Understanding the Scaling Effect of Self-Evolving Negatives for Large Language Model Alignment

Abstract

Large Language Models (LLMs) have advanced significantly, but aligning them with human intentions remains challenging due to costly feedback annotation. We introduce a theoretical framework for understanding the scaling effect of self-evolving negatives in LLM alignment and propose SELF-CONTRAST, an algorithm that effectively scales these negatives. By modeling performance equivalence as gradient matching in direct preference optimization, we reveal conditions where self-evolving negatives approximate standard preference pair performance. According to these insights, SELF-CONTRAST increases distributional variance of self-evolving negatives by similarity filtering, significantly enhancing alignment performance during the scaling. Experiments on three datasets show SELF-CONTRAST achieves equivalent performance to 2-3 times the annotated data used in standard methods. Our work provides both theoretical insights and a practical, annotation-free algorithm for efficient LLM alignment. Code and data are provided at https://anonymous.4open.science/r/Self-Contrast-dev-0E66/.

1 Introduction

Large Language Models (LLMs) such as GPT-3 (Brown et al., 2020), PALM (Chowdhery et al., 2022), OPT (Zhang et al., 2022), and LLaMA (Touvron et al., 2023) have made significant strides in producing accurate and useful outputs in human contexts. A critical aspect of directing these pre-trained LLMs towards understanding human intentions is the concept of alignment (Ouyang et al., 2022; Bai et al., 2022b), primarily achieved through Supervised Fine-Tuning (SFT) and Reinforcement Learning from Human Feedback (RLHF) stages. Specifically, RLHF techniques (Schulman et al., 2017; Rafailov et al., 2023; Zhao et al., 2023; Wang et al., 2023), which utilize human or AI preferences to provide feedback on LLM responses, are seen as essential for LLM alignment.

A significant challenge in scaling RLHF lies in the feedback annotation process, which can be costly and time-consuming. Hence there have been plentiful efforts to harness self-evolution (Tao et al., 2024) strategies (i.e., self-play (Chen et al., 2024; Wu et al., 2024), self-rewarding (Yuan et al., 2024)) for LLM preference optimization to avoid annotation. These methods usually employ LLMs themselves to self-generate responses, and then self-criticize for filtering or directly assume all of these responses as dispreferred (i.e., negative) data against a SFT dataset. Some methods also involve iterative training. Empirically, these approaches demonstrate decent performances and could sometimes even outperform preference optimization based on human annotation.

However, it remains largely unexplored to understand the latent mechanism and scaling effect of these self-evolving negatives. For example, a common setting is that given a fixed SFT dataset $\mathcal{D} = \{(x_i, y_{\text{target}_i})\}$, why and to what extent self-evolving responses as dispreference would have equivalent performance to balanced annotated preference pairs in the scaling. To comprehend the problem, we model this performance equivalence as a problem of gradient matching between self-generated and ideal dispreferred responses against ideal preferred responses, following the common algorithmic context of direct preference optimization (DPO) in literature.

Let l denote number of standard preference pairs, m denote number of self-evolving responses grouped to each preferred response as negatives. Given the parameter negative exploiting potential λ, when $l < \frac{1}{1-\lambda}$, $\exists\, m \geq \frac{\lambda}{\lambda + \frac{1}{l} - 1}$ so that for the target gradient direction $\nabla\theta_{target}$,

$$\mathbb{E}\Big[\nabla\theta_{target} - \overline{\nabla}\theta_m\Big] \leq \mathbb{E}\Big[\nabla\theta_{target} - \overline{\nabla}\theta_l\Big]$$

Figure 1: Equivalent performance curves of scaling SELF-CONTRAST and standard DPO on 3 LLM alignment datasets. Annotation-free SELF-CONTRAST is competitive to standard DPO training with up to 3 times of preference feedback labels.

which means that under such condition, by using m annotation-free self-evolving negatives, we can approximate the alignment performance of using l standard DPO preference pairs. Additionally, by increasing λ, a distribution-dependent parameter, alignment performance with self-evolving negatives can become more effective.

Based on our theoretical findings, we develop SELF-CONTRAST, a new LLM alignment algorithm by effectively scaling self-evolving negatives. To improve λ of dataset distribution, we employ a simple similarity filtering strategy which encourages the variance of self-evolving negatives (i.e., σ_n in Equation 7) to significantly increase. By that means, λ is consequently increased, elevating the performance upper-bound of LLM alignment with self-evolving negatives.

We examine the SELF-CONTRAST on 3 typical LLM alignment datasets: UltraChat (Cui et al., 2023), Nectar (Zhu et al., 2023), and HH-RLHF (Bai et al., 2022a). Results in Figure 1 show that given a dataset, by merely scaling self-evolving negatives, SELF-CONTRAST can achieve equivalent performance with 2 to 3 times of annotated preference data using standard DPO training and other self-evolution algorithms, such as SPIN (Chen et al., 2024). We also justify that increasing σ_n for λ do enhance the alignment performance of using self-evolving negatives.

