text{AUC}(c_{\text{comb}}, \mathcal{D}^{\text{test}}_{\text{sus}} \cup \mathcal{D}^{\text{test}}_{\text{val}}) \leq \text{AUC}(c_{\text{text}}, \mathcal{D}^{\text{test}}_{\text{sus}} \cup \mathcal{D}^{\text{test}}_{\text{val}}), \tag{2}$$

where $\text{AUC}(c, \mathcal{D})$ denotes the AUC of a classifier c on a dataset $\mathcal{D}$. We note that, the AUC comparison does not consider the pairwise relationship between each target data point and held-out point sharing the same prefix. Therefore, we introduce the *difference comparison t-test*. Concretely, we calculate the difference between the prediction scores of each target/held-out pair. Intuitively, the better-performing model should have a larger difference in the prediction scores. Therefore, we statistically verify if this prediction difference is significantly larger for c_{comb} than for c_{text}. The null hypothesis of difference comparison t-test is formalized as follows:

$$\mathcal{H}_0 : \mathbb{E}_{x^{\text{test}}_{\text{val}} \in \mathcal{D}^{\text{test}}_{\text{val}}}[c_{\text{comb}}(x^{\text{test}}_{\text{val}}) - c_{\text{comb}}(x^{\text{test}}_{\text{sus}})] \leq \mathbb{E}_{x^{\text{test}}_{\text{sus}} \in \mathcal{D}^{\text{test}}_{\text{sus}}}[c_{\text{text}}(x^{\text{test}}_{\text{val}}) - c_{\text{text}}(x^{\text{test}}_{\text{sus}})]. \tag{3}$$

Here, the groundtruth label $x^{\text{test}}_{\text{val}}$ is defined as 1 and $x^{\text{test}}_{\text{sus}}$ as 0. The difference comparison t-test is performed multiple times with different random seeds, and the p-values are aggregated with Sidac correction (Šidák, 1967).

By introducing a dual-classifier approach along with two statistical tests, we can statistically distinguish distributional shifts caused by actual membership signals from those caused by generation. Further results in Section 5.4 show that this approach can prevent false positives in dataset inference effectively.

4.3 Weight Constraint

In this section, we explain why and how we apply a weight constraint when computing the importance of different MIA scores. In the original DI, the aggregated MIA score is compared between the held-out and the suspect sets. We define the difference in aggregated MIA score between the two sets y_{diff} as follows:

$$\begin{aligned} y_{\text{diff}} &= \mathbb{E}[\sum_{i=1}^{n} w_i \text{MIA}_i(x_{\text{val}})] - \mathbb{E}[\sum_{i=1}^{n} w_i \text{MIA}_i(x_{\text{sus}})] = \sum_{i=1}^{n} w_i (\mathbb{E}[\text{MIA}_i(x_{\text{val}})] - \mathbb{E}[\text{MIA}_i(x_{\text{sus}})]) \\ &> 0 \text{ if } \mathcal{D}_{\text{sus}} \text{ is member set, otherwise} \leq 0. \end{aligned} \tag{4}$$

Here, $w_i \in \mathbb{R}$ is the weight for the MIA score MIA_i. Assuming that $\mathcal{D}_{\text{sus}}$ and $\mathcal{D}_{\text{val}}$ are i.i.d., we have $\mathbb{E}[\text{MIA}_i(x_{\text{val}})] > \mathbb{E}[\text{MIA}_i(x_{\text{sus}})]$ on member set and $\mathbb{E}[\text{MIA}_i(x_{\text{val}})] \approx \mathbb{E}[\text{MIA}_i(x_{\text{sus}})]$ on non-member set for each MIA score. Therefore, we have y_{diff} close to 0 on the non-member set, regardless of the weights w_i. However, when we synthesize the held-out set with a generator, there can be a small distributional shift between $\mathcal{D}_{\text{sus}}$ and $\mathcal{D}_{\text{val}}$. With this shift, we can have $\mathbb{E}[\text{MIA}_i(x_{\text{val}})] < \mathbb{E}[\text{MIA}_i(x_{\text{sus}})]$ on non-member set. This is often the case for generated text, because the generator usually produces held-out texts that are *simpler* than human-written texts, therefore causing the generated held-out texts to have smaller perplexity. This affects most perplexity-based methods, such as LOSS, Min-K%, and Zlib ratio. Consequently, the linear regression algorithm can assign negative weight w_i to such MIA scores, which causes $y_{\text{diff}} > 0$ on the non-member set and therefore high false positive rates. To ensure that this generation shift does not add up to a falsely high y_{diff}, we constrain the weights to be positive. Concretely, the weights are projected from $\mathbb{R}$ to $(0, 1)$ with Sigmoid function $\sigma(x) = \frac{1}{1+e^{-x}}$. With such a weight constraint, the linear regression only assigns a small weight w_i for MIA_i if $\mathbb{E}[\text{MIA}_i(x_{\text{val}})] < \mathbb{E}[\text{MIA}_i(x_{\text{sus}})]$, avoiding false positives in many cases. We also present the empirical analysis of the weight constraint in Section 5.4.

