Checkpoint Merging via Bayesian Optimization in LLM Pretraining

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Abstract

The rapid proliferation of large language models (LLMs) such as GPT-4 and Gemini underscores the intense demand for resources during their training processes, posing significant challenges due to substantial computational and environmental costs. To alleviate this issue, we propose checkpoint merging in pretraining LLM. This method utilizes LLM checkpoints with shared training trajectories, and is rooted in an extensive search space exploration for the best merging weight via Bayesian optimization. Through various experiments, we demonstrate that: (1) Our proposed methodology exhibits the capacity to augment pretraining, presenting an opportunity akin to obtaining substantial benefits at minimal cost; (2) Our proposed methodology, despite requiring a given heldout dataset, still demonstrates robust generalization capabilities across diverse domains, a pivotal aspect in pretraining.

1 Introduction

With the rapid development of LLMs, such as GPT-3 (OpenAI, 2023), GPT-4 (OpenAI et al., 2023), PaLM (Chowdhery et al., 2023) and Gemini (Team et al., 2023), which boasts tens to hundreds of billions of parameters, the demand for new LLMs and the research aimed at enhancing their capabilities have significantly increased. But we should note that the training requirements for these LLMs are substantial, not only in terms of computational resources, human resources, and capital resources, but also regarding energy consumption and environmental impact. For instance, training the LLaMA2 70B model with 2T tokens necessitates 1,720,320 GPU hours (Touvron et al., 2023), and the development of a transformer with 213 million parameters through neural architecture search can lead to environmental burdens equivalent to the lifetime

CO₂ emissions of five cars over their entire lifespans (Strubell et al., 2019; Faiz et al., 2023). Consequently, reducing consumption and costs during the pretraining phase has emerged as a key challenge in this field.

In response to this challenge, researchers have adopted various strategies in LLM pretraining, including mixed-precision training (Shoeybi et al., 2019), zero-redundancy optimizer (Rajbhandari et al., 2020), continuous retraining (Qin et al., 2022), pipeline parallelism (Liu et al., 2023) and depth up-scaling methods (Kim et al., 2023). Although these approaches contribute to efficient pretraining and cost reduction, they primarily focus on model architecture or optimization processes, rather than directly reducing resource consumption in the pretraining phase (Hou et al., 2022).

Unlike these studies, we focus on the model merging strategy, a classic topic in machine learning (Granger, 1989; Utans, 1996; Chen et al., 2017; Wortsman et al., 2022; Sanyal et al., 2023; Singh and Jaggi, 2023), to enhance LLM pretraining in this paper. In particular, we employ checkpoints saved during pretraining and average these checkpoint parameters to improve pretraining without requiring substantial resources, since merged checkpoints can reduce the variance of the combined output relative to the output of the individual checkpoint while not increasing the bias (Utans, 1996).

However, conducting checkpoint merging is not trivial in pretraining, because different local minima may be found in averaging parameters (Utans, 1996; Chen et al., 2017). Therefore it is important to investigate the basic characters of checkpoint merging and wisely determine the merging weight.

To this end, we make the following effort: (1) we conduct some pilot experiments to explore the characters of checkpoint merging; (2) Based on the findings in the pilot experiments, we propose a method rooted in Bayesian optimization to find the optimal or near-optimal merging weight. In detail,

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we first explore three research questions: "Which checkpoints in the pretraining trajectory should be merged?", "How many checkpoints should be merged?" and "How to merge checkpoint?" via various pilot experiments. Then, based on findings in pilot experiments, we leverage Bayesian optimization to optimize the expensive, black-box, and derivative-free objective function of checkpoint merging, and determine the checkpoint merging weight.

Through various experiments, we mainly find that: (1) Our proposed approach has the potential to enhance pretraining, offering nearly a free lunch; (2) Besides superior performance, the merged soup ¹, determined by a specific held-out dataset same as Wortsman et al. (2022); Matena and Raffel (2022), still exhibit a strong generalization capability across various domains, a crucial aspect in pretraining.