To sum up, we make the following contributions:

- We set up a theoretical framework to understand the scaling effect of self-evolving negatives for LLM alignment, which explains why and how much we can align LLMs via self-evolving negatives.

Figure 2: Intuition of why scaling self-evolving negatives for LLM alignment helps. When the number of preference data pairs is very limited, there is a gap between the average preference optimization direction of the dataset and the true preference optimization direction. This can be addressed by increasing data pairs, which raises costs, or by cheaply adding more negative samples to reduce directional variances.

- Based on the framework, we design SELF-CONTRAST, an annotation-free algorithm for LLM alignment by encouraging distributional variances of self-evolving negatives.
- Extensive experiments over 3 datasets verify its advantage over standard DPO and other self-evolution alignment methods. We also show empirical evidences and insights for the scaling behavior of self-evolving negatives.

2 Understanding Self-Evolving Negatives in LLM Alignment

Self-evolving negatives, or dispreferred responses, have been widely adopted in recent LLM alignment algorithms (Chen et al., 2024; Yuan et al., 2024). However, few work dives into understanding its latent theoretical mechanism and demonstrating its effect in scaling. In this section, we provide a theoretical framework for understanding the scaling effect of self-evolving negatives in LLM alignment.

2.1 Theoretical Framework

Generally speaking, more preference pair data leads to achieve better alignment performance. However, annotating preference data is always difficult. Even obtaining positive samples of preference data alone requires a certain amount of cost. However, on the contrary, obtaining negative samples from self-evolution is cheap and simple. If an equivalent level of performance can be achieved through the scaling of negative samples, it would

significantly reduce the cost of data annotation.

Thereby, under the common LLM alignment algorithm DPO (Rafailov et al., 2023), in this section we are to demonstrate that **increasing self-evolving negative samples can achieve an approximate optimization effect as increasing preference data pairs**. As written in Equation 1,

$$\mathcal{L}_{DPO} = - \mathbb{E}_{(x,p,n)\sim D}\Big[\log \sigma(\beta \log \frac{\theta(p|x)}{\theta_{SFT}(p|x)} \\ - \beta \log \frac{\theta(n|x)}{\theta_{SFT}(n|x)})\Big] \quad (1)$$

the optimization objective of DPO includes increasing the probability of positive samples and reducing the probability of negative samples.

Consider the gradient, positive sample and negative samples determine an optimization direction:

$$\nabla_\theta \mathcal{L}_{DPO} = -\beta \mathbb{E}_{(x,p,n)\sim D}\Big[\sigma(\hat{r}(x,n) \\ - \hat{r}(x,p))(\nabla_\theta \log \theta(p|x) - \nabla_\theta \log \theta(n|x))\Big] \quad (2)$$

where $\hat{r}(x,y) = \beta \log \frac{\theta(y|x)}{\theta_{SFT}(y|x)}$.

We can understand Equation 2 as both positive and negative samples contributing an optimization gradient each, and the final optimization gradient is the difference between the two.

Definition 1 (Preference Gradient) *We denote the gradient contributed by a preference pair* (x_i, p_i, n_i) *as* $\nabla\theta_i$. *For gradients induced by the positive and the negative sample, we denote as* $\nabla\theta_{p_i}$ *and* $\nabla\theta_{n_i}$ *correspondingly:*

$$\nabla\theta_{p_i} = -\beta\sigma(\hat{r}(x,n_i) - \hat{r}(x,p_i))\nabla_\theta \log \theta(p_i|x)$$
$$\nabla\theta_{n_i} = -\beta\sigma(\hat{r}(x,n_i) - \hat{r}(x,p_i))\nabla_\theta \log \theta(n_i|x)$$

In this case, $\nabla\theta_i$ *can be represented as the difference between two points:*

$$\nabla\theta_i = -\beta\sigma(\hat{r}(x,n) - \hat{r}(x,p))(\nabla_\theta \log \theta(p_i|x_i) \\ - \nabla_\theta \log \theta(n_i|x_i)) = \nabla\theta_{p_i} - \nabla\theta_{n_i} \quad (3)$$

Definition 2 (Multi-pair Preference Gradient) *We define the gradient for* l *positive-negative sample pairs* $(x_i, p_i, n_i)_{i=l}^l$ *as* $\overline{\nabla\theta}_l$, *and*

$$\overline{\nabla\theta}_l = \frac{1}{l}\sum_{i=1}^l \nabla\theta_i = \frac{1}{l}\sum_{i=1}^l (\nabla\theta_{p_i} - \nabla\theta_{n_i})$$
$$= \frac{1}{l}(\sum_{i=1}^l \nabla\theta_{p_i} - \sum_{i=1}^l \nabla\theta_{n_i}) \quad (4)$$

The wanted target optimization gradient can be defined as:

$$\nabla\theta_{target} = \lim_{l\to\infty} \overline{\nabla\theta}_l \quad (5)$$

