Simulating Training Data Leakage in Multiple-Choice Benchmarks for LLM Evaluation

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Abstract

The performance of large language models (LLMs) continues to improve, as reflected in rising scores on standard benchmarks. However, the lack of transparency around training data raises concerns about potential overlap with evaluation sets and the fairness of reported results. Although prior work has proposed methods for detecting data leakage, these approaches primarily focus on identifying outliers and have not been evaluated under controlled simulated leakage conditions. In this work, we compare existing leakage detection techniques, namely `permutation` and `n-gram`-based methods, under a continual pretraining setup that simulates real-world leakage scenarios, and additionally explore a lightweight method we call `semi-half` question. We further introduce two efficient extensions, `permutation-R` and `permutation-Q`. While `semi-half` offers a low-cost alternative, our analysis shows that the `n-gram` method consistently achieves the highest `F1-score`, performing competitively with `permutation-Q`. We also refine these techniques to support instance-level detection and reduce computational overhead. Leveraging the best-performing method, we create cleaned versions of MMLU and HellaSwag, and re-evaluate several LLMs. Our findings present a practical path toward more reliable and transparent evaluations, and we recommend contamination checks as a standard practice before releasing benchmark results. [1]

1 Introduction

The development of Large Language Models (LLMs) has shown competitive performance on multiple-choice question answering (Brown et al., 2020; OpenAI et al., 2024; Qwen et al., 2025; Team et al., 2024a; Grattafiori et al., 2024). These models are evaluated on benchmark datasets designed to assess specific competencies such as knowledge and reasoning. However, many LLMs do not disclose their pre-training data (Piktus et al., 2023), raising concerns that benchmark evaluation sets were included in training.

This lack of transparency raises a critical question: *Do current evaluation results reflect the true generalization abilities, or are they barely a product of memorization?* Suppose a model has been trained on evaluation datasets during training. In that case, it doubts the fairness of comparison as its ability to answer questions might originate from data memorization (Carlini et al., 2023) rather than reasoning or generalization. This issue, referred to as data contamination (Magar and Schwartz, 2022; Balloccu et al., 2024) poses significant concerns for reliable benchmarking.

Recent studies have introduced various methods to detect data contamination in multiple-choice question (MCQ) benchmarks for LLMs (Ni et al., 2024; Xu et al., 2024; Li, 2023). However, these approaches primarily focus on identifying outliers and have not been systematically evaluated under controlled leakage conditions. Furthermore, there is limited understanding of their relative effectiveness (Hu et al., 2022; Samuel et al., 2024; Fu et al., 2025), and no consensus on the optimal configurations for detecting training data leakage. To address these gaps, we benchmark existing leakage detection methods under controlled simulations, focusing on two widely used MCQ datasets in LLM evaluation: the Massive Multitask Language Understanding (MMLU) dataset (Hendrycks et al., 2021a) and the HellaSwag dataset (Zellers et al., 2019).

Our key contributions are as follows:

- We compare three leakage detection methods under simulated training data leakage via continual pre-training: (1) the `semi-half` method, which tests whether a truncated ver-

[1]Code and dataset are available at `https://github.com/nailashfrni/mcq-leakage-detection-code`

sion of a question still results in the correct answer; (2) the `permutation` method, originally proposed by Ni et al. (2024), which evaluates whether the original option order yields the highest likelihood among all permutations; and (3) the `n-gram` method, which assesses the similarity between a generated option sentence and the original, following Xu et al. (2024).

- We improve the `permutation` method by introducing two variants, `permutation-R` and `permutation-Q`, which reduce computational overhead while improving `F1-score`. We also refine the `n-gram` method to support instance-level detection.

- We construct and release a subset of the MMLU and HellaSwag dataset verified to be free of contamination across several popular LLMs. Furthermore, we re-evaluate these models on the clean subset to observe shifts in performance ranking.

2 Related Work

2.1 Evaluation Benchmark of LLM

Language model evaluation has shifted from classical NLP tasks—such as named entity recognition and part-of-speech tagging—toward benchmarks that assess knowledge and reasoning, driven by advances in fluency and coherence. These evaluations commonly adopt a multiple-choice format, exemplified by MMLU (Hendrycks et al., 2021a), which compiles questions of 57 subjects from a wide range of school exams across different education levels. Other popular reasoning benchmarks include HellaSwag (Zellers et al., 2019), PIQA (Bisk et al., 2020), BoolQ (Clark et al., 2019), Social–IQa (SIQA) (Sap et al., 2019), and TruthfulQA (Lin et al., 2021).

MMLU is one of the most widely used datasets for evaluating the knowledge capabilities of LLMs. To improve its quality and robustness, prior work has introduced several variants. MMLU-Pro (Wang et al., 2024) enhances the dataset by increasing question difficulty through filtering, expanding answer choices from four to ten, and incorporating expert review. Separately, Gema et al. (2025) released MMLU-Redux, a cleaned version that addresses issues such as ambiguous phrasing, multiple correct answers, and incorrect ground truths. However, despite these improvements, both variants primarily focus on question quality and coverage. Neither MMLU-Pro nor MMLU-Redux incorporates systematic filtering or analysis to detect overlap with pretraining data, leaving open the risk that benchmark scores may reflect memorization rather than true generalization.

2.2 Data Contamination Detection

Numerous methods have been proposed to detect data contamination in LLMs, broadly falling into logit-based, generation-based, and hybrid categories. Logit-based methods analyze the model's output probabilities or internal states; for example, Ni et al. (2024) compare log-probabilities across different option orders, while Li (2023) use perplexity to detect dataset-level leakage. However, these approaches primarily focus on outlier detection, offer limited support for instance-level analysis, and have not been evaluated under controlled training leakage simulations. In contrast, generation-based methods assess whether the model can reconstruct reference content when prompted. Golchin and Surdeanu (2024) use "time-travel" prompts incorporating dataset-specific cues to regenerate partial instances and compare them to the original text. Xu et al. (2024) introduce a hybrid approach combining n-gram similarity with perplexity, though their focus is on GSM8K (Cobbe et al., 2021) and MATH datasets (Hendrycks et al., 2021c). Importantly, these methods have not been tested on the multiple-choice question (MCQ) format, which remains the most widely used prominent structure in LLM evaluation benchmarks.