5 Experimental Evaluation

We start by introducing our experimental setup, further detailed in Appendix E. Then, we present the results of DI executed based on our generated held-out data.

Table 2: Distributional shifts between the suspect set and generated held-out set measured by BoW classifier vs GPT2.

Generation Method	BoW AUC (%)	GPT2 AUC (%)
ICL Paraphrasing	76.2	99.0
Preference Optimization	50.2	58.9
Suffix Completion	**50.0**	**52.2**

Table 3: Results for single author blog posts. Here, p-value < 0.05 indicates the suspect set is member set.

True Membership	AUC $_{\text{Text}}$ (%)	AUC $_{\text{Comb}}$ (%)	P-value	Inferred Membership
✓	53.8	55.6	0.01	✓
×	53.8	53.9	0.13	×

Table 4: Results for different Pile subsets. *True* represents the true membership while *Inferred* denotes the inferred membership. Our generation is successful if these two align.

Subset	Github		Euro-Parl		Phil-Papers		Hacker-News		Enron-Emails		Stack Exchange		PubMed Abstract		USPTO Back.	
True	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×
AUC $_{\text{Text}}$ (%)	54.0	53.3	51.3	51.9	58.5	58.1	56.4	57.1	56.9	58.4	54.0	52.7	54.9	54.7	56.7	55.8
AUC $_{\text{Comb}}$ (%)	59.3	51.9	65.0	47.7	57.0	55.3	57.5	56.3	58.2	53.8	60.0	50.8	59.9	53.0	58.1	55.7
P-value (AUC)	<0.001	1.0	<0.001	1.0	1.0	1.0	0.01	0.98	0.005	1.0	<0.001	1.0	<0.001	1.0	<0.001	1.0
P-value (Diff)	<0.001	1.0	<0.001	1.0	<0.001	0.13	<0.001	0.14	0.001	0.99	<0.001	1.0	<0.001	0.66	<0.001	0.13
Inferred	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×

5.1 Experimental Setup

Single author data. We collect 1400 blog posts from a single author. All figures, tables, videos, and hyperlinks are removed during pre-processing and only plain text is used for evaluation. We sample 450 posts as member data, and finetune a Pythia 410M deduplicated model for 1 epoch as target model. The other posts are held out as non-member and held-out sets for the evaluation.

More Complicated Dataset and Model. We also evaluate our method on the Pile dataset (Gao et al., 2020), which is much more complicated and has subsets of diverse types of texts. We use the de-duplicated version of Pythia 410M model as the target model. The training split of the Pile dataset is used as member data, and the test split as non-member. Here, we only evaluate Pile subsets that are free from copyright issues. Please also refer to Appendix D for detailed configuration on the Pile.

Generation. We finetune a Llama 3 8B model (Dubey et al., 2024) with LoRA as the generator. For both types of datasets, we split 2,000 sequences as the generator inference set, and the others as the generator training split. Therefore, our proposed t-test is conducted on 2,000 synthetic held-out data and 2,000 suspect data for each dataset.

Text and Combined Classifiers. For both the text and the combined classifier, we leverage the basic architecture of the GPT2 classfier with an extra linear layer. Specifically, the classifier has only two layers, with an embedding dimension of 1600 and an attention head number of 25. As explained in Section 4.3,, we apply a weight constraint to the linear layer. The GPT2-based classifier is optimized for 20 epochs, and the linear layer is further optimized for 200 epochs.

