DCLLM: Effects of Decontaminating a Contaminated LLM in Knowledge Distillation

Abstract

Knowledge Distillation (KD) allows larger "teacher" models to inform smaller "student" models that can mitigate the heavy computational demands of large language models (LLMs). LLMs are trained on extensive publicly available data, and they are susceptible to being "contaminated" through exposure to the evaluation data. Consequently, a contaminated teacher LLM can artificially inflate the performance of its student model in a KD setting. Although previous research has examined the efficacy of unlearning methods in removing undesirable information from LLMs and explored various KD approaches utilizing LLMs, the challenge of addressing contamination in teacher LLMs and minimizing the effects of such contamination on student models has been notably underexplored. In this work, we propose a novel framework, named DCLLM, that effectively evaluates the performance of a student LLM distilled by a contaminated teacher across different KD settings, decontaminates it utilizing a variety of unlearning algorithms, and further evaluates the student model's performance distilled by the decontaminated teacher. Our framework demonstrates that these unlearning methods effectively decontaminate the teacher and improve the performance of the distilled student model by up to 3% in terms of Rouge-L score.

1 Introduction

With the introduction of Large Language Models (LLMs), Knowledge Distillation (KD) (Bommasani et al., 2021; Mann et al., 2020; Chowdhery et al., 2023; Han et al., 2021; OpenAI, 2023) has emerged as a way of reducing the computational demand of LLMs (Hinton et al., 2015) by leveraging the intermediate hidden state and output distribution of the larger LLMs (i.e., teacher models) to inform smaller LLMs (i.e., student models) (Shirgaonkar et al., 2024).

A key challenge in KD using LLMs lies in selecting an appropriate teacher model, which is typically larger in terms of model parameters compared to the student model (Sanh et al., 2019; Wang et al., 2020). Given that LLMs are pretrained on a vast amount of data, they are vulnerable to being "contaminated" via exposure to the evaluation benchmark data (Huang et al., 2022; Carlini et al., 2022; Staab et al., 2023). A contaminated teacher model may contaminate its student model and, as a result, inflate the performance on the evaluation data.

Previous works (Kim and Rush, 2016; Song et al., 2020; Gu et al., 2024b; Chiang et al., 2023; Taori et al., 2023) explore how various KD approaches that leverage LLMs affect the performance on the evaluation data. The effect of a contaminated teacher model in evaluating a student model has also been explored (Mansurov et al., 2024). Moreover, a separate dimension of research area focuses on the efficacy of unlearning algorithms applied to LLMs (Maini et al., 2024; Yuan et al., 2024; Ji et al., 2024; Jia et al., 2024; Jin et al., 2024). However, to the best of our knowledge, no prior research has explored the performance of unlearning methods applied to a contaminated teacher model and how the decontaminated teacher model impacts the corresponding student model performance in a KD setting.

In this study, we introduce a novel framework named **DCLLM**, which evaluates a contaminated teacher model on the evaluation data and assesses the effectiveness of unlearning methods in decontaminating it. During fine-tuning, the teacher model is deliberately contaminated with data labeled as a forget set (Maini et al., 2024). In a KD setting, we distill the student model from the contaminated teacher. During decontamination, we utilize the forget set to evaluate the degree of decontamination achieved, while the retain set is employed to assess the model's performance on the data we wish to retain. Subsequently, we analyze

Figure 1: Illustration of DCLLM framework. We first contaminate an uncontaminated model using fine-tuning. Next, we apply unlearning methods on the contaminated model to decontaminate it.

the performance of the student model distilled by the decontaminated teacher on the evaluation data to investigate the effects of unlearning methods on it and whether there is any performance improvement.

We utilize DCLLM (illustrated in Figure 1), to evaluate teacher LLMs that range from 3B to 8B dimensions, employing an instruction-following approach that covers a diverse range of downstream NLP tasks, including brainstorming, classification, closed QA, creative writing, general QA, information extraction, open QA, and summarization. We utilize LLaMA (Touvron et al., 2023), as it is one of the most widely adopted open-source LLMs in practice. We evaluate the performance of LLaMA3-1B as a student model and LLaMA3-3B and 8B as teacher models, on four evaluation datasets utilizing Rouge-L (Lin, 2004), a lexical similarity metric, and BERTScore (Zhang et al., 2019), an embedding-based similarity metric. Our experiments indicate that (1) unlearning methods, such as Gradient Ascent, Direct Preference Optimization (DPO) (Rafailov et al., 2023), and Negative Preference Optimization (NPO) (Zhang et al., 2024), are effective in decontaminating the teacher model across all the evaluation datasets. (2) Notably, in a KD setting, NPO decontaminates the teacher model, and the decontaminated teacher generates a better-quality decontaminated student, which outperforms the directly and indirectly contaminated (through distillation from a contaminated teacher) student by approximately 3% in terms of Rouge-L.

2 Related Work

2.1 Large Language Models (LLMs)

Since their emergence, Large Language Models (LLMs) (Mann et al., 2020; OpenAI, 2023; Chowdhery et al., 2023; Anil et al., 2023; Thoppilan et al., 2022) have consistently outperformed previous state-of-the-art methods in all downstream NLP tasks by leveraging conditional text generation. Recent research involving LLMs has employed an instruction-following approach (Wei et al., 2021; Sanh et al., 2021; Chung et al., 2024) or incorporated human feedback (Bai et al., 2022; Ouyang et al., 2022) to enhance text generation and develop intelligent assistants (OpenAI, 2022, 2023; Touvron et al., 2023). Moreover, significant efforts have been made to inspire research and development in this domain, utilizing open-source LLMs (Biderman et al., 2023; Touvron et al., 2023; Zhang et al., 2022). However, one of the key challenges in deploying LLMs is their substantial computational cost due to their considerable model size (Wei et al., 2022; Kaplan et al., 2020). Consequently, researchers often seek computation-efficient methods (Hu et al., 2022; Han et al., 2024; Dettmers et al., 2023) when working with these models.