3 Leakage Detection Method

To detect whether a model has been exposed to a particular question, especially in multiple-choice question (MCQ) tasks, the problem can be formulated as a *leakage detection* task: given a model $\mathcal{M}$, a question q, options O, and contexts C, the goal is to predict whether $\mathcal{M}$ has memorized them, labeled as either *Leakage* (L) or *Not Leakage* (NL). Since no ground-truth labels exist for this task, we simulate training data leakage using continual pre-training and compare the effectiveness of three detection methods: `semi-half`, `permutation` (Ni et al., 2024), and `n-gram` (Xu et al., 2024). To improve efficiency, we introduce a simplified variant of `permutation`, called `permutation-R`, and

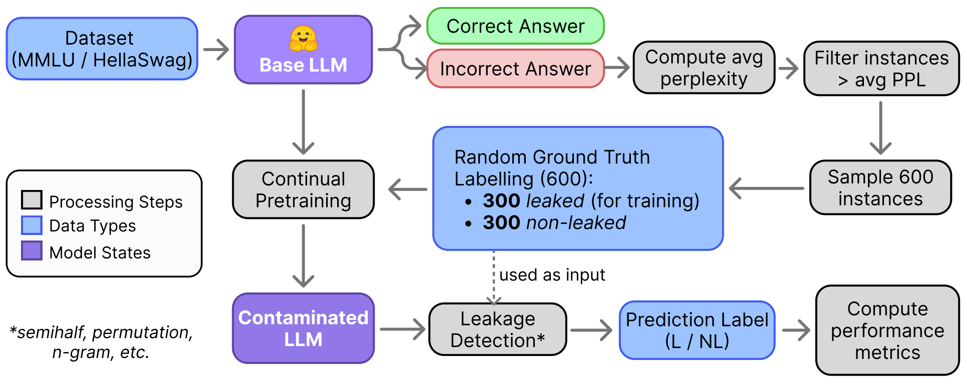
Dataset (MMLU / HellaSwag)
Base LLM
Correct Answer
Incorrect Answer
Compute avg perplexity
Filter instances > avg PPL
Processing Steps
Data Types
Model States
Continual Pretraining
Random Ground Truth Labelling (600):
• 300 leaked (for training)
• 300 non-leaked
Sample 600 instances
used as input
*semihalf, permutation, n-gram, etc.
Contaminated LLM
Leakage Detection*
Prediction Label (L / NL)
Compute performance metrics

Figure 1: Workflow for simulating data leakage and evaluating detection methods. Boxes represent different components: processing steps (gray), data types or datasets (blue), and model states (purple).

propose a new method, `permutation-Q`, built on the same foundation.

3.1 Leakage Simulation

Figure 1 illustrates our controlled simulation of intentional data leakage. We start by selecting questions from MMLU (Hendrycks et al., 2021b) and HellaSwag (Zellers et al., 2019) that the model initially answers incorrectly. From this set, we randomly sample 600 instances with above-average perplexity to ensure unfamiliarity and minimize the chance of prior exposure during pre-training. We use 300 of these samples for continual pre-training via Low-Rank Adaptation (LoRA) (Hu et al., 2021), simulating data leakage. After training, all detection methods are applied to the full set of 600 instances. The 300 examples included in pre-training are labeled as "Leaked", while the remaining 300 serve as "Not Leaked". We assess detection performance using `Precision`, `Recall`, and `F1-score`.

3.2 `Semi-half` Detection Method

To answer a multiple-choice question, a model relies on both the question and the options (Robinson et al., 2023). If it can still select the correct answer after the first half of the question is removed, this may suggest prior exposure during pre-training. Motivated by this, we propose a simple truncation-based method that retains only the final seven words of each question, providing minimal context while aligning with the autoregressive nature of decoder-based LLMs. The seven-word limit reflects the average half-length of the MMLU questions. Figure 2 illustrates a semi-half truncation example: if the model has seen the question during pre-training, it may still produce the correct answer despite the limited input; otherwise, the model is unlikely to produce the correct answer due to insufficient context.

`Semi-half` Truncation Example

Original Question: 'A plant grows in the opposite direction of the gravitational force. This is an example of'

A. positive thignotropism
B. negative phototropism
C. positive phototropism
D. negative gravitropism

`Semi-half` Question: 'gravitational force. This is an example of'

A. positive thignotropism
B. negative phototropism
C. positive phototropism
D. negative gravitropism

Figure 2: Semi-half truncation example

3.3 `Permutation` Method

Ni et al. (2024) proposed a method to detect contamination by evaluating how a language model assigns probabilities across different orders of multiple-choice answer options. The key idea is that if the model consistently assigns the highest probability to the original option order (e.g., A-B-C-D), it may have memorized that specific multiple-choice instance during training and indicated potential contamination.

The detailed method is explained in Appendix A. The algorithm complexity for this method is dominated by computing log-probability scores for each option order variation in a question. In big-Oh notation, the complexity is stated as $O(n!)$, where n denotes the number of options. This is considered a costly approach, and we modified this method to better achieve a less complex algorithm.

`Permutation-R`. Our main concern with the `permutation` method is its computational cost in computing the log-probability for all permutation variations. To address this, we eliminate permutations that have nearly similar log-probability distributions for all questions, then retain only a representative permutation subset.

To determine which permutation pairs show similar distributions, we employ Mean Absolute Difference (MAD) to measure the discrepancy in log-probability scores between two permutations. Let p_{ji} and p_{ki} represent the log-probability scores for permutations j and k on question i, respectively, and let z denote the number of questions. The mean absolute difference between permutations j and k, denoted by $\texttt{Diff}(j, k)$ is computed as:

$$\texttt{Diff}(j, k) = \frac{1}{z} \sum_{i=1}^{z} |p_{ji} - p_{ki}| \, .$$

We experiment with three different models: Qwen2.5-7B (Qwen et al., 2025), LLaMA-3.1-8B (Touvron et al., 2023), and Gemma-7B (Team et al., 2024b). For each experiment, we compute $\texttt{Diff}(j, k)$ for all possible permutation pair j and k and average the ranking across experiment. Since lower MAD indicates more similar distribution, we sort the average rank in increasing order. From that order, we retain only one permutation from each pair. To determine the optimal number of permutations used, we experiment with various proportion values p to observe which setting best balances computational cost and performance. The optimal p is then selected and used as the final configuration for the `permutation-R` method.