Similarly, we define the gradient for 1 *positive sample and* m *negative samples as* $\overline{\nabla\theta}_m$, *and the gradient of that positive sample as* $\nabla\theta_{p_0}$:

$$\overline{\nabla\theta}_m = \frac{1}{m}\sum_{i=1}^m \nabla\theta_i = \frac{1}{m}\sum_{i=1}^m (\nabla\theta_{p_0} - \nabla\theta_{n_i}) \\ = \nabla\theta_{p_0} - \frac{1}{m}(\sum_{i=1}^m \nabla\theta_{n_i}) \quad (6)$$

Supposing $\nabla\theta_p$ and $\nabla\theta_n$ outcomes in a particular gradient space are distributed as follows:

$$(\nabla\theta_p, \nabla\theta_n) \sim N(\mu_p, \mu_n; \sigma_p^2, \sigma_n^2; \rho)$$

we can now show that by leveraging massive self-generated negative responses, we can effectively approximate the gradient effect of standard preference pairs:

Definition 3 (Negative Exploiting Potential) *We define* λ, *a parameter decided by training dataset distribution, as the potential to reduce the gradient estimation error by adding negative samples. The larger the* λ, *the more gradient error can be reduced by increasing negative samples:*

$$\lambda = \frac{\sigma_n^2}{\sigma_p^2 + \sigma_n^2 - 2\sigma_p\sigma_n\rho} \quad (7)$$

and then we can derive the following approximation theorem:

Theorem 1 (Self-Contrast Approximation) *Given the number of negatives* m *and the negative exploiting potential* λ, *when* $l < \frac{1}{1-\lambda}$, $\exists\, m \geq \frac{\lambda}{\lambda+\frac{1}{l}-1}$ *so that*

$$\mathbb{E}\Big[\nabla\theta_{target} - \overline{\nabla\theta}_m\Big] \leq \mathbb{E}\Big[\nabla\theta_{target} - \overline{\nabla\theta}_l\Big] \quad (8)$$

which means by 1 positive and m *negatives, we can effectively approximate the gradient error of* l *standard (i.e., 1:1 positive and negative responses) preference pairs.*

Proof. Please refer to Appendix A.

Interpretation of Theorem. Theorem 1 shows that when l and λ meet certain conditions, increasing

negative samples m can achieve better optimization stability than using multiple pairs of preference data. When $m \to \infty$, we reach the upper limit of the method: attain an effect of approximately $l = \frac{1}{1-\lambda}$ preference data pairs.

2.2 SELF-CONTRAST

From Theorem 1, we can now understand the latent mechanism of harnessing self-evolving negatives for LLM alignment. To guarantee alignment performance of using the strategy, we should improve the distribution-dependent parameter λ. It refers to the negative exploiting potential as defined in Equation 7, which is controlled by distribution variances σ_p, σ_n and variance correlation ρ.

Method: Similarity Filtering. To justify the theoretical observation, we propose to increase σ_n, the distribution variance of self-evolving negatives, as an example in this work. To achieve the goal, we have to encourage diversity of the self-evolving negatives. While it should be fundamentally resolved by reducing mutual similarities between negatives, the computation cost would be quadratic as the number of self-evolving negatives increases. Thereby, here we make a simplification to enhance dissimilarities between each self-evolving negative and the target.

Given a similarity model θ_E, for every prompt x_i, we calculate the similarity between the target $\theta_E(y_{\text{target}_i})$ and self-evolving responses $\{\theta_E(y_{i_j})\}_{j=1}^{M}$, which yields

$$s(y_{\text{target}_i}, y_{i_j}) = \text{Similarity}(\theta_E(y_{\text{target}_i}), \theta_E(y_{i_j}))$$

We consider taking the $a\%$ least similar responses as the self-evolving negatives we use for alignment training. When synthesizing the preference dataset with multiple negatives, we extract m nonidentical self-generated responses from the remaining $a\%$.

In this context, $a\%$ is a hyperparameter. To gain a better understanding of how $a\%$ affects both the data and model performance, please refer to Section 4.1's ablation study.

3 Experiments

This section studies the effectiveness of our method, which arises mainly from two aspects. First, we prove that increasing the number of negative samples can continuously improve model performance. Second, we demonstrate the efficacy of using the embedding model to filter negative samples.

3.1 Experiment Settings

We conduct our experiments on **Mistral-7B-v0.1** (Jiang et al., 2023) and Meta-Llama-3-8B (Dubey et al., 2024). For the embedding model used in response filtering, we use **UAE-Large-V1** (Li and Li, 2023). Our training code is based on the **LLaMA-factory** . We use **vLLM** to sample responses.

Datasets. We conduct experiments on two general-purpose datasets, Nectar (Zhu et al., 2023) , Ultra-Chat (Ding et al., 2023; Tunstall et al., 2023), and a safety preference dataset HH-RLHF (Bai et al., 2022a).