2.2 Knowledge Distillation

To address the heavy computational demands associated with LLMs, researchers employ knowledge distillation (KD) techniques (Hinton et al., 2015). These methods transfer knowledge from a

larger teacher model to a smaller student by harnessing the intermediate hidden states (Sun et al., 2019; Jiao et al., 2019) and output distributions of a teacher (Liang et al., 2020; Song et al., 2020; Zhang et al., 2023). This process enhances the performance of a student model, which is smaller in terms of parameters, while maintaining efficiency and performance that approaches that of the teacher (Gou et al., 2021; Rusu et al., 2015; Sanh et al., 2019). Previous studies have demonstrated that KD approaches utilizing forward KL divergence (Sanh et al., 2019), often referred to as *forward KD*, show effectiveness in text classification and generation tasks (Taori et al., 2023; Peng et al., 2023; Chiang et al., 2023; Kim and Rush, 2016). KD approaches that utilize reverse KL divergence (Gu et al., 2024b), referred to as *reverse KD*, show superior performance in instruction-tuned text generation (Chen et al., 2018; Huszár, 2015; Ji et al., 2023; Nowozin et al., 2016).

2.3 Machine Unlearning

Early machine unlearning efforts focus on text classification (Bourtoule et al., 2021), and prominent unlearning algorithms aim to optimize model parameters to remove the influence of targeted data (Jang et al., 2022; Maini et al., 2024; Yuan et al., 2024; Zhang et al., 2024; Jia et al., 2024; Yao et al., 2024; Wang et al., 2025; Li et al., 2024; Ishibashi and Shimodaira, 2023; Gu et al., 2024a; Lu et al., 2024; Tian et al., 2024; Liu et al., 2024; Tamirisa et al., 2024). These approaches rely on a predefined forget set, which is used to fine-tune the model so that it will *unlearn* the specified information. To the best of our knowledge, no prior work has investigated the effectiveness of unlearning algorithms when applied to a contaminated teacher model within KD for the purpose of assessing the impact on student models.

3 Methodology

In our proposed framework, DCLLM, we utilize an LLM that samples a response, y, containing T tokens from the probability distribution, p_x, conditioned on the prompt, x. To explore KD, we employ open-source LLMs so that we can leverage the intermediate hidden state and output distribution from a teacher LLM, contributing to richer knowledge sharing (Zhang et al., 2022; Touvron et al., 2023) with a potential student LLM.

3.1 Knowledge Distillation (KD) Methods

We evaluate DCLLM using two widely adopted KD approaches for LLMs: one that minimizes the forward Kullback-Leibler (KL) divergence and the other that minimizes the reverse KL divergence.

3.1.1 KD with Forward KL divergence

Traditional KD methods employ minimizing the forward KL divergence as the optimization problem. This involves calculating the divergence between the output distribution of the student model, $q_\phi(y|x)$, and that of the teacher model, $p(y|x)$, where ϕ denotes the parameters of the student model. This method is commonly referred to as *forward KD* and mathematically expressed as follows:

$$KL[p||q_\phi] = \mathbb{E}_{x \sim p, y \sim p'}[\log \frac{p(y|x)}{q_\phi(y|x)}] \quad (1)$$

where p' denotes the distribution of the data.

3.1.2 KD with Reverse KL divergence

Gu et al. proposed MiniLLM (Gu et al., 2024b), a novel approach to KD, especially for the task of text generation. MiniLLM minimizes the divergence between the output distributions of the teacher model, $p(y|x)$, and that of the student model, $q_\phi(y|x)$, utilizing reverse KL divergence. Therefore we refer to it as *reverse KD*. The authors argued that forward KD performs better in classification tasks due to a relatively simple output space compared to that of text generation tasks. This approach can be mathematically formulated as follows:

$$\phi = argmin_\phi KL[q_\phi||p]$$
$$= argmin_\phi(-\mathbb{E}_{x \sim p, y \sim p'}[\log \frac{p(y|x)}{q_\phi(y|x)}]) \quad (2)$$

3.2 Unlearning Methods

We selected unlearning-finetuning as our preferred method for unlearning, as it is most widely adopted and focuses on optimizing the parameters (Yao et al., 2024; Maini et al., 2024; Zhang et al., 2024; Liu et al., 2024; Jia et al., 2024; Jin et al., 2024). Through parameter optimization, unlearning-finetuning effectively modifies the internal state of the model selected for unlearning.

We evaluate the efficacy of unlearning on both the target data that we aim to unlearn, termed as

forget set, D_F, using forget loss and the data that we want to retain, termed as retain set, D_R, using retain loss.

3.2.1 Forget Loss

Unlearning can be targeted or untargeted. Targeted unlearning involves training the model to output the desired answers. For targeted unlearning, we select Direct Preference Optimization (DPO).