The algorithm complexity is $O\left(p.[n!]\right)$, where n denotes the number of options and p is for percentage of permutations used. This improvement might not be significant in the big-Oh notation since it still has permutation complexity. However, in practice, the reduced variation factor contributes to reducing computation time.

`Permutation-Q`. In practice, `permutation-R` improves efficiency by introducing a fractional term upfront. However, challenges arise when dealing with tasks that involve more than four answer choices, such as MMLU-Pro (Wang et al., 2024), with 10 options. To address this, we propose `permutation-Q` method, that replaces the factorial component with a more tractable quadratic approximation. The idea is to employ only two options in each log-probability calculation.

Suppose that we have an instance $x = [q, o_1, o_2, ..., o_n]$ where q denotes the question and o_n is the last option answer. We generate permutation P_2^n from $o = \{o_1, o_2, ..., o_n\}$ to only two options. We calculate the log-probability score for all possible permutations of two options. If the original option order (A-B) produces the maximum log-probability among all orders, we consider the instance x as 'Leakage', otherwise not.[2] The algorithm is presented in Algorithm 1 in Appendix B.

The complexity of the above method is centered on log-probability calculation for all possible combinations of options. The big-Oh notation is computed as:

$$O(P_2^n) = O(n.(n-1)) = O(n^2 - n) = O(n^2).$$

The complexity is reduced from factorial to quadratic, which is an improvement in detecting a leakage in a particular model.

3.4 `N-Gram` Method

The `n-gram` method builds on the approach introduced by Xu et al. (2024), which uses n-gram accuracy to detect potential data contamination during pre-training. The core idea is to test whether a model has memorized benchmark answer options by evaluating its ability to generate them. While the original method generates n tokens per prompt and compares them to a reference sequence, we modify it to generate an entire option sentence in a single inference. Other than that, while Xu et al. (2024) focus on detecting leakage at the dataset-split level by comparing metric differences between original and synthetic data, we adapt it to work at the instance level. This modification allows the method to identify contamination on a per-example basis and allows the analysis to be more comprehensive. The full details of the method and its algorithm are presented in Appendix C.

4 Experiment

4.1 Set-Up

We experiment with four models and two evaluation benchmarks—MMLU (Hendrycks et al., 2021b) and HellaSwag (Zellers et al., 2019)—to simulate data contamination in LLMs. The model list detailed in Table 5 in Appendix E. Each model

[2] The key idea is to compare the original 2-option pairs with its permutations, regardless of whether the correct answer is present in the pair.

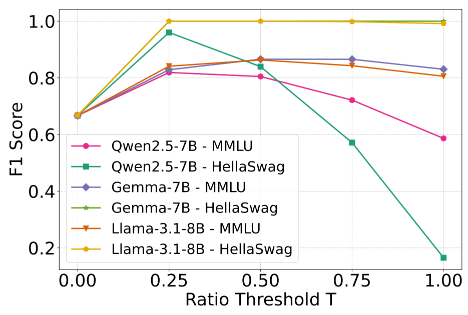

Figure 3: Comparison of `n-gram` detection F1-score performance under varying ratio thresholds T.

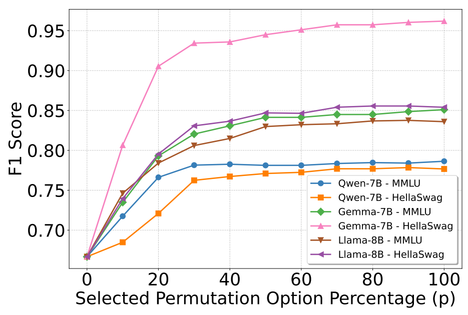

Figure 4: Performance of `permutation` at different percentages p, used to reduce computational complexity.

undergoes continual pre-training on each benchmark. Using the Adam optimizer, we set the learning rate to $1e-5$ for the language model head and $5e-4$ for other parameters. Each model is trained for 10 epochs with a weight decay of 0.01, a warmup ratio of 0.1, and a cosine learning rate scheduler. We also record the loss at each epoch for monitoring. For experiments involving LLaMA-3.1-8B base and Gemma-7B, we utilize an H100 SXM GPU with 80GB VRAM. For all other models, we use an A40 GPU with 48GB VRAM.

After completing the continual pre-training for all eight settings, we tune the threshold of `n-gram` and optimize the `permutation` method first. We then use this configuration to evaluate all methods and compare their performance.

4.2 Preliminary Results

Varying `N-Gram` Method's Threshold. We explore the effect of varying the threshold T in the `n-gram` method, which determines its sensitivity to determine an instance as 'Leakage'. The results of this comparison are presented in Figure 3. Across all experiments, a threshold of $T = 0.25$ consistently yields the best or comparable `F1-score`. Notably, in Qwen2.5-7B on HellaSwag, `F1-score` drops sharply as T increases. For LLaMA-8B and Gemma-7B on HellaSwag, `F1-score` remains at 100% for $T = 0.25$, 0.5, and 0.75, with only a slight decrease at $T = 1.0$. A similar trend appears in MMLU, where `F1-score` peaks at $T = 0.5$ but still exceeds 80% at $T = 0.25$.

These results suggest that $T = 0.25$ offers the best balance of sensitivity and reliability for detecting data contamination. This approach ensures that all potentially suspicious questions, even if only a single option is successfully replicated, are treated as 'Leakage'. This ensures comprehensive detection and allows us to capture as many contaminated instances as possible.

Reducing Permutation Variation. Using the Mean Absolute Difference (MAD), we compute the difference scores between log-probability distributions for each permutation pair. We rank all pairs by similarity for each model and average these rankings to identify the top 24 most similar pairs (see Table 3 in Appendix D). Notably, many of these differ by only two character swaps, suggesting such changes have minimal effect on the log-probabilities.

Based on this observation, we vary the proportion p to find an optimal trade-off between performance and efficiency. The full list of permutation used for each p is detailed in Table 4 in Appendix D. The impact of varying this percentage threshold on performance is illustrated in Figure 4.

An interesting finding is that using 50% or 100% of the permutations yields no significant difference in performance. The `F1-score` remains relatively stable across this range. This empirically supports the idea that using only a subset of permutations can still yield high performance, as some permutations may produce similar log-probabilities. To balance computational cost and detection quality, we adopt $p = 50\%$ as the default threshold for the `permutation-R` method in the subsequent comparison.

`Permutation-Q` Experiment. We experiment `permutation-Q` in six different model and dataset settings to observe its performance. We compare the result with `permutation-R` and the original `permutation`. The `F1-score` comparison is presented in Figure 5.