In summary, the contribution of this paper is threefold: (1) We propose merging checkpoints in the pretraining trajectory to reduce pretraining costs, offering nearly a free lunch. (2) To find the optimal merging weight, we leverage Bayesian optimization, which excels at optimizing expensive black-box derivative-free objective functions. (3) Through various experiments, we denote our method exhibits superior performance and the newly merged checkpoint maintains strong generalization across different domains.

2 Pilot Experiments

This section presents phenomena observed during our pilot experiments on checkpoint merging. Specifically, we mainly explore the following three research questions: **RQ1:** Which checkpoints in the pretraining trajectory should be merged? **RQ2:** How many checkpoints should be merged? **RQ3:** How to merge checkpoints?

2.1 Experiment Setup

In the pilot experiments, we use 11 checkpoints of Baichuan2 (Yang et al., 2023) at various stages of pretraining from 200 billion tokens up to the full 2.6 trillion tokens. Meanwhile, we select two representative benchmark datasets as the tested: C-Eval (Huang et al., 2023), a comprehensive evaluation benchmark comprising over 10k multiple-choice questions spanning 52 diverse disciplines

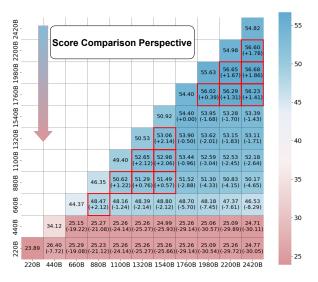


Figure 1: The performance of conducting pairwise checkpoint merging via greedy soup in C-Eval.

and four difficulty levels; CMMLU (Li et al., 2023), a general Chinese evaluation benchmark designed to assess the knowledge and reasoning abilities of law masters.

2.2 Which Checkpoints in the Pretraining Trajectory Should be Merged?

To answer the RQ1, we examine all possible pairwise merging scenarios, totaling 55 combinations (C_{11}^2) , and evaluated their performance on the C-Eval and CMMLU test sets using the greedy soup strategy (Wortsman et al., 2022), where checkpoints are sequentially added to the soup if they improve accuracy on the development data.

The results on C-Eval are presented in the Figure 1. From the figure, we can find that: (1) In the C-Eval dataset, except for the merging of Baichuan2-220B with Baichuan2-440B and Baichuan2-440B with Baichuan2-660B, merging two checkpoints from adjacent training stages generally yields better performance compared with individual checkpoint, e.g., merging Baichuan2-1980B with Baichuan2-2200B can achieve a 56.65% accuracy, but the Baichuan2-2200B can only achieve a 54.98% accuracy. Moreover, merging Baichuan2-1980B with Baichuan2-2200B (achieving a 56.65% accuracy) can exceed the final checkpoint (Baichuan2-2420B, achieving a 54.82%) a lot, improving 1.83% in test accuracy. Meanwhile, the same trend is also evident in the CMMLU dataset, presented in the Appendix. (2) Merging distant checkpoints can result in great performance decline, e.g., in the C-Eval dataset,

¹According to Wortsman et al. (2022), the merged result is called "soup".

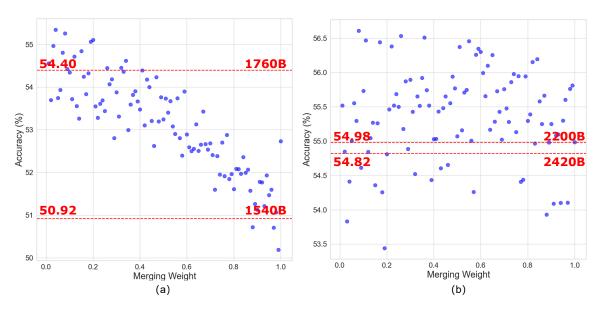


Figure 2: (a) The result on merging Baichuan2-1540B with Baichuan2-1760B via the merging weight uniformly sampled from [0, 1]. (b) The result of merging Baichuan2-2200B with Baichuan2-2420B via the merging weight uniformly sampled from [0, 1].