Nectar is a preference dataset that included 7 ranked responses. To construct an SFT dataset Nectar_{SFT}, we select the rank one response as the SFT target. We exclusively utilize samples with a length of less than 1024. The final SFT dataset contains 144k samples. For Self-Contrast and other baselines, we randomly sample an 18k subset from Nectar, referred to as Nectar_{18k} in the following passage. For UltraChat, we randomly take 16k samples with a length of less than 2048 and only use the first turn. In addition, to compare our methods with DPO, we also run DPO on a 16k subset of `ultrafeedback_binarized`[1] (Cui et al., 2023), named $\text{UltraFeedBack}_{16k}$ as a baseline.

To further investigate the effectiveness of our method, we also conduct a set of independent experiments on HH-RLHF. Referring to the original DPO work, we use 160k samples within 1024 tokens with the chosen response as the SFT target to construct an SFT dataset HH-RLHF_{SFT}. For Self-Contrast and other baselines, we randomly select 16k samples from the training set for DPO. We also extract 2.6k single-turn dialogues from the test set to serve as our evaluation dataset HH-RLHF_{test}.

Baselines. To compare the performance, we have established the following comparison methods: SFT, DPO_{std}, SPIN (Chen et al., 2024), and three variants of SELF-CONTRAST (Cf. Apppendix B.1 for more details).

Evaluation Benchmarks. We report mainly the performance of our method on the MT-bench(Zheng et al., 2023) and Alpaca-Eval(Li et al., 2023). Additionally, we employ `Starling-RM-7B-alpha`[2] to calculate the accuracy of the data between the chosen response and

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[1] https://huggingface.co/datasets/HuggingFaceH4/ultrafeedback_binarized
[2] https://huggingface.co/berkeley-nest/Starling-RM-7B-alpha

the rejected response in the preference dataset used during training. `Starling-RM-7B-alpha` is a reward model trained on Nectar, which also includes UltraChat and HH-RLHF.

We also evaluate several NLP tasks related to the Open LLM Leaderboard, including RC-Challenge (Clark et al., 2018), TruthfulQA (Lin et al., 2022), Winogrande (Sakaguchi et al., 2019), GSM8k (Cobbe et al., 2021), HellaSwag (Zellers et al., 2019) and MMLU (Hendrycks et al., 2021). To obtain more accurate results, we use `GSM8K-eval` [3] to evaluate GSM8k. The others are evaluated by `lm-evaluation-harness`.

For HH-RLHF, we use `Starling-RM-7B-alpha` to measure the Win Rate between the SFT target and the model response on the single-turn dialogue. When sampling responses, we set temperature = 1.0.

3.2 Results

Results on UltraChat and Nectar. We test the effectiveness of SELF-CONTRAST on Nectar and UltraChat under the evaluation of MT-Bench and Alpaca-Eval, which targets general alignment evaluation of LLMs. The main results are presented in Table 1.

Our results in UltraChat and Nectar suggest that leveraging self-generated responses as negative samples effectively contributes to the enhancement of model performance on the MT-Bench. When potential positive responses are removed, the MT-Bench score is increased even further. We hypothesize that this occurrence is primarily due to an improvement in the precision of negative examples. We provide an analysis of this phenomenon in Section 4.1. More to the point, the utilization of multiple negative examples results in a continuous increase compared to the use of a single negative example. It indicates the feasibility of improving the performance by adding negative samples.

We also notice that our methods outperform DPO_{std} where use responses generated by other models. We believe that in addition to employing multiple negative samples, the use of the model's own output as negative samples, rather than the output of other models, plays a crucial role.

Results on HH-RLHF$_{test}$. On HH-RLHF, we test our methods by setting $a\%$ to 100% (unfiltered), 75%, and 50% with 1, 2, 4, 8, and 16 negative samples, and we plot their Win Rate in Figure 3.

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[3] https://github.com/Guangxuan-Xiao/GSM8K-eval/

We choose $a\% = 75\%$ to represent our methods, as shown in Table 2. The results further substantiate the efficacy of our approach. Furthermore, we note that the value of $a\%$ exerts a significant influence on the results of our experiments, which we investigate in detail in Section 4.1.

Addition experiments with Meta-Llama-3-8B. To examine our methods on a stronger model, we conducted a set of experiments on Meta-Llama-3-8B (Dubey et al., 2024), setting $a\%$ to 75%. We list our best attempts alongside the baselines in Figure 3.

4 Ablation Studies

Our main experimental results indicate that Self-Contrast is a promising approach. Therefore, in order to further investigate the impact of negative sample size and response filtering on the model, we conduct detailed ablation experiments.

4.1 Response Filtering

In order to further investigate the impact of filtering negative samples on the final model alignment performance, we conduct the following experiments on UltraChat$_{16k}$.

We construct several preference datasets in different negative sample filtering parameters. As stated in Section 2.2, when filtering out possible positives and referring to the left as negatives, we remove the top $1 - a\%$ responses closed with the SFT target in the embedding space measured by cosine similarity and use the left $a\%$ as negatives, where $a\%$ is a parameter. $a\%$ will affect the proportion of false positives presented in negative samples in training data. To measure the false negative rate, we use **Starling-RM-7B-alpha** as our RM and compute negative rewards with the SFT target reward. We consider negative rewards that are smaller than the SFT target reward as true negatives. The ratio of true negatives is defined as data accuracy.