By using only two options per log-probability computation, `permutation-Q` achieves competitive `F1-score` scores and, in some settings, even

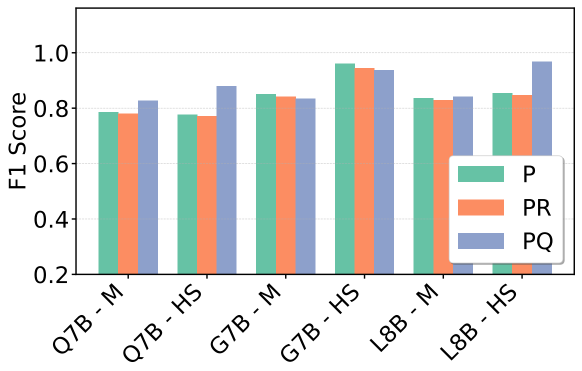

Figure 5: Performance of `permutation`-based methods: the original (P), reduced variant `permutation-R` (PR), and quick variant `permutation-Q` (PQ), evaluated on MMLU (M) and HellaSwag (HS). Model abbreviations: Q = Qwen, L = Llama, G = Gemma.

outperforms both the original `permutation` and `permutation-R` methods. These results highlight its ability to reduce complexity while potentially improving performance.

4.3 Main Results

Detection Performance Across Methods with Tuned Thresholds. Using the selected thresholds and configurations for the `n-gram` and `permutation-R` methods, along with other original approaches, we compare detection performance across eight evaluation settings. The results are presented in Table 1. Since each experiment uses a different subset of data, depending on the base model's initial ability to answer the questions, the metrics should only be compared across detection methods within the same experiment, not across different models or benchmarks.

Across experiments, the `n-gram` method consistently achieves over 81% `F1-score` and outperforms other methods in Qwen-0.5B (MMLU) and all HellaSwag settings. `Permutation-Q` shows strong performance as well, outperforming other methods in Qwen-7B and LLaMA-8B, while the original `permutation` achieves the best `F1-score` in Gemma-7B. Overall, `permutation-Q` performs competitively and often matches or exceeds the performance of `n-gram`.

Interestingly, combining multiple methods tends to increase `Recall` as more instances are flagged as 'Leakage', but this often leads to a decrease in `F1-score` (see Table 6 in Appendix F), likely due to a rise in false positives and lower `Precision`. A closer look at the HellaSwag results reveals that `n-gram` almost perfectly detects 'Leakage' across all settings. This may be attributed to the nature of the HellaSwag task, which involves predicting the most coherent continuation of a given context. This objective closely aligned with how `n-gram` generates options based on prefix patterns. It is also possible that `n-gram` benefits from the continual pretraining objective, which focuses on next-token prediction. Regardless of the cause, `n-gram` remains highly effective and competitive. Furthermore, since it does not require access to model logits, it can be applied to closed-weight models. For these reasons, we adopt `n-gram` as the primary detection method for both MMLU and HellaSwag.

Leakage Detection Results on Full Benchmarks. After applying the `n-gram` method to the full MMLU and HellaSwag datasets, we identified several instances flagged as 'Leakage'. Figure 6 illustrates the proportion of detected leakage across different models. Qwen2.5-7B shows a relatively higher tendency for potential leakage in both benchmarks, followed by LLaMA-3.1-8B on MMLU and Qwen2.5-0.5B on HellaSwag. These observations align with the findings of Ni et al. (2024), who also highlighted potential risks of leakage in the Qwen model family, despite using a different methodology. We additionally tested DeepSeek (Liu et al., 2024) and Gemini (Team et al., 2023) models: DeepSeek ranks third with 35% on MMLU and 0.17% on HellaSwag, while Gemini-2.0-Flash exhibits minimal indications of leakage across both datasets.

We observe that MMLU shows a higher potential for leakage across models compared to HellaSwag, likely due to its widespread use in NLP research, making its content more likely to appear in training data. Additionally, the `n-gram` method is sensitive to the length of the option text, as it generates tokens sequentially to match the reference, resulting in slower detection for longer options. In contrast, `semi-half` and `permutation`-based methods require only a single inference step per instance, making them more efficient.

Leakage $\neq$ Model Understanding. We observe that models do not always correctly answer leaked instances, both in our leakage simulation and full-benchmark evaluations. As illustrated in Table 2, models frequently fail to provide correct responses to flagged examples, indicating that memorizing input sequences does not equate to genuine understanding or reasoning. Nonetheless, instances

Benchmark	Model	S	P	PR	PQ	N	S+PQ	S+N	PQ+N
MMLU	Qwen-0.5B	55.68	82.78	82.12	86.63	<u>88.23</u>	79.16	79.84	85.47
	Qwen-7B	56.88	78.64	78.12	<u>82.68</u>	81.89	78.79	78.37	80.59
	Gemma-7B	68.59	<u>85.10</u>	84.14	83.45	82.87	77.12	75.95	80.32
	LLaMA-8B	50.51	83.59	82.98	<u>84.27</u>	84.11	80.00	79.84	81.63
HellaSwag	Qwen-0.5B	60.86	81.13	80.73	94.94	<u>99.83</u>	80.61	82.99	96.46
	Qwen-7B	67.92	77.67	77.10	87.93	<u>96.01</u>	73.48	75.79	95.67
	Gemma-7B	71.04	96.20	94.50	93.69	<u>100.00</u>	74.91	75.76	94.19
	LLaMA-8B	68.71	85.40	84.70	96.77	<u>100.00</u>	75.09	75.66	96.77

Table 1: Detection performance (`F1-score`) for various methods across different models and benchmarks. The methods are coded as follows: S = `Semi-half`, P = `Permutation`, PR = `Permutation-R`, PQ = `Permutation-Q`, and N = `N-Gram`. For combined methods (denoted by '+'), an instance is classified as Leakage if at least one of the methods detects it. <u>Underlined</u> scores represent the best method among the model & benchmark combinations.