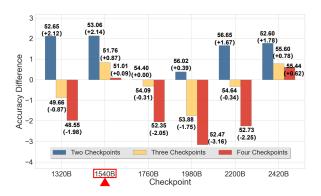


Figure 3: Assessing the accuracy disparities in C-Eval from merging two adjacent checkpoints, three adjacent checkpoints and four adjacent checkpoints by using greedy soup.

merging Baichuan2-220B with Baichuan2-2200B can only achieve a 25.26% accuracy, which is near to the performance of the undertrained Baichuan2-220B (23.89%).

2.3 How Many Checkpoints Should be Merged?

Based on the first pilot experiment, we further conducted some experiments to investigate the effect on performance while combining varying numbers of checkpoints in the pre-trained phase. Specifically, using the C-Eval dataset as the testbed, we leverage the greedy soup strategy (Wortsman et al., 2022) to merge adjacent three or four checkpoints across different pretraining stages.

The experimental results are present in the Fig-

ure 3. From the figure, we can find that: Compared with pairwise merging, merging three or four checkpoints does not show a significant advantage in performance. For example, when merging two models, such as merging Baichuan2-1320B with Baichuan2-1540B, performance notably increases to 53.06% (+2.14), however, merging three checkpoints (Baichuan2-1100B, Baichuan2-1320B, and Baichuan2-1540B) leads to a performance increase to 51.76% (+0.84), and merging four checkpoints (Baichuan2-880B, Baichuan2-1100B, Baichuan2-1320B, and Baichuan2-1540B) resulted in a further reduced performance of 51.01% (+0.09).

2.4 How to Merge Checkpoints?

In checkpoint merging, the most critical question lies in determining the proportion (merging weight) to combine checkpoints in the LLM parameter space. To probe this question, we select merging representative Baichuan2-1540B with Baichuan2-1760B and Baichuan2-2200B with Baichuan2-2420B in the C-Eval dataset, meanwhile, uniformly sample 100 points in the entire merging weight distribution space ([0, 1]) for in-depth testing.

The experimental results are present in the Figure 2. From the figure, we can find that: (1) As shown in Figure 2(a), there is a huge performance gap between Baichuan2-1540B and Baichuan2-1760B. In this case, we observe a certain monotonic trend between the performance of merged

soup and merging weight. as higher merging weight is assigned to the checkpoint with better performance, the performance of the merged soup gradually improves. Besides, there are 13% of weights showing improvement beyond the superior base model (Baichuan2-1760B, which can achieve higher accuracy compared to Baichuan2-1540B).(2) In the Figure 2(b), due to reaching the late stage of pretraining, Baichuan2-2200B and Baichuan2-2420B show the similar performance. The monotonic trend shown in merging Baichuan2-1540B and Baichuan2-1760B disappears. Meanwhile, 76% merging weights have the potential to elevate the merged soup beyond the superior checkpoint. To further verify this finding, we also conduct the same experiment on merging DeepSeek-1800B and DeepSeek-2000B, a 7B LLM trained by DeepSeek (DeepSeek-AI et al., 2024). We find that the experimental results are consistent with that on Baichuan 2, shown in the Appendix.

3 Method

In this section, we first illustrate the formulation of checkpoint merging in subsection §3.1. Then, we introduce the implementation of our method in subsection §3.2, which can effectively and efficiently determine the merging weight

3.1 Preliminary: Checkpoint Merging

When conducting LLM pretraining, we have already saved multiple checkpoints at the time t, denoted as $\{\Theta_1, \Theta_2, ..., \Theta_t\}$. The linear combination of these multiple checkpoints in parameter space is referred to as "Checkpoint Soup" and can be represented as:

$$\widetilde{\Theta}_t = \sum_{i=1}^t \lambda_i \Theta_i \quad \text{s.t.} \sum_{i=1}^t \lambda_i = 1$$
 (1)

where $\lambda_i \in \mathbb{R}$ represents merging weight. According to the key findings in pilot experiments, in this paper, we only focus on pairwise merging, therefore, the Equation 1 can be reformulated as:

$$\widetilde{\Theta}_t = \lambda_t \Theta_t + (1 - \lambda_t) \Theta_{t-1} \tag{2}$$

As shown in pilot experiments, the performance of $\widetilde{\Theta}_t$ can surpass that of Θ_t when an appropriate λ_t is assigned. Therefore, for each checkpoint merging iteration, the primary challenge is to find the optimal or near-optimal merging weight λ_t .