5.2 Results for Single Author Dataset

The experimental results on the single author dataset are presented in Table 3. On the member set, the combined classifier c_{comb} outperforms the text classifier c_{text}, by a large margin of 1.8% AUC score. Moreover, the observed p-value of 0.01 strongly supports the alternative hypothesis, indicating that the superior performance of c_{comb} over c_{text} is statistically significant. This enables our method to correctly identify that the target set is part of the training set. For the non-member set, c_{comb} and c_{text} achieve comparable AUC scores, with a p-value of 0.13 that significantly exceeds the threshold of 0.05. This result confirms the ability of our approach to correctly identify non-member texts as such, thus avoiding the false positives that occur with the original LLM DI approach. We also refer the readers to Section 3, where we show that a distributional shift exists even among the single author's data. Without our approach, this shift causes significant false positives to DI.

5.3 Results for Pile Datasets

The results on different Pile subsets are shown in Table 4, while those on other subsets can be found in Appendix B. We observe that DI correctly predicts the membership of datasets from diverse domains and styles, including plain text, academic writing, and code using our method for generating the held-out data. The results also show that our generation method generalizes well to documents with different lengths, ranging from 1KB (Wikipedia) to 70KiB (PhilPapers). Notably, the p-values for our difference comparison t-test are significantly lower than 0.05 on all the evaluated member sets, and higher than 0.1 on all the non-member sets.

5.4 Ablation on Post-hoc Dataset Inference

We conduct ablation studies to separately analyze the contribution of the three components in our held-out data generation: suffix completion, calibrating, and weight constraint. We also refer readers to Appendix F for further analysis of sample size in our method.

Table 5: Ablation studies for three components in our approach.

Configuration	True Membership	P-value	Inferred Membership
w/o Suffix Completion	✓	1.0	×
(ICL Paraphrasing)	×	1.0	×
w/o Post-hoc Calibration	✓	<0.001	✓
(Original T-test in DI)	×	<0.001	✓
w/o Weight Constraint	✓	0.004	✓
	×	0.43	×
Ours	✓	<0.001	✓
	×	1.0	×

Suffix Completion. We replace our generation scheme with ICL paraphrasing and present the p-values on the generated data in Table 5. The p-values for both member and non-member sets are 1.0, which indicates that the c_{text} has better or similar performance when compared with c_{comb}. The reason behind the observation is that the distributional shift caused by the generation is much larger than the shift induced by the membership signal, such that c_{comb} does not outperform c_{text} even with extra membership inputs on the member set. Consequently, the DI predicts both sets as non-member and suffers from false negative.

Post-hoc Calibration. We replace our calibration method with the original DI without calibration. Specifically, only a linear classifier is optimized to aggregate different MIA metrics and output the final prediction score. Furthermore, the t-test is conducted directly between the predictions on the target set and the ones on the held-out set. We observe that the p-values under this condition are extremely low for both member and non-member sets, and DI has false positive in this case. This observation aligns with results in Section 3, where we show that even a small distributional shift causes a significantly small p-value in the original DI. Therefore, our post-hoc calibration approach is crucial to evaluating the distributional shift caused only by membership signals.

Weight constraint. As explained in Section 4.3, the weight constraint avoids summing the distributional shift caused by generation to the final MIA prediction when the direction of the generation shift is different from that caused by the membership signal. As shown in Table 5, applying the constraint leads to a much lower p-value on the member set and much higher on non-member set, which helps our method make a more accurate prediction about the membership.

6 Conclusions

We propose how to *synthetically generate* an in-distribution held-out dataset to enable the real-world application of DI. Therefore, we solve two critical challenges, namely (1) creating high-quality, diverse synthetic data that accurately reflects the original distribution and (2) bridging likelihood gaps between real and synthetic data. Our solution relies on designing a data generator training scheme based on a suffix-based completion task and post-hoc calibration to align the likelihood gaps between real and synthetic data. Through extensive experimental evaluation, we highlight that our method enables a robust DI and correctly identifies training data while achieving a low false positive rate. This shows our method's reliability to support copyright owners to make legitimate claims on data usage for real-world litigations.