- **Direct Preference Optimization (DPO):** When evaluating the DPO (Rafailov et al., 2023) loss on the forget set, D_F, it treats the samples in D_F as negative and the sample rejection answers are treated as positive. This can be mathematically formulated as follows:

$$L_{NPO}(D_F; \phi) = -\frac{2}{\omega}\mathbb{E}_{(x,y)\sim D_F}$$
$$[log\sigma(\omega \log \frac{p(y|x;\phi)}{p(y|x;\phi_{ref})})] \quad (3)$$

  Here, ω represents a hyperparameter, σ represents a sigmoid function, and ϕ_{ref} represents the reference model prior to unlearning.

  On the other hand, in case of untargeted unlearning, the behavior of the unlearned model on the forget set remains uncertain. For untargeted unlearning, we adopt the following two methods:

- **Gradient Ascent (GA):** The optimization of gradient ascent is fundamentally the opposite of the training objective, as it maximizes the prediction loss of the forget set. It can be mathematically formulated as follows:

$$L_{GA}(D_F; \phi) = \frac{1}{D_F}\sum_{x\in D_F} l(x, \phi) \quad (4)$$

  Here, the loss on an instance $x \in D_F$ is denoted by $l(x, \phi)$.

- **Negative Preference optimization (NPO):** NPO (Zhang et al., 2024) addresses the challenge of unlearning by treating the samples in the forget set as negative ones, while ignoring the positive component of Direct Preference Optimization (DPO) (Rafailov et al., 2023) loss. This can be mathematically formulated as follows:

$$L_{NPO}(D_F; \phi) = -\frac{2}{\omega}\mathbb{E}_{(x,y)\sim D_F}$$
$$[log\sigma(-\omega \log \frac{p(y|x;\phi)}{p(y|x;\phi_{ref})})] \quad (5)$$

3.2.2 Regularization Loss

While the forget loss addresses the task of unlearning, it is equally important to maintain the performance on the retain set, D_R. The regularization loss is calculated on D_R to ensure that the overall unlearning framework preserves the model utility. We select the traditional gradient descent (GD) for evaluating the regularization loss.

- **Gradient Descent (GD):** GD is performed on D_R while observing the prediction loss during training.

$$L_{GD}(D_R; \phi) = \mathbb{E}_{(x,y)\sim D_R}[- \log p(y|x;\phi)] \quad (6)$$

With three variations of forget loss and a regularization loss, we experiment with three variations of the unlearning method: GA with GD, NPO with GD, and DPO with GD.

4 Experimental Evaluation

4.1 Data

We evaluate DCLLM using the databricks-dolly-15k[1] dataset, containing approximately 15k instruction-following samples spanning eight downstream NLP tasks: brainstorming, classification, closed QA, creative writing, general QA, information extraction, open QA, and summarization. We partition the dataset into 500 samples for testing, 1000 for validation, and the remainder for training. The distribution of the training data across tasks is illustrated in Figure 2.

Additionally, we evaluate the trained model on three additional test datasets to ensure a robust assessment of the framework.

- **Self-Instruct (Wang et al., 2022a):** Self-Instruct comprises 252 instruction-following samples in the test set.

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[1]https://huggingface.co/datasets/databricks/databricks-dolly-15k

Figure 2: Task distribution of `databricks-dolly-15k` training data.

- **S-NI (Wang et al., 2022b):** Super-NaturalInstructions consists of approximately 9,000 test samples of 119 diverse topics. For our framework evaluation, we focus on samples that are longer than ten tokens.

- **Vicuna (Chiang et al., 2023):** Vicuna constitutes 80 instruction-response pairs, adding complexity to the task.

Further details about the test data distribution are shown in Appendix Section E.

4.2 KD Evaluation Metrics

We utilize two metrics to determine lexical similarity and embedding-level similarity. For lexical similarity, we use the standard Rouge-L metric, and for embedding-level similarity, we select BERTScore.

- **Rouge-L (R-L):** Rouge-L (Lin, 2004), denoted by $Rouge - L(\hat{y}, y)$, measures the similarity between the model predictions, y and the gold labels, $\hat{y}$, at the word-level. This metric is applied in the evaluation of both KD and unlearning performance.

- **BERTScore (BS):** Without restricting our evaluation at the word-level, we utilize BERTScore (BS) (Zhang et al., 2019), to capture the inherent semantic similarity of the samples with more precision, especially in text generation. BS leverages a pre-trained transformer model (Vaswani et al., 2017), BERT, (Devlin et al., 2019) to calculate the sample embedding.

4.3 Experimental Setup

We follow the MiniLLM (Gu et al., 2024b) experimental configuration for evaluating the KD approaches and the TOFU benchmark (Maini et al., 2024) for the unlearning methods. We conduct our experiments on two KD model configuration, where we utilize LLaMA3-3B and LLaMA3-8B (Touvron et al., 2023) as the teacher models, and LLaMA3-1B as the student model. For forward KD evaluation, we fine-tune the student model with supervision from the output distribution of the teacher model. For KD with reverse KL divergence, we follow the experimental configuration set by (Gu et al., 2024b).

During the unlearning experiments, we treat all the "closed QA" examples of `databricks-dolly-15k` train split as the forget set and the rest as the retain set. For each instance in the forget set, we leverage the `LLaMA3-8B-Instruct` model to generate a paraphrased version of the instruction-response pair, which represents the same question and answer with different words. Moreover, we construct five different perturbed versions of the response that are structurally similar but factually incorrect, so that we can measure the truth ratio (TR) as mentioned in Section C.1. We list our complete hyperparameter setting in the Appendix Section A.