3.2 Checkpoint Merging via BayesOpt

To find the optimal or near-optimal merging weight, we resort to Bayesian optimization (short for "BayesOpt"). BayesOpt is an effective global optimization strategy widely used to find optimal solutions for functions that are costly or difficult to evaluate directly. BayesOpt consists of three main components: an objective function to be optimized, a Bayesian statistical model for modeling the objective function, and an acquisition function for deciding where to sample next (Frazier, 2018).

Objective Function in Checkpoint Merging. The objective function to be optimized in checkpoint merging during the pretraining phase can be formulated as

$$\max_{\lambda_t \in [\alpha, 1]} f(\lambda_t | \Theta_t, \Theta_{t-1}, \text{LLM}, D)$$
 (3)

where given the LLM equipped with the parameter $\widetilde{\Theta}_t$ (defined in the Equation 2) and a certain held out labeled dataset D, the objective function $f(\cdot)$ can project the merging weight λ_t to the overall performance of the LLM in D, e.g., F1 score in the named entity recognition task and BLEU score in the translation task. Besides, to reduce the search space, the range of the merging weight is controlled by a hyperparameter $\alpha \in [0,1)$.

Gaussian Process: A Bayesian statistical model. To model the object function in Equation 3, Gaussian process (GP) regression (Seeger, 2004) is utilized. In detail, given a finite collection of merging weight $\lambda_t^{1:k} = \lambda_t^1, ..., \lambda_t^k$, it is able to collect the object function's values at these points together into a vector $f(\lambda_t^{1:k}) = [f(\lambda_t^1), ..., f(\lambda_t^k)] \in \mathbb{R}^k$. Note that, we omit the condition in $f(\cdot)$ for convenience. In GP, this prior distribution is supposed to be multivariate normal, with a particular mean vector and covariance matrix, which is denoted as

$$f\left(\lambda_t^{1:k}\right) \sim \text{Normal}\left(\mu_0\left(\lambda_t^{1:k}\right), \Sigma_0\left(\lambda_t^{1:k}, \lambda_t^{1:k}\right)\right)$$
(4)

where μ_0 and Σ_0 are mean function and covariance function with learnable parameters, which can be estimated by maximum likelihood estimation. $\mu_0\left(\lambda_t^{1:k}\right) = \left[\mu_0\left(\lambda_t^1\right), \ldots, \mu_0\left(\lambda_t^k\right)\right] \in \mathbb{R}^k \text{ and } \Sigma_0\left(\lambda_t^{1:k}, \lambda_t^{1:k}\right) = \left[\Sigma_0\left(\lambda_t^1, \lambda_t^1\right), \ldots, \Sigma_0\left(\lambda_t^1, \lambda_t^k\right); \ldots; \Sigma_0\left(\lambda_t^k, \lambda_t^1\right), \ldots, \Sigma_0\left(\lambda_t^k, \lambda_t^k\right) \right] \in \mathbb{R}^{k \times k}.$

Using Bayes' rule, we have a posterior probability distribution:

$$f(\lambda_t) \mid f\left(\lambda_t^{1:k}\right) \sim \text{Normal}\left(\mu_k(\lambda_t), \sigma_k^2(\lambda_t)\right)$$
 (5)

Algorithm 1 Checkpoint Merging Via BayesOpt

- 1: for k = 1 to N do
- Fit the parameters of the Gaussian process given observation history $(\lambda_t^{1:k}, f(\lambda_t^{1:k}))$ 2:
- Compute the acquisition function based on the posterior distribution (Equation 5). 3:
- 4:
- 5:
- 6:
- Evaluate the maximizer λ_t^{k+1} of the acquisition function. Conducting checkpoint merging $\widetilde{\Theta}_t^{k+1} = \lambda_t^{k+1} \Theta_t + (1 \lambda_t^{k+1}) \Theta_{t-1}$ Using $\widetilde{\Theta}_t^{k+1}$ to obtain $f(\lambda_t^{k+1})$ on the held out dataset D Append the new observation pair $(\lambda_t^{k+1}, f(\lambda_t^{k+1}))$ to the observation history. 7:

$$\mu_k(\lambda_t) = \Sigma_0 \left(\lambda_t, \lambda_t^{1:k}\right) \Sigma_0^{-1} \left(\lambda_t^{1:k}, \lambda_t^{1:k}\right) \cdot \left(f\left(\lambda_t^{1:k}\right) - \mu_0\left(\lambda_t^{1:k}\right)\right) + \mu_0(\lambda_t)$$
(6)

$$\sigma_k^2(\lambda_t) = \Sigma_0(\lambda_t, \lambda_t) - \Sigma_0\left(\lambda_t, \lambda_t^{1:k}\right) \cdot \Sigma_0^{-1}\left(\lambda_t^{1:k}, \lambda_t^{1:k}\right) \Sigma_0\left(\lambda_t^{1:k}, \lambda_t\right)$$
(7)

From the above equations, we find that: (1) The posterior mean $\mu_n(\lambda_t)$ is a weighted average between the prior $\mu_0(\lambda_t)$ and an estimate based on the data $f(\lambda_t^{1:k})$. (2) The posterior variance $\sigma_n^2(\lambda_t)$ is equal to the prior covariance $\Sigma_0(\lambda_t, \lambda_t)$ less a term that corresponds to the variance removed by observing $f(\lambda_t^{1:k})$.

Acquisition Functions. Suppose we have $\lambda_t^{1:k}$ and $f(\lambda_t^{1:k})$, and currently we find the best solution is f_*^k , we need to use the acquisition function to determine where to sample new merging weight (next evaluation point). The acquisition function serves as a cheap-to-evaluate utility function to guide the sampling decisions.

One acquisition function used in this paper is Expected Improvement (EI) (Močkus, 1975; Jones et al., 1998). In detail, we want to choose λ_t^{k+1} so that the performance of the LLM $(\cdot | \Theta_t)$ can be improved enhanced. Since $f(\lambda_t | \Theta_t, \Theta_{t-1}, LLM, D)$ is unknown until after the pass all data in D through the LLM, what we can do is to take the expected value of the improvement and choose λ_t^{k+1} to maximize it. We define the expected improvement as:

$$EI_k(\lambda_t) := E_k[max(f(\lambda_t) - f_*^k, 0)]$$
 (8)

Here, $E_k[\cdot]$ indicates the expectation taken under the posterior distribution (present in the Equation 5) given observations of $f(\cdot)$ at $\lambda_t^1, ..., \lambda_t^k$. Then we evaluate the merging weight at the point with the largest expected improvement,

$$\lambda_t^{k+1} = \operatorname{argmax} \operatorname{EI}_k(\lambda_t) \tag{9}$$

Another acquisition function used in this paper is Upper Confidence Bound (UCB) (Srinivas et al., 2009). Compared with the EI, the UCB tries to guide the search from an optimistic perspective, which is defined as:

$$UCB := \mu_k(\lambda_t) + \beta \cdot \sigma_k(\lambda_t) \tag{10}$$

where $\beta > 0$ is a learnable parameter to navigate the exploitation-exploration trade-off. Considering the objective function $f(\cdot)$ can be complex and non-convex, it may be the case that no single acquisition function will perform the best over the entire optimization. Therefore, a mixed strategy in which the acquisition function samples from a pool at each iteration might work better than any single acquisition (Hoffman et al., 2011).

Note that, the proposed checkpoint merging via BayesOpt is not limited to pairwise checkpoint merging, but can also handle merging multiple checkpoints in the same way as pairwise merging. The overall procedure of checkpoint merging via BayesOpt is illustrated in Algorithm 1.

Experiments

Experimental Setups

Datasets: Besides C-Eval (Huang et al., 2023) and CMMLU (Li et al., 2023) used in the pilot experiments, we further select three benchmark datasets as the testbed: MMLU (Hendrycks et al., 2021), a large-scale multi-task language understanding benchmark consisting of multiple-choice questions on academic subjects; and GSM8K (Cobbe et al., 2021), a well-known mathematics-focused evaluation benchmark.