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A Visualization of DI on Single Author Data

In Section 3, we show that there is a distributional shift between the non-member data and held-out data, even for texts composed by a single author. Here, we show this distributional shift in texts also lead to a shift in the MIA score. As presented in Figure A1, the distributional shift in perplexities exists not only between member and held-out sets, but also between *non-member and held-out sets*. This shows that the inherent distributional shift among documents is entangled with the shift caused by membership signals in the MIA score, and makes DI fail to determine membership by simply detecting any distributional shift in the MIA score.

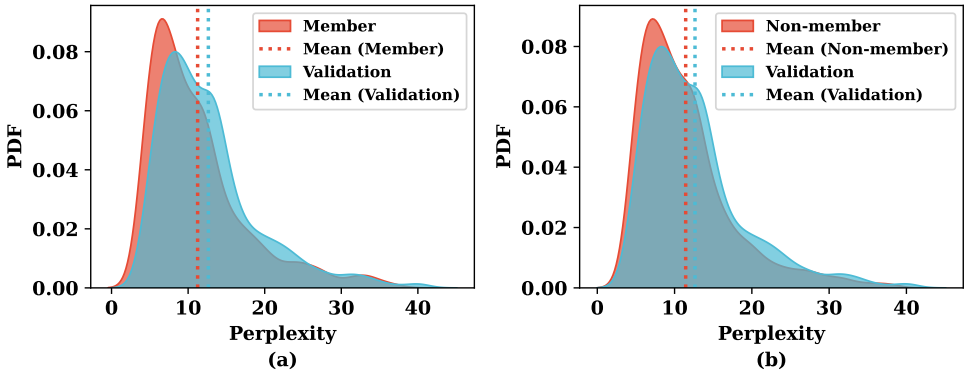

Figure A1: Probability distribution function of target model perplexities on different sets. We show the comparison between (a) the member and held-out, and (b) the non-member and held-out sets.

B Results for Other Pile Subsets

Here, we present the results for other Pile subsets in Table A1. The results demonstrate that our method successfully predicts the membership of all evaluated subsets, which aligns with the observation shown in Section 5.3,

Table A1: Results for other Pile subsets. *True* represents the true membership while *Inferred* denotes the inferred membership. Our generation is successful if these two align.

Subset	Pile-CC		Wiki-pedia		ArXiv		NIH Exporter		Free-Law		Ubuntu IRC		PubMed Central	
True	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×
AUC $_{\text{Text}}$ (%)	53.1	52.5	51.7	52.2	53.9	53.1	51.4	53.3	55.6	51.6	52.7	52.5	54.1	52.4
AUC $_{\text{Comb}}$ (%)	60.3	48.3	58.6	52.0	57.3	44.7	54.1	51.6	56.7	51.6	54.5	54.2	54.4	49.5
P-value (AUC)	<0.001	1.0	<0.001	0.98	<0.001	1.0	<0.001	1.0	<0.001	0.49	<0.001	0.03	0.30	1.0
P-value (Diff)	<0.001	1.0	<0.001	0.43	<0.001	1.0	0.005	1.0	0.003	0.84	0.002	0.12	0.004	0.66
Inferred	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×	✓	×

C Details of ICL Generation

We test two types of templates to prompt GPT-4-Turbo model with in-context-learning (ICL). One is to paraphrase the given sample based on the examples, and the other is to complete the text with part of the sentence.

C.1 Text Completion Prompt

In the text completion prompt, we give ten examples from the author provided documents, and prompt the GPT-4-Turbo model to complete the given sample, which is shown at the end of the prompt. Here is an example of this kind of queries:

Input:

```
I have some text samples. Please help me complete the last sample
   based on my example samples.
A device may be provided to sense an environment's present
   temperature. For example, [...] a thermistor that is robust
   and reliable and that can be fabricated at a reasonable cost.
[...]
This invention relates to a method of synthesizing musical tones.A
    musical tone or natural tone produced by an acoustic or
   natural musical instrument can [...]  With the music
   synthesizer it is considerably difficult to obtain dynamic
   audio spectra.pneumoniae.
Radio communications receivers commonly receive and decode
   messages which contain information. A part of this information
    may be [...]a single radio will transmit messages to the
   remainder of the group. These radio
```