5 Results and Analysis

We present our evaluation of DCLLM in two distinct phases, including training evaluation and test evaluation.

5.1 Training Set Evaluation

We evaluate both the teacher models (LLaMA3-3B and LLaMA3-8B) and the student model (LLaMA3-1B) in the zero-shot and fine-tuning settings. During fine-tuning the student model, we fine-tune it with the data, including the retain and forget set. During fine-tuning the teacher models, once we fine-tune them with only the retain set data, and in another setting, we fine-tune them with both the retain and forget sets. When distilling the student model from the teacher model, we contaminate the teacher model such that the forget set is exposed during training. As illustrated in Table 1, in the case of all the unlearning methods, when combined with GD as a regularization loss in forward and reverse KD settings, the performance of the student

#Parameters	Method	Dolly	
		R-L	BS
Student:1B	Zero-Shot	8.91	41.99
	Finetuned with forget set	86.97	93.05
Teacher:3B	Zero-Shot	11.52	45.53
	Finetuned with forget set	88.75	93.95
	Finetuned w/o forget set	84.57	91.53
	(DPO+GD)	32.15	61.79
	(NPO+GD)	34.80	64.11
	(GA+GD)	34.75	64.15
Teacher:8B	Zero-Shot	12.87	44.86
	Finetuned with forget set	89.43	94.32
	Finetuned w/o forget set	85.50	92.01
	(DPO+GD)	8.96	40.86
	(NPO+GD)	8.98	40.92
	(GA+GD)	8.95	40.80
Student Model distilled by Contaminated Teacher			
Teacher:3B	FKD	86.62	92.86
Student:1B	RKD	84.68	91.89
Teacher:8B	FKD	86.83	92.97
Student:1B	RKD	85.61	92.32
Student Model distilled by Decontaminated Teacher using (DPO+GD)			
Teacher:3B	FKD	85.61	92.30
Student:1B	RKD	83.28	91.09
Teacher:8B	FKD	21.44	54.52
Student:1B	RKD	8.81	34.79
Student Model distilled by Decontaminated Teacher using (NPO+GD)			
Teacher:3B	FKD	85.11	92.08
Student:1B	RKD	83.74	91.37
Teacher:8B	FKD	21.49	54.47
Student:1B	RKD	9.13	35.08
Student Model distilled by Decontaminated Teacher using (GA+GD)			
Teacher:3B	FKD	85.03	92.04
Student:1B	RKD	83.49	91.25
Teacher:8B	FKD	21.30	54.42
Student:1B	RKD	8.74	34.79

Table 1: Evaluation on Train set. R-L and BS stand for Rouge-L scores and BERTScores, respectively. The methods FKD and RKD refer to Forward Knowledge Distillation and Reverse Knowledge Distillation, respectively.

model LLaMA3-1B, distilled by the decontaminated teacher LLaMA3-3B, is reduced compared to that of a student distilled by the contaminated teacher. This indicates that these methods are effective both in decontaminating the teacher model and preserving the true model's performance across different KD settings.

5.2 Evaluation on Test Data

We evaluate both the contaminated and decontaminated models across four different challenging variations of test data to measure the robustness of our overall framework. We observe in Table 2 that almost all the unlearning algorithms have a significant impact on the test set performance. We notice a significant decline in the teacher model's performance after unlearning, indicating the efficacy of these approaches in decontamination.

On the contrary, NPO substantially reduces the contamination exposure, while improving the performance on the remaining data. In both the forward and reverse KD settings, the student (LLaMA3-1B) model distilled by the decontaminated teacher (LLaMA3-3B), leveraging NPO, outperforms the directly contaminated student on the S-NI data by 1.99% and 3.36%, respectively, and performs comparably on the rest of the data in terms of Rouge-L score. The student LLaMA3-1B distilled by the decontaminated (using NPO) LLaMA3-3B in the forward KD setting improves upon the student with the contaminated teacher in the same setting on most test datasets. Furthermore, in the reverse KD setting, the same decontaminated teacher enhances the student model's Rouge-L score over the contaminated teacher by 1.27% and 2.41% on the Dolly and S-NI data, respectively, while maintaining comparable performance on the remaining test data. Additionally, in both KD settings, the student LLaMA3-1B model distilled by the decontaminated LLaMA3-3B teacher, leveraging DPO, demonstrates superior performance compared to the directly contaminated student on the S-NI data by 1.08% and 2.09%, respectively, in the Rouge-L metric. Similarly, GA, when employed to decontaminate the LLaMA3-3B model, performs comparably in all the experimental settings. We conduct a paired bootstrap test to determine whether the performance improvement of student model LLaMA3-1B distilled by the decontaminated LLaMA3-3B using various unlearning methods is significant compared to the fine-tuned student. As we can observe in Figure 3, almost