During the experiment, we varied the value of a from $\frac{1}{1} \times 100\%$ to $\frac{1}{16} \times 100\%$. We created a single negative preference dataset, where we filtered negatives from 32 prompt responses and randomly chose one from the filtered negatives to compose the preference data with the SFT target. We then evaluated the accuracy of the data and the performance of the final model on MT-Bench.

As a reference, we perform an experiment using RM as the filter as an upper bound of the data

Dataset	Method	MT-Bench	Alpaca-Eval Win Rate	Alpaca-Eval LC Win Rate	ARC	TruthfulQA	Winogrande	GSM8k	HellaSwag	MMLU	Avg.
UltraChat	SFT	5.90	70.36	57.35	57.1	40.3	_76.6_	_38.7_	81.5	_58.1_	58.7
	DPO$_{pub}$	6.64	84.66	72.46	58.2	40.9	**77.7**	**40.6**	82.4	**58.6**	**59.7**
	SPIN (Chen et al., 2024)	6.55	90.11	78.48	_58.7_	_41.8_	76.2	38.1	_82.5_	57.6	59.1
	Self-Contrast$_1$ (ours)	6.75	91.36	**84.89**	_58.7_	41.4	76.1	37.3	82.4	57.6	58.9
	Self-Contrast$_8$ (ours)	**6.88**	_91.71_	_83.21_	**58.8**	**42.6**	75.9	37.6	**82.5**	57.5	_59.2_
	Self-Contrast$_{16}$ (ours)	_6.87_	**92.63**	81.68	58.1	41.5	76.0	38.2	82.6	57.5	59.0
Nectar	SFT	6.78	93.57	84.67	58.8	49.6	**78.1**	41.2	80.1	59.2	61.2
	DPO$_{pub}$	7.22	96.02	85.64	60.2	53.4	**78.1**	46.7	81.3	59.7	63.2
	SPIN (Chen et al., 2024)	7.06	95.14	85.45	_60.8_	53.1	_77.4_	46.3	82.6	**59.8**	63.3
	Self-Contrast$_1$ (ours)	7.28	95.90	_87.37_	60.6	52.9	_77.4_	_47.5_	82.6	59.2	_63.4_
	Self-Contrast$_8$ (ours)	_7.39_	_96.14_	87.12	**61.1**	**54.9**	76.7	**47.9**	**83.5**	59.7	**64.0**
	Self-Contrast$_{16}$ (ours)	**7.41**	**96.27**	**88.71**	60.5	_53.5_	77.1	46.6	_82.8_	59.2	63.3

Table 1: Main results on UltraChat and Nectar subsets. SFT and DPO$_{std}$ are trained with preference feedback datasets. Self-Contrast$_i$ indicates using i filtered self-generated negatives. Self-Contrast$_1$ has a significant improvement compared to SFT, DPO on original data, and SPIN (Chen et al., 2024). Furthermore, Self-Contrast$_8$ achieved additional progress compared to Self-Contrast$_1$ by simply increasing the number of negative samples, without any increase in the number of positive samples.

Method	Win Rate	Avg. Reward
SFT	40.02	0.089
DPO$_{std}$	80.74	0.325
SPIN (Chen et al., 2024)	78.53	0.317
Self-Contrast$_1$ (ours)	82.26	0.355
Self-Contrast$_8$ (ours)	_83.72_	_0.367_
Self-Contrast$_{16}$ (ours)	**85.45**	**0.375**

Table 2: Results of on HH-RLHF$_{test}$. SFT and DPO$_{std}$ are trained with the original preference feedback dataset. We report Win Rate and Avg. Reward following (Rafailov et al., 2023).

Dataset	Method	MT-Bench
UltraChat	SFT	6.76
	DPO$_{std}$	6.76
	SPIN (Chen et al., 2024)	_6.87_
	Self-Contrast (ours)	**7.03**
Nectar	SFT	6.89
	DPO$_{std}$	_7.33_
	SPIN (Chen et al., 2024)	6.90
	Self-Contrast (ours)	**7.51**

Table 3: Experiments conducted on Nectar and Ultrachat with Meta-Llama-3-8B.

accuracy, where we randomly chose a response with lower reward than the SFT target as negative.

Figure 5 shows that the accuracy of the negatives decreases with $a\%$. The proportions of positive and negative samples are high in responses similar and dissimilar to SFT targets, respectively. However, the performance of the model does not always increase with the accuracy of the data. From $\frac{1}{1} \times 100\%$ to $\frac{1}{16} \times 100\%$, the performance decrease with data accuracy.

The phenomenon could be explained. A response that significantly deviates from the SFT target is more likely to be incorrect. However, it is also more likely to be unrelated to the problem or to be too easy to distinguish, and thus a weak negative sample. Therefore, we need to select a ratio that not only filters out potential positives but also maintains strong and relevant negatives to the problem.