Baseline Methods: We compared our merging method with the following strong baselines: (1) **Checkpoints before Merging** To better showcase the performance changes after model merging, we report the performance of checkpoints before merging. (2) Uniform Soup (Wortsman et al., 2022)

Dataset	Baichuan2-1980B	Baichuan2-2200B	Uniform Soup	Greedy Soup	Fisher	RegMean	Ours
C-Eval	55.63	54.98	53.00	55.63	55.73	55.21	56.17(+0.44)
CMMLU	55.68	56.29	54.20	56.29	56.13	55.21	56.88(+0.59)
MMLU	54.00	51.27	54.30	55.39	54.25	54.77	55.44(+ 0.05)
GSM8K	23.28	21.99	23.96	23.28	20.92	23.73	24.02(+0.29)
Average	47.15	46.13	46.37	47.65	46.76	47.23	48.13(+0.48)

Dataset	Baichuan2-2200B	Baichuan2-2420B	Uniform Soup	Greedy Soup	Fisher	RegMean	Ours
C-Eval	54.98	54.82	54.93	55.64	54.44	54.55	56.23(+0.59)
CMMLU	56.29	56.78	56.71	56.78	56.62	56.46	56.97(+0.19)
MMLU	51.27	53.97	54.62	54.82	54.16	54.77	54.56(-0.26)
GSM8K	19.64	21.00	20.92	21.92	22.44	23.88	24.32(+0.44)
Average	45.55	46.64	46.80	47.29	46.92	47.42	48.02(+0.50)

Table 1: The results of merging Baichuan2-1980B with Baichuan2-2200B and merging Baichuan2-2200B with Baichuan2-2420B across various benchmark datasets.

Dataset	DeepSeek-1400B	DeepSeek-1600B	Uniform Soup	Greedy Soup	Fisher	RegMean	Ours
C-Eval	38.80	39.40	41.26	40.70	40.24	39.55	41.79(+0.55)
CMMLU	40.27	40.94	42.18	42.25	41.76	41.80	42.55(+0.30)
MMLU	41.94	42.60	43.87	43.88	43.95	43.27	43.85(-0.03)
GSM8K	11.30	13.27	14.18	14.03	15.39	15.04	15.70(+0.41)
Average	33.08	34.05	35.37	35.22	35.34	34.92	35.97(+0.53)

Dataset	DeepSeek-1800B	DeepSeek-2000B	Uniform Soup	Greedy Soup	Fisher	RegMean	Ours
C-Eval	43.05	44.36	44.61	44.70	44.81	43.95	45.82(+1.01)
CMMLU	45.31	46.82	46.84	46.82	46.49	47.12	47.15(+0.03)
MMLU	47.68	49.29	49.02	49.29	48.73	49.07	49.43(+0.14)
GSM8K	16.60	18.88	17.82	18.88	18.73	18.56	19.04(+0.22)
Average	38.16	39.84	39.57	39.92	39.69	39.68	40.36(+0.44)

Table 2: The results of merging DeepSeek-1400B with DeepSeek-1600B and merging DeepSeek-1800B with DeepSeek-2000B across various benchmark datasets.

implements an equitable averaging of models, disregarding individual performance metrics to ensure uniform contribution. Note that LAWA (Sanyal et al., 2023) is also a particular case of uniform soup. (3) Greedy Soup (Wortsman et al., 2022), conversely, selectively incorporates checkpoints based on their demonstrated ability to augment model accuracy, adopting only those that yield tangible performance improvements in the held-out dataset. (4) Fisher Weighted Averaging (Matena and Raffel, 2022) (short for "Fisher") strategically utilizes Fisher information to allocate weights to model parameters, thereby maximizing the ensemble's joint posterior likelihood for superior efficiency. (5) RegMean (Jin et al., 2022) applies regression techniques to reduce prediction variance across models, thereby bolstering the ensemble's overall robustness and performance.

LLM Checkpoints Besides checkpoints of pre-

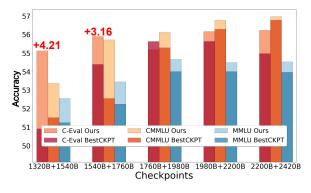


Figure 4: This result of comparing our method with the checkpoint with superior performance before merging.

training Baichuan2-7B (Yang et al., 2023), we also leverage intermediate checkpoints of training Deepseek 7B (DeepSeek-AI et al., 2024).