#Parameters	Method	Dolly R-L	Dolly BS	Self-Instruct R-L	Self-Instruct BS	S-NI R-L	S-NI BS	Vicuna R-L	Vicuna BS
Student:1B	Zero-Shot	9.08	42.50	6.81	40.62	8.39	39.35	14.37	50.98
	Finetuned with forget set	28.51	61.29	18.88	52.25	29.10	56.01	18.33	57.85
Teacher:3B	Zero-Shot	12.22	46.55	10.37	44.18	13.48	44.07	17.77	56.66
	Finetuned with forget set	31.11	62.87	21.98	54.27	33.27	59.89	18.60	58.35
	Finetuned w/o forget set	30.40	62.32	22.69	55.35	35.04	59.50	18.64	58.42
	(DPO+GD)	12.61	49.23	8.26	44.53	8.48	42.65	17.10	55.29
	(NPO+GD)	14.65	50.60	10.06	46.09	12.33	46.75	19.30	56.14
	(GA+GD)	14.62	50.54	10.00	46.06	12.36	46.73	19.23	56.00
Teacher:8B	Zero-Shot	12.70	45.22	12.35	45.05	16.41	46.70	16.53	54.10
	Finetuned with forget set	30.65	61.67	23.00	55.23	32.91	59.10	19.50	59.00
	Finetuned w/o forget set	30.95	62.36	23.42	56.29	35.37	59.25	20.12	59.22
	(DPO+GD)	9.25	41.77	7.94	41.99	8.94	39.52	16.23	52.88
	(NPO+GD)	9.24	41.68	7.95	42.13	8.95	39.43	16.25	53.01
	(GA+GD)	9.22	41.21	7.88	41.82	8.99	39.80	16.21	52.70
Student Model distilled by Contaminated Teacher									
Teacher:3B	FKD	28.20	60.94	19.40	51.72	30.29	56.43	17.93	56.92
Student:1B	RKD	27.44	60.13	19.08	53.11	30.05	56.88	18.20	57.81
Teacher:8B	FKD	28.19	60.56	19.59	52.44	30.00	56.35	17.54	57.08
Student:1B	RKD	28.22	60.74	18.68	51.70	29.74	56.58	17.14	56.62
Student Model distilled by Decontaminated Teacher using (DPO+GD)									
Teacher:3B	FKD	**28.88**	60.92	17.84	51.30	30.18	56.39	17.19	56.30
Student:1B	RKD	**28.27**	**60.77**	19.07	52.85	**31.19**	55.82	17.71	57.47
Teacher:8B	FKD	16.71	51.52	11.09	46.26	16.97	47.92	16.18	55.14
Student:1B	RKD	8.82	35.17	6.57	35.56	8.71	32.55	10.82	43.35
Student Model distilled by Decontaminated Teacher using (NPO+GD)									
Teacher:3B	FKD	**28.86**	**61.10**	19.71	**52.27**	**31.09**	**57.30**	17.09	56.70
Student:1B	RKD	**28.71**	**60.80**	18.85	51.95	**32.46**	56.61	16.91	56.95
Teacher:8B	FKD	16.24	51.30	10.74	45.89	16.56	47.81	16.11	54.32
Student:1B	RKD	8.71	35.21	6.77	35.89	10.25	33.78	11.06	43.68
Student Model distilled by Decontaminated Teacher using (GA+GD)									
Teacher:3B	FKD	**28.51**	60.95	19.67	51.98	**30.81**	**56.69**	16.81	56.36
Student:1B	RKD	**28.69**	**60.80**	19.52	52.69	29.55	56.32	16.09	55.86
Teacher:8B	FKD	16.04	51.24	11.68	46.22	16.73	47.77	15.67	53.97
Student:1B	RKD	8.56	35.11	6.42	35.54	9.43	33.39	9.38	41.90

Table 2: Evaluation on Test set. R-L and BS stand for Rouge-L scores and BERTScores, respectively. The methods FKD and RKD refer to Forward Knowledge Distillation and Reverse Knowledge Distillation, respectively. We bold-face a score if a KD approach with a student model distilled by a decontaminated teacher has outperformed the same student distilled by the contaminated teacher, and underline a score if it improves the corresponding directly contaminated student model.

all the distilled student models' improvement is statistically significant. Further details about this test are listed in the Appendix Section D.

We further observe in Table 5 that, when evaluating on the Dolly data in a forward KD setting, the student model LLaMA3-1B distilled by the decontaminated teacher LLaMA3-3B, leveraging NPO, improves the student model distilled by the con-

Figure 3: Pairwise Bootstrap Testing to compare student models distilled by decontaminated teacher models with the directly contaminated (fine-tuned) student model. DPO_FKD_LLaMA3_1B_3B, DPO_RKD_LLaMA3_1B_3B, NPO_FKD_LLaMA3_1B_3B, NPO_RKD_LLaMA3_1B_3B, GA_FKD_LLaMA3_1B_3B, GA_RKD_LLaMA3_1B_3B represent LLaMA3-1B distilled by decontaminated LLaMA3-3B using DPO in forward KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using DPO in reverse KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using NPO in forward KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using NPO in reverse KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using GA in forward KD, and LLaMA3-1B distilled by decontaminated LLaMA3-3B using GA in reverse KD, respectively.

taminated teacher across a range of tasks, specifically classification by 3.15% and summarization by 1.81%, while performing comparably on the remaining topics. Moreover, the Rouge-L score in the closed QA task is reduced by 5.10%, indicating that NPO effectively decontaminates the teacher model from data of similar distribution. This clearly demonstrates that the contamination transferred from the contaminated teacher model to the student has been significantly reduced. One potential reason for NPO's superior performance may be that the unlearning experimental setup favored the method, allowing it to clearly discern between positive and negative samples, while minimizing data interference with the model's pre-trained knowledge.