Figure 6 shows the distribution of negative samples selected by response filtering. The data distribution filtered by reward modeling is our ideal distribution. When $a\% = 100\%$, no filtering is performed. The distribution of filtered true negative samples is very close to the distribution of reward modeling, but there is also a large number of false negative samples. When $a\%$ approaches 0, the number of false negative samples decreases significantly. However, in true negative samples, we selected fewer hard negative samples that deviated from the distribution of reward modeling. Thus, trade-offs between maintaining a low level of false negatives and preserving as many hard negatives as possible is necessary. In our case, we choose $a\% = 25\%$.

4.2 Negative Sample Quantity

Although response filtering has greatly improved the accuracy of data and the performance of models, there is still a gap compared to reward modeling methods due to the lack of negative sample quality. However, in addition to data quality, we can still

Figure 3: Comparison of the impact of varying the quantity of negative samples on MT-Bench for Nectar, UltraChat, and HH-RLHF$_{test}$. With an increase in the number of negative samples, the performance of SELF-CONTRAST exceeds that of the DPO$_{std}$ method using the standard preference dataset. Moreover, increasing the number of negative samples achieved the same effect as increasing preference data without increasing the number of positive samples.

improve performance through the quantity of data.

To clarify the correlation between the quantity of negative samples and the performance of the model, we performed experiments using varying numbers of negative samples. The aim is to determine whether the model performance improved consistently with an increasing number of negative samples.

We conduct our experiment on UltraChat$_{16k}$ and Nectar$_{18k}$, using 1, 2, 4, 8, and 16 filtered or unfiltered samples. The negative samples used for training are randomly chosen from the last 25% similar responses to the SFT target out of a set of 32 responses. Figure 3 shows the results.

The results indicate that increasing the number of negative samples, regardless of whether they have been filtered or not, can effectively improve the model performance. In Self-Contrast(unfiltered), although the accuracy of the data is not high, it still outperforms DPO$_{std}$ by adding negative samples.

4.3 Compare with More Preference Data

According to Theorem 1, increasing the quantity of negative samples is equivalent to adding more preference data pairs. Since collecting preference data incurs a cost, this method has the potential to significantly decrease the data cost for alignment, if its effectiveness is demonstrated.

Therefore, we compared the performance on the MT-Bench between DPO using more preference data and Self-Contrast with more negative samples. For DPO, the data are randomly sampled from Nectar. For Self-Contrast, we use Nectar$_{18k}$.

From Figure 1 we can know that on the MT-Bench, the performance improvement brought by adding negative samples and adding certain pref-

erence data is equivalent. Although more negative samples in total may be required to achieve the same effect, obtaining negative samples is efficient and inexpensive, so increasing negative samples has significant advantages in improving performance.

It has also been observed that the advantages of increasing the number of negative samples decrease with time. This aligns with our hypothesis that there exists a maximum threshold for enhancing performance by increasing negative samples.

5 Related Work

Reinforcement Learning from AI Feedback. RLAIF (Lee et al., 2023) is an intriguing field due to its potential to automate learning and improvement. Compared to previous RLHF works (Stiennon et al., 2022; Ouyang et al., 2022; Glaese et al., 2022; Touvron et al., 2023), the use of AI feedback rather than manual annotation effectively reduces the use of human annotations. RLAIF uses the LLM-as-a-Judge (Zheng et al., 2023; Liu et al., 2023; Ke et al., 2023) style prompting to generate the preference dataset from a larger model to align a smaller model. However, although RLAIF has eliminated the cost of manual annotation, the feedback from strong LLMs such as PaLM 2 (Anil et al., 2023) or GPT-4 (OpenAI et al., 2023) still remains expensive.

Self-Alignment. Self-Alignment, whether training-based (Bai et al., 2022b; Yuan et al., 2024) or prompting-based (Cheng et al., 2023), offers a novel opportunity to produce syntactic data from self-generated responses without human or other AI annotation. Principle-Driven Self-Alignment (Sun et al., 2023) improves re-

Figure 4: In the model responses released by Alpaca Eval, it was found that across all domains, the similarity between negative samples is lower than that between positive samples. Moreover, positive samples are more similar to the target responses compared to negative samples.

Figure 5: The impact of parameter $a\%$ on data accuracy and performance. While a smaller a leading to consistently higher accuracy of selected negatives, it harms LLM alignment when it becomes too small.

Figure 6: The negative distributions with different last $a\%$ similar thresholds. There is a trade-off between less false positive and more strong negatives when selecting a.

sponse quality by specifying special rules, using these responses for self-distillation to enhance performance. Self-critique methods, such as Constitutional AI (Bai et al., 2022b) and SELF-REFINE (Madaan et al., 2023), improve self-generated data quality iteratively. Self-Rewarding language models (Yuan et al., 2024) use LLM-as-a-Judge prompting to provide high-quality reward signals and add labeled EFT data during the SFT stage. Adversarial methods like Self-Play fInetuNing (SPIN) (Chen et al., 2024) directly use self-generated responses as rejected samples to produce syntactic preference data but require multiple iterations and may include false-positive rejections.