Output:

```
messages are selectively received by the grouped radios which
   decode the identity information within the [...] and secure
   group communications in diverse and often challenging
   operational environments.
```

C.2 Paraphrasing Prompt

In the paraphrasing prompt, we give ten examples from the author provided documents, and prompt the GPT-4-Turbo model to paraphrase the last. Here is an example of this kind of queries:

Input:

```
Paraphrase the last sample according to the other samples.
1. Field of the Invention This invention relates generally to
   fluid injectors. More particularly, this invention relates to
   a proportional needle control fuel injector having a [...] The
    needle valve is moveable between a first position closing the
    injection fuel outlet port and a second position to open to
   injection fuel outlet.
[...]
The present invention relates to the structure of a casing of a
   miniature portable [...] is forcibly urged away from the
   casing by a tool, it is likely that the casing is scratched or
    the base plate is deformed.
This invention relates to fuel cells and, in particular, to
   improvements in the catalyst used in internal  [...]  fuel
   cell in which the catalyst assembly has minimum displacement
   and permits vertical and horizontal orientations of the fuel
   cell.
```

Output:

```
This invention pertains to fuel cells, specifically addressing
   enhancements in catalysts utilized  [...] and efficiency of
   internal reforming fuel cells by mitigating previous
   limitations and improving overall system functionality.
```

C.3 Distribution Shift Analysis

The distributional shifts are quantified in BoW AUC and GPT2 AUC as shown in Table A2. As observed, both types of prompt templates produces synthetic texts with large distributional shifts to

the suspect sets. Notably, the BoW classifier can already achieve as much as an AUC of 79.2%, and the GPT2-based classfier can obtain more than 99.0% AUC for both types of templates. The reason is that there are many words (such as "remarkable" and "moreover") that appear much more frequently in the synthetic text than in the human-written text. These words can be easily detected even with a simple BoW classifier.

Table A2: Distributional shifts between the suspect set and GPT-4-Turbo generated validation set.

Template Type	BoW AUC(%)	GPT2 AUC(%)
ICL Text Completion	79.2	99.2
ICL Paraphrasing	76.2	99.0

D Pile Dataset Segmentation

We present the details for the configurations of Pile subset in Table A3. We note that, it is claimed that the following Pile subsets may have copyright issues and cannot be included for evaluation: Books3, OpenWebText2, Gutenberg (PG-19), OpenSubtitles. BookCorpus2, and YoutubeSubtitles. For most subset there are documents that are much longer than the other documents, which causes that too many snippets are sample from these documents if all snippets are used. Therefore, we set a maximum snippet for each document on each subset according to the median lengths of the documents. Also, we note that our approach can achieve good performance on most subsets with only 32 tokens. For certain subsets, we use a token length of 64 for a stronger membership signal. The average token number for the Pile subset is 45. In practical applications, we suggest choosing the token numbers when the text-classifier has the minimal AUC to avoid distributional shift as much as possible. As a more conservative approach, this avoids making false accusations of copyright violation.

Table A3: Segmentation configurations for different Pile subsets.

Subset	Number of Test Set in Pile	Chosen Split Size	Max. Snippets per Document	Number of Tokens per Snippet
Pile-CC	>4000	4000	20	32
StackExchange	>4000	4000	5	64
PubMed Abstracts	>4000	4000	20	64
Wikipedia (en)	>4000	4000	5	32
USPTO Backgrounds	>4000	4000	20	64
PubMed Central	>4000	4000	10	32
FreeLaw	>4000	4000	5	32
ArXiv	>4000	4000	10	32
NIH ExPorter	>3000	3000	10	32
HackerNews	>3000	3000	10	64
Github	>1000	1000	30	32
Enron Emails	1957	1957	30	64
EuroParl	290	290	200	32
PhilPapers	132	132	500	64
Ubuntu IRC	43	43	500	32

E Implementation Details

E.1 Generator

The LoRA rank for the generator is 32. The generator is trained for 100 epochs, and the learning rate is set to 2×10^{-4}. We set a warm-up ratio of 0.03, and a linear scheduler is used to dynamically adjust the learning rate.