4.2 Main Results

Figure 4 illustrates the performance improvement of our method over the best base checkpoint performance (short for "BestCKPT") value on the C-Eval dataset during the mid to late stages of pretraining. Meanwhile, in Table 1, we present two merging combinations that are characterized by notable score improvements. For example, the merging of the Baichuan2-1980B and Baichuan2-2200B achieves a 0.59% improvement on the CMMLU dataset compared with the Baichuan2-2200B. Similarly, the merging of the Baichuan2-2200B and Baichuan2-2420B demonstrates significant gains, achieving a 0.57% improvement on the C-Eval dataset compared to the Baichuan2-2420B.

In addition to surpassing baseline checkpoints, our approach also significantly outperforms other merging baselines across various datasets. On the CMMLU dataset, applying our proposed method to merge the Baichuan2-1980B with the Baichuan2-2200B can surpass Uniform Soup, Greedy Soup, Fisher Weighted Averaging, and RegMean by 2.68%, 0.59%, 0.75%, and 1.67%, respectively. A similar trend is also observed on the C-Eval dataset, with our method outperforming others by substantial margins.

To further validate our proposed method, we apply it to the DeepSeek 7B. Results are shown in Table 2, testing the merging of the DeepSeek-1800B with DeepSeek-2000B on the C-Eval dataset, achieving a score of 45.82, thereby outperforming Uniform Soup, Greedy Soup, Fisher Weighted Averaging, and RegMean by 1.34%, 1.24%, 0.57%, and 1.87%, respectively. These results not only underscore the robustness and applicability of our proposed method but also its effectiveness in enhancing model performance across different pretraining stages and models.

4.3 Can the Merged Soup Generalize to Unseen Domains?

Since the merging weight is determined in a certain held-out labeled dataset D (Equation 3), therefore, it is a very important question needs to be answered: "Can the merged soup perform well in unseen datasets?" To answer this question, we investigate the out-of-domain generalization capability of various merged soups. In our experiment, we use the C-Eval to determine the merging weight, and test merged soups on CMMLU, MMLU and GSM8K.

Dataset	Greedy Soup (IND/OOD)	Fisher (IND/OOD)	Ours (IND/OOD)
CMMLU	56.78/56.78	56.62/56.72	56.97/56.91
MMLU	54.82/54.54	54.16/54.54	54.56/55.29
GSM8K	21.92/23.65	22.44/24.34	24.32/24.40
$\Delta(\downarrow)$	2.01	2.38	1.05

Table 3: The results of testing the merged soups on the out-of-domain dataset. We use the C-Eval dataset to determine the merging weight and test the merged soups on the out-of-domain dataset, CMMLU, MMLU and GSM8K. "IND" and "OOD" denote "In-domain" and "Out-Of-Doamin", respectively. Δ denotes the total difference in performance between IND and OOD on this three out-of-domain datasets.

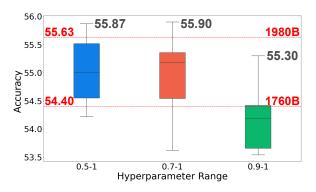


Figure 5: The results of varying merging weight searching space size on merging Baichuan2-1760B and Baichuan2-1980B, were tested on the C-Eval dataset.

The results are displayed in the Table 3. From the table, we can find that: (1) Although determining the merging weight in a Chinese dataset, merged soups obtained by various merging methods consistently perform well in English datasets, like MMLU and GSM8K, which means merging pretraining checkpoints in the parameter space does not compromise the generalization of checkpoints. (2) Compared with Greedy Soup and Fisher Weighted Averaging, our proposed method presents a better result, since the difference in performance between the in-domain setting (determining weight and testing the merged soup using the data from the same domain) and out-of-domain setting is the smallest, indicating a high probability that the merging weight found on IND setting and OOD setting may be the same.

C-Eval	1/4	1/2	3/4	1
Ours	56.61	56.08	55.80	56.23

Table 4: "This is the result of studying the variation in the size of the held-out dataset after merging on the 2200B and 2420B checkpoints.