6 Conclusions

In this paper, we have introduced SELF-CONTRAST, a novel algorithm that leverages self-evolving negatives to achieve efficient and effective LLM alignment, demonstrating performance equivalent to methods using 2-3 times more annotated data. Our theoretical framework provides insights into the scaling effect of self-evolving negatives, explaining why and how they can be used to approximate standard preference pair performance in LLM alignment. These findings not only advance our understanding of LLM alignment processes but also offer a practical, annotation-free approach that could significantly reduce the cost and time associated with aligning large language models to human preferences.

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A   Self-Contrast with Massive Negatives

In this section, we demonstrate Theorem 1.

Under Theoretical Framework in Section 2.1, we have:

$$\overline{\nabla\theta_l} \sim N(\mu_1 - \mu_2, \frac{1}{l}(\sigma_1^2 + \sigma_2^2 - 2\sigma_1\sigma_2\rho))$$

$$\overline{\nabla\theta_m} \sim N(\mu_1 - \mu_2, \sigma_1^2 + \frac{\sigma_2^2}{m} - 2\sigma_1\sigma_2\rho)$$

$$\nabla\theta_{target} = \mu_1 - \mu_2 \qquad (9)$$

Equalization 8 can be write as:

$$\mathbb{E}\left[\nabla\theta_{target} - \overline{\nabla\theta_m}\right] \leq \mathbb{E}\left[\nabla\theta_{target} - \overline{\nabla\theta_l}\right]$$

$$\Leftrightarrow \sigma_1^2 + \frac{\sigma_2^2}{m} - 2\sigma_1\sigma_2\rho \leq \frac{1}{l}(\sigma_1^2 + \sigma_2^2 - 2\sigma_1\sigma_2\rho)$$

$$\Leftrightarrow \frac{\sigma_2^2}{\lambda} + \frac{\sigma_2^2}{m} - \sigma_2^2 \leq \frac{\sigma_2^2}{l\lambda}$$

$$\Leftrightarrow \frac{1}{m} \geq 1 - \frac{1}{\lambda}(1 - \frac{1}{l}) \qquad (10)$$

When $l < \frac{1}{1-\lambda}$, Equalization A has a solution:

$$m \geq \frac{\lambda}{\lambda + \frac{1}{l} - 1} \qquad (11)$$

B   Main Experiment Details

Although our method is simple and efficient, there are still many important details in the implementation process. This chapter will provide a detailed description of these details to provide traversal for reproduction. Additionally, all experiments were conducted on machines equipped with 8 NVIDIA A800 GPUs.

B.1   Baselines

We include the following comparison methods in our work:

- **SFT**: For Nectar, we fine-tune `Mistral-7B-v0.1` on Nectar$_{SFT}$ for 1 epoch. For UltraChat, we use `zephyr-7b-sft-full` (Cf. Appendix B). For HH-RLHF, we fine-tune `Mistral-7B-v0.1` on HH-RLHF$_{SFT}$ for 1 epoch.

- **DPO$_{std}$ (Rafailov et al., 2023)**: We conduct DPO on θ_{SFT} using the standard available preference feedback data (positive:negative = 1:1) from Nectar$_{18k}$, UltraFeedBack$_{16k}$, or HH-RLHF$_{train}$. For Nectar, the sample ranked the first is selected as the chosen sample, while the one rejected is randomly chosen from the remaining responses being ranked behind.

- **SPIN (Chen et al., 2024)**: The method samples one random response from θ_{SFT} as the rejected to run DPO given the SFT target. We use the AdamW optimizer instead of the RMSProp used in the original paper to align settings with our other experiments (in fact, we find AdamW outperforms RMSProp). Additionally, we conduct only the first iteration (Cf. Appendix B) as SELF-CONTRAST does.

- **Self-Contrast$_1$ (ours)**: We use 1 rejected samples filtered from 32 different θ_{SFT} responses to run the DPO, setting $a\%$ to 25% on Ultra-Chat and Nectar, 75% on HH-RLHF$_{test}$.

- **Self-Contrast$_8$ (ours)**: We use 8 rejected samples filtered from 32 different θ_{SFT} responses to run the DPO, setting $a\%$ to 25% on Ultra-Chat and Nectar, 75% on HH-RLHF$_{test}$.

- **Self-Contrast$_{16}$ (ours)**: We use 16 rejected samples filtered from 64 different θ_{SFT} responses to run the DPO, setting $a\%$ to 25% on UltraChat and Nectar, 75% on HH-RLHF$_{test}$.

B.2 Experiment on Nectar

Before conducting the experiment in Nectar, we first pre-process the dataset according to the following steps:

- Remove samples with a combined length of prompts and responses that exceeds 1024 tokens.

- Designate the highest-ranked response as the SFT target.

The basic information after data processing is shown on the Tabel 4.