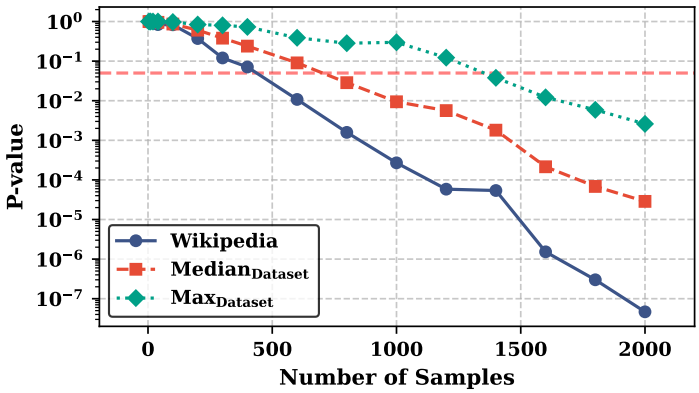

Figure A2: The p-values of member sets with change in sample size. Median$_{\text{Dataset}}$ denotes the median p-value of different datasets, and Mean$_{\text{Dataset}}$ is the maximum p-value of all subsets. Number of samples refers to the total size of both suspect and validation sets.

F Analysis of Sample Size

We also set out to analyze how the sample size in our proposed t-test affects the statistical confidence of DI with our generated held-out data. Here, the sample size is the total number of the suspect and held-out set, which is also the number of queries made to the target model. The two sets are of the same size, as they are produced in a pairwise manner. We observe from Figure A2 that, as the number of samples increases, DI exhibits improved detection capability of training data. Notably, with fewer than 1,000 samples, DI achieves statistical significance ($p < 0.05$) across most of the evaluated datasets. When increasing the sample size to 2k queries, the method demonstrates even stronger statistical significance ($p < 0.01$) consistently across all datasets.

G Examples of Synthetic Texts

In this section, we provide some examples of the synthetic texts on the Pile dataset. Here, prefix denotes the first half of the generated text, real suffix refers to the original suffix of the natural text, and generated suffix refers to the synthetic completion based on the prefix. We observe that, the generated suffixes are reasonable continuation of the prefixes. The generated suffixes also align with the style of each dataset and do not overfit to the content of the real suffixes.

G.1 Pile-CC

Prefix:

```
are excited about and also what we hoped to see from this years E3
    !
```

Real suffix:

```
From the surprising new Spider-Man PS4 game to the bizarre We
    Happy Few and
```

Generated suffix:

```
Let us know your thoughts on this monologue as we are preparing
    for our next
```

G.2 StackExchange

Prefix:

```
var FKEntityListWithCastCopy = new debiteur().GetType().
   GetProperty(\""
```

Real suffix:

```
schakeling\").GetValue(dbEntry) as List<FKEntity>;//Just
```

Generated suffix:

```
FKEntityList\").GetValue(instance, null);\n            foreach(var
    t in FKEntity
```

G.3 PubMed Abstracts

Prefix:

```
were calculated using the Kaplan-Meier method. Of the 117 patients
    in
```

Real suffix:

```
whom data were analyzed, 103 had follow-up MR or CT images and 14
   patients were
```

Generated suffix:

```
the study (76 with UC and 41 with DC), 45 patients required
   proctocolic resection
```

G.4 Wikipedia (en)

Prefix:

```
Em is going away for a while. While it's not up to the standard
```

Real suffix:

```
of "Mockingbird," it is more fully realized than the two other new
```

Generated suffix:

```
of their three previous albums, cattle call is still an enjoyable
   romp,
```

G.5 USPTO Backgrounds

Prefix:

```
1. Field of the Invention\nThis invention relates to a storage
   device for athletic equipment and, in particular, to a
   portable storage device for transporting and retaining
```

Real suffix:

```
elongate items of athletic equipment such as hockey sticks and
   related athletic equipment.\n2. Discussion of Related Art\
   nNumerous team athletic activities require individual players
   on the
```

Generated suffix:

```
multiple pairs of basketballs.\n2. Description of the Related Art\
   nDuring the summer and other periods when there is an extended
    break from an athletic school or program
```

G.6 PubMed Central

Prefix:

```
example, both cycles apply Lewis acidic metal centers to bind the
    monomers (ep
```