6 Conclusion

In this paper, we introduce DCLLM, a novel framework that effectively assesses the impact on a student model that learns from the teacher through KD and evaluates most commonly used unlearning methods to decontaminate a teacher model exposed to contamination during fine-tuning. Our research demonstrates that most of the unlearning methods show a lot of promise in decontamination. Upon further analysis, we observe that the student model distilled by the decontaminated teacher, leveraging NPO as an unlearning method, outperforms the student distilled by the contaminated teacher in unlearning contamination while maintaining model utility. Moreover, the student model distilled by the decontaminated teacher with NPO improves the directly contaminated student model prediction by around 2-3% across all the evaluation data, demonstrating the robustness of the decontaminated model. We strongly believe that our experiments will motivate a new research dimension and encourage researchers to explore this area extensively.

Limitations

Although we are the pioneers for exploring the decontamination effects within a contaminated teacher model and have introduced a novel framework, DCLLM, to assess the effectiveness of unlearning algorithms, our work has two significant limitations.

- We selected LLaMA as our primary open-source LLM to evaluate the performance of DCLLM. In the future, we intend to expand our framework to include support for further open-source LLMs during evaluation.

- During the unlearning phase, we employed DPO as our only targeted unlearning method. We intend to evaluate our framework with other targeted unlearning techniques to enhance its robustness.

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A Training Details

A.1 Knowledge Distillation Experiments

During the knowledge distillation (KD) phase, we conduct our experiments across different settings, ranging from zero-shot, fine-tuned, world-level KD, and KD utilizing reverse KL divergence. For models $> 1B$, the fine-tuned and KD experiments are conducted on four NVIDIA A100 40GB GPUs, using DeepSpeed with ZeRO2 to reduce memory footprints. In case of forward KD, we adopt the approach outlined in (Gu et al., 2024b), mixing the distillation loss equally with the supervised language modeling loss based on the gold labels. The final checkpoints for each setting are chosen according to the Rouge-L scores from the validation set. Further hyperparameter details are listed in Table 3.

Hyperparameters	Value
No. of Epochs	10
Training Batch Size	[32, 64]
Learning Rate	$[5X10^{-6}, 1X10^{-5}, 5X10^{-5}]$

Table 3: Hyperparameters used in the knowledge distillation (KD) experiments. For all models, we select the best learning rate and batch size from the given range.

A.2 Unlearning Experiments

During the unlearning phase, all experiments are conducted using two NVIDIA A100 GPUs with 40GB of memory. We follow the TOFU (Maini et al., 2024) repository and utilize DeepSpeed with ZeRO3 to reduce memory footprints. During the unlearning process, we apply a linear warm-up learning rate in the first epoch, followed by a linearly decaying learning rate in the later epochs. Both the α and β parameters are set to 0.1. We provide additional hyperparameter details in Table 4.

B Task-wise Evaluation on Test Data

We provide a detailed task-wise evaluation of `databricks-dolly-15k` test data in different settings in Table 5. When evaluating the Dolly data, we can observe that decontaminated LLaMA3-3B utilizing NPO improves the fine-tuned LLaMA3-1B prediction across a range of tasks, with a 0.99% increase in brainstorming and a 1.21% increase in

Hyperparameters	Value
No. of Epochs	5
Training Batch Size	32
Learning Rate	$1X10^{-5}$
Optimizer	AdamW
Weight Decay	0.01
β	0.1
α	0.1

Table 4: Hyperparameters used in the unlearning experiments.

open QA. Moreover, the decontaminated LLaMA3-3B model, utilizing DPO and GA, outperforms the corresponding fine-tuned student model in brainstorming, information extraction, and open QA across all the KD settings.

C Evaluation on Unlearning

C.1 Unlearning Evaluation Metrics

To evaluate the performance of the unlearned model, we follow the "TOFU: A Task of Fictitious Unlearning for LLMs" (Maini et al., 2024), which effectively assesses unlearning by accounting for the different generation behaviors of the model. Moreover, we leverage three additional metrics (Yuan et al., 2024) for an adequate evaluation of the unlearned model utilizing the forget set, D_F, and the retain set, D_R.

- **Probability (P):** We compute the conditional probability, $P(y|x)$, where given an instruction, x, the probability that the model outputs a correct answer, y_c can be calculated as:

$$P(y|x) = \frac{P(y_c|x)}{\sum_{i=1}^{n} P(y_i|x)} \qquad (7)$$

- **Rouge (R-L):** We use the standard Rouge-L metric as mentioned before in 4.2.

- **Truth Ratio (TR):** Truth ratio calculates the likelihood ratio of the answer being correct compared to an incorrect one. Since we train our model based on a particular phrasing of the gold label, it is possible for the model to assign a higher probability weight to that version compared to others. Given y_{pert} be a set of perturbed versions of the gold label, and $\tilde{y}$ be the paraphrased version of the gold label, we can compute the truth ratio as follows:

#Parameters	Method	BST	CLF	CQA	CW	GQA	IE	OQA	SM
Student:1B	Zero-Shot	6.83	8.96	7.59	11.25	10.95	8.61	7.95	14.65
	Finetuned with forget set	19.68	59.54	38.82	18.43	17.42	35.11	20.73	37.71
Teacher:3B	Zero-Shot	10.47	11.16	14.65	12.49	13.11	12.35	11.84	14.72
	Finetuned with forget set	21.53	59.89	40.70	17.98	17.29	38.31	27.76	38.50
	Finetuned w/o forget set	20.82	56.93	39.62	18.76	17.38	30.47	25.92	38.05
	(DPO+GD)	10.60	12.07	13.06	16.94	13.30	13.38	10.82	20.44
	(NPO+GD)	12.24	14.10	16.69	18.03	15.71	14.96	12.24	24.76
	(GA+GD)	12.12	14.27	16.39	17.82	15.58	14.90	12.23	25.14
Teacher:8B	Zero-Shot	10.71	13.68	17.42	11.68	11.85	14.92	11.90	14.93
	Finetuned with forget set	22.19	60.14	42.73	17.53	16.96	33.10	26.09	40.39
	Finetuned w/o forget set	23.27	59.24	41.05	18.46	17.07	37.57	23.70	40.17
	(DPO+GD)	7.85	7.28	9.49	12.14	11.08	10.65	8.15	13.12
	(NPO+GD)	7.84	7.26	9.51	12.08	11.07	10.62	8.11	13.15
	(GA+GD)	7.83	7.23	9.58	12.05	10.99	10.59	8.08	13.11
Contaminated									
Teacher:3B	FKD	19.98	55.41	44.00	18.23	16.15	35.79	21.46	35.87
Student:1B	RKD	18.92	54.83	40.67	17.16	17.47	34.54	20.14	34.89
Teacher:8B	FKD	18.11	57.29	39.92	17.86	16.42	30.63	22.47	40.08
Student:1B	RKD	18.50	57.11	43.98	18.66	17.03	36.41	20.57	36.06
Decontaminated with (DPO+GD)									
Teacher:3B	FKD	**21.46**	**56.26**	41.40	16.95	**16.93**	**35.81**	**22.34**	**39.37**
Student:1B	RKD	**19.80**	**57.86**	39.95	**17.37**	17.25	33.19	**21.31**	**36.60**
Teacher:8B	FKD	10.48	28.25	21.99	14.07	14.44	21.29	13.61	17.23
Student:1B	RKD	6.04	9.64	12.16	6.38	8.30	9.18	8.90	12.76
Decontaminated with (NPO+GD)									
Teacher:3B	FKD	**20.67**	**58.56**	38.90	17.33	**16.88**	33.64	**21.94**	**37.68**
Student:1B	RKD	**20.42**	**57.27**	40.52	**17.34**	16.86	34.33	**22.32**	**38.95**
Teacher:8B	FKD	10.72	26.88	19.44	12.53	14.28	15.09	14.30	19.54
Student:1B	RKD	5.75	8.24	11.28	7.64	8.02	10.99	7.48	21.54
Decontaminated with (GA+GD)									
Teacher:3B	FKD	**20.00**	56.33	41.30	18.07	**16.90**	35.93	**22.36**	35.38
Student:1B	RKD	**20.00**	**57.99**	**41.07**	16.12	16.30	**36.76**	**22.52**	**36.60**
Teacher:8B	FKD	10.59	26.98	20.66	12.96	13.57	15.88	13.71	18.85
Student:1B	RKD	6.15	8.87	9.33	6.53	8.15	11.11	8.35	14.73

Table 5: Task-wise Rouge-L Score of test split on `databricks-dolly-15k` data. BST, CLF, CQA, CW, GQA, IE, OQA, and SM represent Brainstorming, Classification, Closed QA, Creative Writing, General QA, Information Extraction, Open QA, and Summarization, respectively, which are the eight tasks of Dolly data. We bold-face a score if a KD approach with a decontaminated teacher model has outperformed that of the contaminated one, and underline a score if it improves the corresponding fine-tuned student model.

$$TR = \frac{\frac{1}{|y_{pert}|} \sum_{y_c \in y_{pert}} P(y_c|x)^{\frac{1}{|y_c|}}}{P(\tilde{y}|x)^{\frac{1}{|\tilde{y}|}}} \quad (8)$$

- **Token Entropy (TE):** One common issue observed is that an unlearned model often generates tokens that lack meaning, even after generating the correct prediction. The token entropy (TE) considers the diversity of tokens

#Parameters	Method	R-L	P	TR	TE	CS	ES	FE	MU
	Forget Set								
	(DPO+GD)	0.44	9.06	40.93	100.00	6.05	0.00	88.70	-
	(NPO+GD)	25.73	0.96	61.59	92.83	54.96	8.65	69.62	-
	(GA+GD)	0.00	0.00	29.06	0.00	9.45	0.00	92.30	-
LLaMA3-3B	Retain Set								
	(DPO+GD)	1.14	8.23	33.51	95.42	7.06	1.67	-	3.37
	(NPO+GD)	23.95	1.66	41.68	87.92	60.36	23.67	-	18.27
	(GA+GD)	0.00	0.00	14.51	0.00	9.38	0.00	-	0.00
	Forget Set								
	(DPO+GD)	30.63	9.38	44.76	67.06	36.31	8.65	74.05	-
	(NPO+GD)	38.09	2.49	55.42	61.34	50.45	9.62	68.79	-
	(GA+GD)	0.00	0.00	65.41	100.00	9.45	0.00	85.03	-
LLaMA3-8B	Retain Set								
	(DPO+GD)	28.15	6.55	34.74	70.71	45.19	44.00	-	33.15
	(NPO+GD)	31.88	2.69	42.22	65.01	55.83	36.00	-	25.93
	(GA+GD)	0.00	0.00	33.88	90.00	9.38	0.00	-	0.00

Table 6: Evaluation of unlearning methods on the forget set and retain set. R-L, P, TR, TE, CS, ES, FE, and MU stand for Rouge-L score, Probability, Truth Ratio, Token Entropy, Cosine Similarity, Entailment Score, Forget Efficacy, and Model Utility, respectively.

within the model prediction. If a model prediction, y, contains T unique tokens and C_{y_i} denotes the unique token y_i's frequency, then we can define TE as follows:

$$TE = \frac{-\sum_{i=1}^{T} C_{y_i} \log_2 C_{y_i}}{\log_2 |C_\phi|} \quad (9)$$

- **Cosine Similarity (CS):** Cosine similarity (CS) is measured by computing the semantic similarity of the predictions before and after the unlearning method is applied. To determine the sample semantic similarity to the gold label, we employ Sentence-BERT (Reimers and Gurevych, 2019) to extract the sample embedding and then calculate the CS.