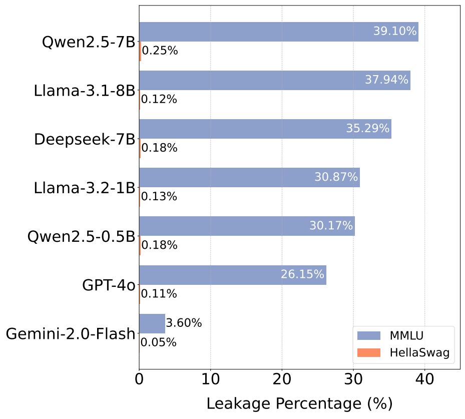

Figure 6: Data leakage rates for each model on MMLU and HellaSwag using the `n-gram` method.

Model	Accuracy on Leaked Set
Deepseek-7B	39.06%
Gemini-2.0-Flash	95.65%
GPT-4o	87.09%
LLaMA-3.1-8B	51.19%
Qwen2.5-7B	64.12%

Table 2: Accuracy scores of models on MMLU instances detected as leakage by `n-gram`.

encountered during pretraining are generally more likely to be answered correctly. This discrepancy may arise from a misalignment between training and evaluation objectives: while continual pretraining does not aim to identify the most likely answer among multiple choices, evaluation typically depends on comparing the log-likelihoods of each option.

Despite this disconnect, computing the log-likelihood of each option (A–D) remains the standard for evaluating multiple-choice questions in LLM. However, since we lack visibility into how each model was exposed to these benchmarks—such as whether answer keys were included during pretraining—we propose two complementary definitions of leakage: (1) Strong leakage: the detection method identifies the instance as 'Leakage' and the model answers it correctly. (2) Weak leakage: the detection method identifies the instance as 'Leakage', regardless of the model's answer.

Benchmark Reduction Under Strong Leakage Definition. By the strong definition of leakage, we remove any correctly answered instance flagged as 'Leakage' by the `n-gram` method in at least one LLM. This results in the removal of 6,547 out of 14,042 instances (46.6%) from MMLU, and 38 out of 10,042 instances (0.38%) from HellaSwag.

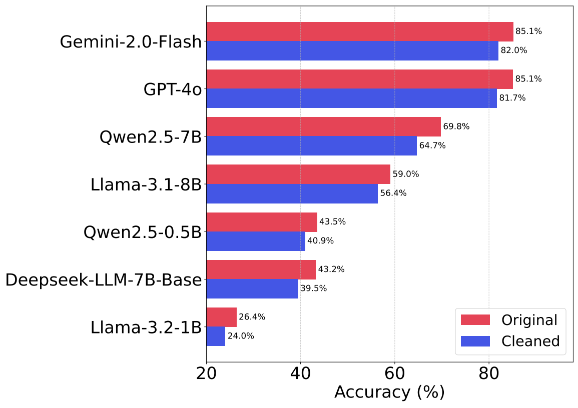

Figure 7: Comparison of model performance on original vs. cleaned MMLU benchmark based on strong definition of leakage.

Figure 7 compares model performance on the original and cleaned versions of MMLU.[3] On

[3]HellaSwag is excluded due to the minimal number of leaked instances (0.38%) and the absence of notable performance differences. GPT-4o remains the top-performing model on both versions.

the cleaned MMLU benchmark, Gemini-2.0-Flash achieves the highest performance among all evaluated models, followed closely by GPT-4o. While the relative ranking across the evaluated models remains largely consistent even after removing 46% of potentially leaked instances, we note that the models differ in size. Therefore, performance shifts could be more pronounced when comparing models within the same parameter scale. To explore this further, we analyze accuracy drops by subject and subject category within the same model in Section 5.

We also tested the LLMs' performance with the weak leakage definition. Since model accuracy on leaked instances is not 100%, removing these instances reduces the number of incorrectly answered examples, resulting in higher accuracy for some models. However, this only affects the performance ranking on the MMLU dataset, where GPT-4o slightly surpasses Gemini 2.0 Flash to become the top-performing model. The ranking positions for the other models remain unchanged.

5 Analysis

5.1 Performance Varies in Specific Subjects

Referring to the strong version of leakage definition, we analyze performance changes across specific MMLU subjects. Figure 8 presents the percentage drop in accuracy after removing potentially leaked instances, which highlights subjects with relatively large performance declines. In particular, model performance on the *Anatomy* subject drops substantially, with Qwen-7B showing the largest decrease (35.4%).

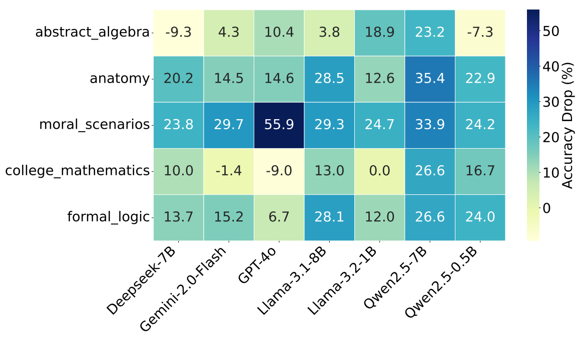

Figure 8: Performance drops in selected MMLU subjects for each model. Qwen-7B shows the largest accuracy drop in these subjects.

Meanwhile, *Moral Scenarios* contains the highest number of detected leaked instances. However, as observed in previous experiments, this subject yields a low `F1-score`. Upon further inspection, we find this is likely due to repetitive option templates used across all questions, such as "*Not Wrong, Not Wrong; Not Wrong, Wrong; Wrong, Not Wrong; Wrong, Wrong*" or "*True, False*." These patterns may increase the chance that the model generates the correct option based solely on surface similarity, leading to false positives under the `n-gram` detection method.

We also observe a noticeable accuracy decline in *Formal Logic* after data cleaning. This suggests that part of the model's original strong performance in this subject could be attributed to memorization rather than genuine reasoning ability. The cleaned results provide a more realistic reflection of the models' logical reasoning skills. We also find that the STEM group is most affected, showing the largest performance difference across subject groups (see Figure 10 in Appendix J for further details).

5.2 Detection Methods: Pros & Cons

As shown in Table 1, the `n-gram` method consistently achieves the highest `F1-score`, followed closely by `Permutation-Q`. However, each method has its own strengths and weaknesses. Table 8 in Appendix H summarizes the strengths and limitations of each method that focusing on computational cost and leakage detection effectiveness, to inform their use in different scenarios.