Nectar	value
samples	177k
avg. prompt length	145.92
avg. response length	256.29
avg. turns	1.54

Table 4: Nectar after pre-process

Rank One Distribution of Nectar

Figure 7: The distribution of the rank-one reply source.

We also perform a statistical analysis of the origins of the models from which the SFT target is derived, presented in Figure 7.

We divide the pre-processed data into a training set with 144k samples D_{Nectar}, the remaining will be used for verification. Each sample in D_{Nectar} contains one prompt x_i and seven responses $\{r_{i_j}\}_{j=0}^6$ sorted by quality:

$$D_{Nectar} = \{(x_i, r_{i_0}, r_{i_1}, r_{i_2}, r_{i_3}, r_{i_4}, r_{i_5}, r_{i_6})\}_{i=1}^{144k}$$

Based on D_{Nectar}, we construct an SFT dataset with x_i and r_{i_0}, using openchat[4] template:

$$\text{Nectar}_{SFT} = \{(x_i, r_{i_0})\}_{i=1}^{144k}$$

We also randomly sampled a 18k subset Nectar$_{18k}$ from D_{Nectar}.

hyper-parameter	value
epoch	1
batch size	128
learning rate	$5e-6$
precision	bfloat16

Table 5: Hyper-Parameter for θ_{SFT}.

hyper-parameter	value
epoch	1
batch size	$128n$
learning rate	$5e-7$
beta	0.1
precision	bfloat16

Table 6: Hyper-Parameter for DPO, where n is the number of negatives. We guarantee that the average number of prompts in a single batch remains constant for each configuration during training.

We then perform SFT on **Mistral-7B-v0.1** to get θ_{SFT} using Nectar$_{SFT}$, the hyper-parameters are shown in Table 5. For experiments with negative sample sizes less than or equal to 8, we sample 32 responses per prompt from θ_{SFT} on Nectar$_{18k}$ using vllm. For the experiment with 16 negative samples, we sample 64 responses per prompt. We use $temperature = 1.0$ and $top\ p = 1.0$.

After constructing the training sets for each setting according to the description in Section 3.1, we conduct DPO following the hyperparameter mentioned in Table 6.

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[4]https://huggingface.co/openchat/openchat_3.5

When conducting experiments in Section 4.3, the batch size for the DPO baselines is $128 \times ceil(\frac{training\ samples}{18k})$, other hyperparameters follow Table 5.

B.3 Experiment on UltraChat

On UltraChat, we start with **zephyr-7b-sft-full** as θ_{SFT}, which is trained on **ultrachat_200k**. We have noticed that there are many versions of **zephyr-7b-sft-full**. To ensure a fair comparison with SPIN, we selected the model version that has MT-bench scores the same as those reported in SPIN. This particular version can be identified by its commit ID, which is $c3160e9$.

To establish the DPO_{pub} baseline, we performed a random sampling of a subset consisting of 16k data points from **ultrafeedback_binarized**. In our other experiments, the preference data for DPO is constructed using a 16k subset from the dataset **ultrachat_200k**. We have used θ_{SFT} to sample 32 or 64 responses per prompt, with $temperature = 1.0$ and $top\ p = 1.0$, which is consistent with the setup used in Nectar. During DPO and SELF-CONTRAST, we use the hyper-parameters the same as in Nectar.

B.4 Experiment on HH-RLHF

We perform SFT on HH-RLHF$_{SFT}$, following the previous hyper-parameters in Table 5.

When synthesizing the SELF-CONTRAST data, we filter the negative responses from 32 model responses with $a\%$ in $[100\%, 75\%, 50\%]$. The remaining hyperparameters are identical to those in Nectar.

When calculating the rewards for the test using **Starling-RM-7B-alpha**, for numerical stability, we added a layer of sigmoid function after the output of the model to map the reward values to $[0, 1]$.

C Experiment Setting for Meta-Llama-3-8B

For our additional experiments conducted on Nectar and Ultrachat with Meta-Llama-3-8B, most of the experimental settings are the same as with Mistral. The main difference is that, due to the model's characteristics, we used an SFT learning rate of 1e-5 and a DPO learning rate of 5e-6 for the experiments with Meta-Llama-3-8B.

D Limitations

Although massive negatives and response filtering have proven to be effective, there are still numerous aspects of our approach that require additional investigation.

Assessing human evaluation is necessary. To evaluate the human preference, we mainly test our model on MT-Bench and alpaca-eval, which is more aligned with GPT preferences. Although the SFT dataset we use is also generated by GPT-4, manual evaluation is still necessary in production to ensure effectiveness.

Safety and ethics still need further research. Although the positive samples we use come from SFT data, they can ensure a certain level of safety and ethics. However, considering the possibility of false negatives in the negative samples, the safety of our training method needs further verification.

Scaling is needed. Although current experiments have shown effectiveness on models with 7B parameters, the effectiveness of the method on larger models still needs further validation. In addition, increasing the data scale or using stronger embedding models also remains to be explored.