Real suffix:

```
oxide or lactone), and both invoke labile metal alkoxide
    intermediates as
```

Generated suffix:

```
oxides or cyclic carbonates), but the axes of the metallacycle in
```

G.7 FreeLaw

Prefix:

```
Court, 638 P.2d 65 (Colo.1981
```

Real suffix:

```
Here, the juvenile court denied the GAL's motions because it did
    not want
```

Generated suffix:

```
), cert. denied, 454 U.S. 1146, 102
```

G.8 Arxiv

Prefix:

```
up and vice versa. In contrast, fundamentalists expect the price
    to track its
```

Real suffix:

```
fundamental value. Orders from this type of agent may be written
    as\n\n$$D
```

Generated suffix:

```
underlying fundamentals up and down, but given sufficient
    acceleration the price might \u201crun away
```

G.9 NIH ExPorter

Prefix:

```
attachment and growth, respectively. Together with an industrial
    sponsor, Vaxiron,
```

Real suffix:

```
Inc., we will develop quality control tools and metrics for
    assessing vaccine antigen formulations,
```

Generated suffix:

```
the applicant has carried out clinical trials of different vaccine
     candidates based on different viruses for
```

G.10 GITHUB

Prefix:

```
.string \"reach only by using a BIKE technique.$\"\n\
   nRoute110_Text_
```

Real suffix:

```
16EEF6:: @ 816EEF6\n\t.string \"Which
```

Generated suffix:

```
16F381:: @ 816F381\n\t.string \"ROUTE {ROAD
```

G.11 ENRON EMAILS

Prefix:

```
Lay.  He went on to say that Kenneth was Dewayne Re
```

Real suffix:

```
es' cousin  and started telling about all of your fine attributes
   and what a
```

Generated suffix:

```
ams' direct \nreport and that it would be extremely difficult for
   Kenneth to get
```

G.12 EUROPARL

Prefix:

```
het mondeling amendement op schrift heeft gekregen.\nIk st
```

Real suffix:

```
el voor om niet te spreken over \"de Raad en de lidstat
```

Generated suffix:

```
akk voor de uitnodiging om tijdens uw volgende bij
```

G.13 PHILPAPERS

Prefix:

```
distribute well among [the gods who fought with him] their titles
   and privileges
```

Real suffix:

```
" (885, cf. 66\u201367 and 74); to swallow
```

Generated suffix:

```
 (17.1). Orderly distribution of praise for the victory is re
```

G.14 UBUNTU IRC

Prefix:

```
about setting up reoccuring status meetings?\n<dfarning> should we
    start
```

Real suffix:

```
holding those or is it too soon?\n<dfarning> Luke will be joining
```

Generated suffix:

```
with a status meeting or a design meeting?\n<manusheel> dfarning
```

G.15 HACKERNEWS

Prefix:

```
Angular (work just uses Dojo).\n\nPeople don't seem to
```

Real suffix:

```
be hungry here.\n\n------\nlewispollard\nWorked for IBM as a
   software engineer on one of
```

Generated suffix:

```
care that it's adding yet another ~20KB per page. We're\nsaying no
```

H OTHER RELATED WORK ABOUT TEST SET CONTAMINATION DETECTION

Test set contamination is a newly identified risk, where the public test benchmarks are involved during LLM training (Balloccu et al., 2024). For example, Roberts et al. (2024) observe that LLMs are better at generating code with more appearances on GitHub, revealing that LLMs can be contaminated with open-source GitHub data and are overestimated on coding tasks. Similarly, Li & Flanigan (2024) demonstrate that some LLMs have a better performance on few-shot benchmarks constructed before the model training, which indicates test set contamination for LLMs. To detect test set contamination, Golchin & Surdeanu (2023) design prompts that guide LLM to reproduce exact or near-exact test set instances, such that the model encloses the contaminated samples memorized during the pre-training phase. Oren et al. (2024) compare the target model predictions between a test set and all of its permutations. However, this method is based on the assumption that the test set is involved in the training set in its exact order, which could be interrupted by a random shuffle before training. Test set contamination can also be a potential application of our method, as the proposed approach can perform training data detection on complex datasets composed by different authors.