6 Conclusion

In this work, we simulate leakage using three methods—`semi-half`, `permutation`, and `n-gram`—and introduce a simplified variant, `permutation-Q`, which uses only two options and achieves strong performance across several settings. Our results identify `permutation-Q` and `n-gram` as the most effective detection methods under our controlled simulation setup, with Qwen-7B showing a high risk of leakage, especially in MMLU STEM subjects, where accuracy drops by up to 8% after filtering. We also observe consistent accuracy reductions across all models once leaked instances are removed. These findings highlight the distinction between memorization and true understanding, reinforcing the need to apply leakage detection before evaluation to ensure that test data remains clean and that the reported results reflect genuine generalization.

Limitations

Detection methods tend to yield a high false positive rate on moral scenario subjects. This is likely due to the repetitive structure of moral scenario questions in MMLU, which remains consistent across instances. In general, this issue arises in questions that use common option formats without referencing a specific domain topic, such as "*True; False*" or "*First; Second; Third; Fourth*". As a result, when the model encounters a new question with a similar option structure, it may mistakenly flag it as a leakage instance. We consider this a limitation of our approach and encourage future work to explore more robust strategies for detecting leakage in cases involving repeated option sentences or generic question formats.

While simulating continual pre-training (CPT), we recognize that using a single benchmark as the sole training corpus does not fully capture real-world LLM training. However, to better reflect practical scenarios, we also performed continual pre-training with the benchmark mixed with additional random data. Detection performance stayed consistent in both setups, and we observed no significant drop in the performance. Finally, our experiments focus on multiple-choice question (MCQ) tasks, and we encourage future work to extend this method to other task types.

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Ethics Statements

This work investigates potential data contamination in benchmark evaluations of large language models. While our methods aim to surface instances likely seen during training, we make no claims about the intentional inclusion of benchmark data or misconduct by model developers. Our findings are intended to support more reliable and transparent evaluation practices. We discourage the use of these results to make unfounded accusations against any specific model or organization.

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A Detailed Permutation Method

For each instance, we compute the log-probability score for all possible permutations of the answer options. Let n be the number of answer options, resulting in $n!$ possible permutations. For each permutation, denoted as $\pi = (o_{\pi(1)}, o_{\pi(2)}, \ldots, o_{\pi(n)})$, we construct the sequence $[q, o_{\pi(1)}, o_{\pi(2)}, \ldots, o_{\pi(n)}]$, where q is the question and $o_{\pi(i)}$ are the permuted answer options. We then tokenize this sequence into $x = (x_1, x_2, \ldots, x_T)$, where T is the total number of tokens.

Given a language model $\mathcal{M}$, we compute the log-probability score starting from the first token of the first answer option. The score is calculated as:

$$\text{Score}(x) = \sum_{i=i^*}^{T} \log P(x_i \mid x_{<i}; \mathcal{M}),$$

where $P(x_i \mid x_{<i}; \mathcal{M})$ is the conditional probability assigned to token x_i given its preceding context; and i^* marks the token index where the first option sentence begins. This scoring function captures how likely the model is to continue generating a specific option sequence, conditioned on the prompt. If the original order (A-B-C-D) has the maximum log-probability across other orders, we consider the model to memorize that version more and the instance as 'Leakage', otherwise not.

B Permutation-Q Algorithm

Algorithm 1 details our refined `permutation-Q` procedure. Its time complexity is lower than that of the original `permutation` method because the factorial term ($O(n!)$) is replaced by a quadratic factor ($O(n^2)$).

C N-gram Algorithm

For each input instance $x = [q, o_1, o_2, \ldots, o_n]$, the model $\mathcal{M}$ is asked to generate each option o_i ($i \leq n$), using the question q and the previous options o_1 to o_{i-1} as context. The generated output $\hat{o}_i$ is then compared to the original o_i using a `ROUGE-L` score (Lin, 2004). If the similarity score is above a threshold $t = 0.75$ (based on Xu et al. (2024)), we consider the option as replicated. We count how many options are replicated in this way and calculate the ratio over the total number of options. If this ratio is higher than a threshold T, we mark the instance x as contaminated for model $\mathcal{M}$. A

Algorithm 1 `Permutation-Q` Detection Method

```
Input: Data $x = [q, o_1, o_2, ..., o_n]$; Model $\mathcal{M}$
Output: "L" (Leaked) or "NL" (Not Leaked)
 1: # Generate all pairs of options
 2: $P \leftarrow$ Permute($\{o_1, o_2, ..., o_n\}, 2$)
 3: # Initialize empty score list
 4: scores $\leftarrow$ [ ]
 5: for each pair $(o_i, o_j) \in P$ do
 6:     # Construct prompt sequence
 7:     seq $\leftarrow [q, o_i, o_j]$
 8:     # Compute log-probability
 9:     scores += $[log(P(\text{seq}; \mathcal{M}))]$
10: end for
11: # Construct original correct sequence
12: seq' $\leftarrow [q, o_1, o_2]$
13: # Has the highest log-probability?
14: if $log(P(\text{seq}'; \mathcal{M})) = \max(\text{scores})$ then
15:     return "L"                          ▷ Leaked
16: else
17:     return "NL"                         ▷ Not Leaked
18: end if
```

full, detailed algorithm is presented in Algorithm 2.

The threshold used for this detection method decides the sensitivity level. If we use $T = 0.25$, meaning an instance is labeled as 'Leakage' if at least one of its options is generated with high similarity to the ground truth, this is intended to capture as many suspicious instances as possible. The smaller the threshold T is, the more sensitive it gets to detect contamination. In this study, we further explore the effect of varying the threshold T. Since both MMLU and HellaSwag benchmarks contain four options per question, we experiment with $T = \{0.00, 0.25, 0.5, 0.75, 1.00\}$, where each value represents the minimum proportion of similar options required to consider a question contaminated.

D Average Ranking Ordering Across Permutations

After we compute Mean Absolute Difference (MAD) for each models, we average the ranking to get the order of most similar permutations, shown in Table 3. These order reflect how similarly a model responds to different answer orderings.