- **Entailment Score (ES):** Entailment Score (ES) measures the factual accuracy of the model prediction against the corresponding gold labels for a set of questions. We utilize a pretrained Natural Language Inference (NLI) model (Sileo, 2023) that predicts the entailment relationship between the model prediction and the corresponding gold label for each set of questions. The final ES is derived by calculating the ratio of the "entailment" relationship across all samples.

Finally, we aggregate all the above unlearning metrics into a single one to determine the forget efficacy and the model utility, measuring performance on the forget set and retain set, respectively.

- **Forget Efficacy (FE):** Forget Efficacy (FE) measures the quality of unlearning on the forget set. We calculate FE by taking the arithmetic mean of all the above metrics and then subtracting this mean from 1.

$$FE = 1 - Mean(P, R-L, \\ TR, TE, CS, ES) \quad (10)$$

- **Model Utility (MU):** Model Utility (MU) measures the overall quality of the unlearning process. Hence, it optimizes the model prediction, ensuring that none of the associated metrics yield values approaching zero. We calculate MU on the retain set simply by taking the harmonic mean of the previously mentioned metrics.

$$MU = HarmonicMean(P, R-L, \\ TR, TE, CS, ES) \quad (11)$$

C.2 Unlearning Evaluation

We evaluate the performance of the unlearning algorithms in terms of their effectiveness in decontamination. We observe in Table 6 that all the

Figure 4: Bootstrap Distribution Plot

unlearning algorithms demonstrate strong performance on the forget set. However, except for NPO, no other unlearning algorithms exhibit significant performance in terms of model utility, indicating they struggle to preserve the true model performance while decontaminating LLaMA3-3B. NPO achieves a TR score of almost 62% on the forget set, indicating its ability to distinguish between correct and incorrect answers more effectively than the other unlearning algorithms. Moreover, DPO performs well in terms of model utility while decontaminating LLaMA3-8B.

D Significance Testing

We conduct a paired bootstrap test, with 10,000 bootstrap resamples, and present the 95% confidence interval (CI) to report whether there is any improvement for a student model, LLaMA3-1B, distilled by a decontaminated teacher, LLaMA3-3B, over a directly contaminated (fine-tuned) student model. In table 7, we enlist the Rouge-L score comparison of the student models, the improvement over the fine-tuned student model, along with their 95% CI on bootstrap testing.

E Test Data Distribution

For robust evaluation of our proposed framework, we employ `Self-Instruct`, `S-NI`, `Vicuna` data, and the test split of `databricks-dolly-15k` data. The `Self-Instruct`, `S-NI`, and `Vicuna` data contain 71, 37, and 9 distinct topics, respectively. Further details about their data distribution are illustrated in Figure 5, 6, 7, and 8.

Model	R-L	Imp.	95% CI
Fine-tuned LLaMA3-1B	27.84	-	-
DPO_FKD_ LLaMA3_1B_3B	28.91	1.08	[0.003, 0.018]
DPO_RKD_ LLaMA3_1B_3B	28.04	0.21	[-0.006, 0.010]
NPO_FKD_ LLaMA3_1B_3B	29.84	2.00	[0.013, 0.027]
NPO_RKD_ LLaMA3_1B_3B	29.22	1.38	[0.007, 0.021]
GA_FKD_ LLaMA3_1B_3B	29.63	1.79	[0.010, 0.026]
GA_RKD_ LLaMA3_1B_3B	28.43	0.60	[-0.001, 0.013]

Table 7: Rouge-L (R-L) Score Comparison of directly contaminated (fine-tuned) student model with the student model distilled by the decontaminated teacher, along with bootstrap significance testing. The column "Imp." indicates the performance improvement of the student model distilled by a decontaminated teacher over the directly contaminated student. DPO_FKD_LLaMA3_1B_3B, DPO_RKD_LLaMA3_1B_3B, NPO_FKD_LLaMA3 _1B_3B, NPO_RKD_LLaMA3_1B_3B, GA_FKD _LLaMA3_1B_3B, GA_RKD_LLaMA3_1B_3B represent LLaMA3-1B distilled by decontaminated LLaMA3-3B using DPO in forward KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using DPO in reverse KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using NPO in forward KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using NPO in reverse KD, LLaMA3-1B distilled by decontaminated LLaMA3-3B using GA in forward KD, and LLaMA3-1B distilled by decontaminated LLaMA3-3B using GA in reverse KD, respectively.

Figure 5: Data distribution of `Self-Instruct` data across 71 distinct categories.

Figure 6: Data distribution of S-NI data across 37 distinct categories.

Figure 7: Data distribution of `Vicuna` data across 9 distinct categories.

Figure 8: Test data distribution of `databricks-dolly-15k` data across 8 distinct categories.