To decide which permutation used for a certain percentage p, we iteratively eliminate one permutation from each highly similar pair. Specifically, we

Algorithm 2 `N-Gram` Detection Method

Input: Data $x = [q, o_1, o_2, ..., o_n]$; Model $\mathcal{M}$; Similarity threshold t; Leakage threshold T
Output: "L" (Leaked) or "NL" (Not Leaked)

```
1:  # Initialize count
2:  count ← 0
3:  for $i = 1$ to $n$ do
4:      # Construct prompt
5:      prompt ← $[q, o_1, o_2, ..., o_{i-1}]$
6:      # Generate prediction
7:      $\hat{o_i}$ ← $\mathcal{M}$(prompt)
8:      # Compute similarity score
9:      score ← ROUGE-L($\hat{o_i}$, $o_i$)
10:     if score ≥ t then
11:         count ← count + 1
12:     end if
13: end for
14: ratio ← count / $n$
15: if ratio ≥ $T$ then
16:     return "L"                ▷ Leaked
17: else
18:     return "NL"               ▷ Not Leaked
19: end if
```

remove the second permutation in the pair, assuming its behavior is already well-represented by the first. This process continues until the desired number of permutations, determined by a percentage threshold p, remains.

The final set of retained permutations for each threshold level p used in the `permutation-R` experiment is detailed in Table 4. This approach ensures that we retain a diverse set of permutations while minimizing redundant evaluation.

E Detailed Model Used in Experiment

Table 5 lists the LLMs used in our experiments. Each model is evaluated on both the MMLU and HellaSwag benchmarks. The models include Qwen (Qwen et al., 2025), Gemma (Team et al., 2024b), and LLaMA (Touvron et al., 2023). All models are accessed via Hugging Face (Wolf et al., 2020).

F Complete Detection Methods Performance Comparison

Table 6 presents the full comparison of detection method performance in different model and evaluation settings. This table provides a more detailed overview of each method's sensitivity in detecting leakage (`Recall`), as well as its effectiveness in identifying true leakage while minimizing false positives (`Precision`).

Permutation Pair	**Average Rank**
ACBD - ACDB	2.67
CDAB - CDBA	3.67
BACD - BCAD	4.67
CADB - CDAB	7.33
ACDB - ADBC	10.33
DBAC - DBCA	10.67
BACD - BADC	15.00
DCAB - DCBA	17.67
ACBD - ADBC	17.67
BDAC - BDCA	18.00
CBDA - CDBA	19.00
ADBC - ADCB	19.33
DBCA - DCBA	20.67
CBAD - CBDA	21.67
CABD - CBAD	24.33
CADB - CDBA	27.00
ACDB - ADCB	27.67
BADC - BCAD	28.33
DBCA - DCAB	33.00
DBAC - DCAB	34.00
ACBD - BACD	35.00
ACDB - BACD	36.67
CADB - CBDA	37.00
ADCB - DABC	41.00

Table 3: Top-24 average rank between permutation pairs in Qwen-7B, LLaMA-8B, and Gemma-7B, sorted in increasing order. Lower average rank indicate higher similarity.

G Experiment with Instruct Model

Besides the experiment with only using base models, we also apply the same procedure to an instruct model. Table 7 shows the performance comparison between base and instruct models. We can see that the `F1-score` in the instruct model mostly produces a larger score than the base model.

H Detailed Detection Methods' Pros & Cons

Table 8 summarizes the advantages and limitations of the leakage-detection methods discussed in this paper across four criteria: computation time, detection effectiveness, risk of misclassification, and compatibility with closed-weight models. Com-

Percentage (p)	Permutations Used
0	ABCD
10	ABCD, ABDC
20	ABCD, ABDC, ACBD, CABD
30	ABCD, ABDC, ACBD, BCDA, CABD, CADB, DBAC
40	ABCD, ABDC, ACBD, BCDA, BDAC, CABD, CADB, DACB, DBAC
50	ABCD, ABDC, ACBD, BACD, BCDA, BDAC, CABD, CADB, DABC, DACB, DBAC, DCAB
60	ABCD, ABDC, ACBD, BACD, BCDA, BDAC, CABD, CADB, CBAD, CBDA, DABC, DACB, DBAC, DCAB
70	ABCD, ABDC, ACBD, ADCB, BACD, BCDA, BDAC, BDCA, CABD, CADB, CBAD, CBDA, DABC, DACB, DBAC, DCAB
80	ABCD, ABDC, ACBD, ADCB, BACD, BADC, BCDA, BDAC, BDCA, CABD, CADB, CBAD, CBDA, DABC, DACB, DBAC, DBCA, DCAB, DCBA
90	ABCD, ABDC, ACBD, ADBC, ADCB, BACD, BADC, BCDA, BDAC, BDCA, CABD, CADB, CBAD, CBDA, CDAB, DABC, DACB, DBAC, DBCA, DCAB, DCBA
100	ABCD, ABDC, ACBD, ACDB, ADBC, ADCB, BACD, BADC, BCAD, BCDA, BDAC, BDCA, CABD, CADB, CBAD, CBDA, CDAB, CDBA, DABC, DACB, DBAC, DBCA, DCAB, DCBA

Table 4: Permutations used at each p percentage level for `permutation-R`.

Model (#Parameter)	Source
Qwen (0.5B)	`Qwen/Qwen2.5-0.5B`
Qwen (7B)	`Qwen/Qwen2.5-7B`
Gemma (7B)	`google/gemma-7b`
LLaMA (8B)	`meta-llama/Llama-3.1-8B`

Table 5: Model sources used in the experiments. All models are accessed via Hugging Face (Wolf et al., 2020).

Method	Metric	MMLU				HellaSwag			
		Qwen-0.5B	Qwen-7B	Gemma-7B	LLaMA-8B	Qwen-0.5B	Qwen-7B	Gemma-7B	LLaMA-8B
S	Recall	50.67	51.00	71.33	41.00	61.67	84.00	90.33	86.00
	Precision	61.79	64.29	66.05	65.78	60.06	57.01	58.53	57.21
	F1-Score	55.68	56.88	68.59	50.51	60.86	67.92	71.04	68.71
P	Recall	87.33	88.33	99.00	97.67	71.67	66.67	97.00	78.00
	Precision	78.68	70.86	74.62	73.07	93.48	93.02	95.41	94.35
	F1-Score	82.78	78.64	**85.10**	83.59	81.13	77.67	**96.20**	85.40
PR	Recall	88.00	88.67	99.00	98.33	74.00	67.33	97.33	79.33
	Precision	76.97	69.82	73.15	71.78	88.80	90.18	91.82	90.84
	F1-Score	82.12	78.12	84.14	82.98	80.73	77.10	94.50	84.70
PQ	Recall	99.33	98.67	100.00	100.00	97.00	85.00	99.00	100.00
	Precision	76.80	71.15	71.60	72.82	92.97	91.07	88.92	93.75
	F1-Score	86.63	**82.68**	83.45	**84.27**	94.94	87.93	93.69	96.77
N	Recall	98.67	98.00	100.00	99.67	99.67	92.33	100.00	100.00
	Precision	79.78	70.33	70.75	72.75	100.00	100.00	100.00	100.00
	F1-Score	**88.23**	81.89	82.87	84.11	**99.83**	**96.01**	**100.00**	**100.00**
S + PQ	Recall	100.00	99.67	100.00	100.00	97.67	97.00	100.00	100.00
	Precision	65.50	65.14	62.76	66.67	68.62	59.15	59.88	60.12
	F1-Score	79.16	78.79	77.12	80.00	80.61	73.48	74.91	75.09
S + N	Recall	99.00	99.67	100.00	99.67	100.00	99.67	100.00	100.00
	Precision	66.89	64.58	61.22	66.59	70.92	61.15	60.98	60.85
	F1-Score	79.84	78.37	75.95	79.84	82.99	75.79	75.76	75.66
PQ + N	Recall	100.00	99.67	100.00	100.00	100.00	99.33	100.00	100.00
	Precision	74.63	67.65	67.11	68.97	93.17	92.26	89.02	93.75
	F1-Score	85.47	80.59	80.32	81.63	96.46	95.67	94.19	96.77

Table 6: Detection performance (Recall, Precision, and F1-score) for various methods across different models and benchmarks. **Bold** scores represent the best F1-score among several leakage detection methods. The methods are coded as follows: S = Semi-half, P = Permutation, PR = Permutation-R, PQ = Permutation-Q, and N = N-Gram.

Method	MMLU		HellaSwag	
	Base	Instruct	Base	Instruct
Semi-half	55.68	76.67	60.86	69.92
Permutation	82.78	87.04	81.13	87.78
Permutation-R	82.12	85.84	80.73	86.74
Permutation-Q	86.63	87.55	94.94	95.01
N-Gram	88.23	88.79	99.83	100.00
Semi-half + Permutation-Q	79.16	80.92	80.61	80.65
Semi-half + N-Gram	79.84	81.87	82.99	82.64
Permutation-Q + N-Gram	85.47	85.67	96.46	95.85

Table 7: `F1-score` comparison across different detection methods between Qwen 0.5B base and instruct models on MMLU and HellaSwag datasets.

patibility with closed-weight models is crucial because many state-of-the-art LLMs do not release their weights, making certain detection methods unusable for their evaluation.

I Performance Changes under the Weak Definition of Leakage

In addition to analyzing performance changes based on the strong definition of leakage, we also examine the shifts that occur under the weak definition. Figure 9 presents the performance comparison on the original versus the cleaned dataset under the weak leakage definition.

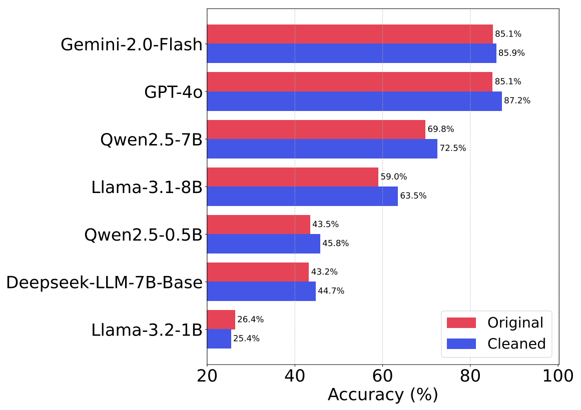
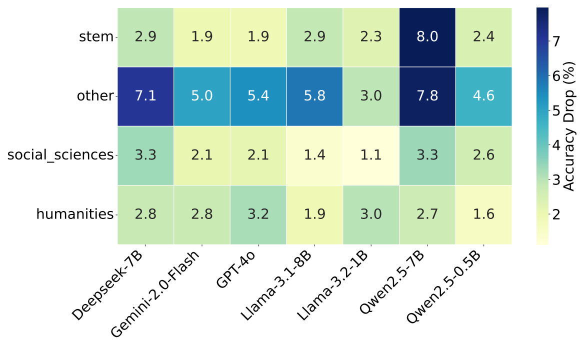


Figure 9: Comparison of model performance on original vs. cleaned MMLU benchmark based on weak definition of leakage.

After cleaning, GPT-4o ranks first, outperforming Gemini-2.0-Flash, while the ranking of the remaining models remains unchanged. Since no model achieves perfect accuracy on leaked instances, removing them leads to a reduction in the proportion of incorrect answers. Consequently, the overall accuracy of all models increases.

J Performance Varies Across Broader Subject Groups

Across broader subject groups (Figure 10), Qwen-7B's performance in the *STEM* group appears more affected, with an observed accuracy drop of up to 8%. All models also experience a decline in the *Other* category, with Qwen-7B again showing the most pronounced decrease.



	Deepseek-7B	Gemini-2.0-Flash	GPT-4o	Llama-3.1-8B	Llama-3.2-1B	Qwen2.5-7B	Qwen2.5-0.5B
stem	2.9	1.9	1.9	2.9	2.3	8.0	2.4
other	7.1	5.0	5.4	5.8	3.0	7.8	4.6
social_sciences	3.3	2.1	2.1	1.4	1.1	3.3	2.6
humanities	2.8	2.8	3.2	1.9	3.0	2.7	1.6

Figure 10: Performance drops by subject group for each model. Qwen-7B shows a marked drop in the STEM group. The 'Other' category exhibits the most performance decline overall.

Method	Computation Time	Detection Effectiveness	Misclassification Risk	Closed-Weight Compatible
Semi-half	Low ($O(n)$)	Low recall and precision	Weak at detecting leaked instances	Yes
Permutation	Very high ($O(n!)$)	Effective (F1-score $78\% - 96\%$)	May misclassify common option questions as leaked	No
Permutation-R	Medium–high ($O(p \cdot [n!])$)	Competitive with Permutation (F1-score $> 80\%$)	Same issue with the common option patterns	No
Permutation-Q	Moderate ($O(n^2)$)	Effective (F1-score $> 82\%$, up to 96% in HellaSwag); often better than original	Same issue with the common option patterns	No
N-Gram	Depends on token length ($O(m)$ where m is token count)	Very effective (F1-score $>$ 81%, up to 100% in HellaSwag)	Same issue with the common option patterns	Yes

Table 8: Comparison of leakage detection methods across key aspects.