5 Discussion

5.1 The Impact of Varying the Held-out Dataset Size on Checkpoint Merging

Same as Wortsman et al. (2022); Matena and Raffel (2022), our proposed need a training set to determine the merging weight. Therefore, it is worth investigating the impact of variations in the held-out dataset size on the result. To this end, we extract some fractions of the C-Eval validation data as the held-out dataset, and test merging Baichuan2-2200B and Baichuan2-2420B.

The result is presented in Table 4. From the result, we find that the size of the held-out dataset appears to exert minimal influence on the efficacy of our method, which maintains commendable performance even when the available dataset is limited. We conjecture the reason is that the impact of dataset size on our proposed method pertains primarily to the assessment phase, therefore, a small dataset can still provide sufficient information to discern the quality of the weight allocation. With the C-Eval dataset, for instance, extracting a fraction of the data can still serve to evaluate the model's capabilities effectively.

5.2 The Impact of Varying Merging Weight Searching Space Size

As shown in Equation 3, the hyperparameter α controls the merging weight searching space. To investigate the impact of this hyperparameter, we conduct some experiments. The experiment results are shown in the Figure 7. It can be observed that setting α to 0.5 or to 0.7 can achieve relatively good results, whereas setting α to 0.9 can result in a noticeable decline in accuracy. Digging deeper, we find that setting α to 0.5 or to 0.7 can both converge on the optimal merging weight within the range of (0.87, 0.89). Besides, in our experience, we also find that when the performance gap between checkpoints is apparent, a narrower searching space is beneficial, predominantly favoring the stronger checkpoint. In contrast, when checkpoints before merging can achieve balanced performance, a broader searching space is preferable.

6 Related Work

Model Merging in LLM: Model merging focuses on the unification of several models into one coherent entity, aiming to harness the collective strengths and mitigate the individual weaknesses of each model (Jolicoeur-Martineau et al., 2023), and has recently emerged as a significant trend in the research of Large Language Models. In detail, Wortsman et al. (2022) proposes model soup to improve accuracy without increasing inference time by averaging weights of multiple fine-tuned models. Jin et al. (2022); Yu et al. (2024); Wan et al. (2024) investigate the problem of merging individual LM fine-tuned on different datasets to obtain a single model that performs well both across all dataset domains or obtain new capabilities. Ramé et al. (2024) proposes using model merging to obtain a reliable and robust reward model in RLHF. However, we find that conducting model merging during pretraining receives little attention.

Bayesian Optimization in NLP: Bayesian Optimization (BayesOpt) can efficiently optimize objective functions that take a long time to evaluate and are widely applied in NLP. In detail, Yogatama et al. (2015) leverage BayesOpt for Text Representations. Ruder and Plank (2017) learn data selection measures using BayesOpt in transfer learning for sentiment analysis and parsing. Simpson et al. (2020) proposes using BayesOpt for community QA and summarization, demonstrating its superiority in tasks requiring nuanced feedback interpretation. Besides, Brochu et al. (2010); Liaw et al. (2018) find that Gaussian process preference learning enables rapid, efficient inference, making it suitable for interactive applications requiring quick user feedback processing. In this paper, unlike previous work, we use BayesOpt to obtain the merging weight for checkpoint merging in LLM pretraining.

7 Conclusion

In this paper, to alleviate the huge computational cost of pretraining LLM, we propose merging checkpoints in the pretraining trajectory. Specifically, we first conduct some pilot experiments to explore the characters of checkpoint merging. Then, based on the findings in the pilot experiments, we propose a method rooted in Bayesian optimization to find the optimal or near-optimal merging weight. Through various experiments, we find that: our

proposed approach has the potential to enhance pretraining, offering nearly a free lunch Besides superior performance, the merged result still exhibits a strong generalization capability across various domains, which means our proposed method does not compromise the generalization of pretraining checkpoints.

Limitations

The limitations of our work are presented as follows: First, the underlying mechanisms of checkpoint merging remain opaque. We cannot precisely delineate the knowledge encapsulated within two checkpoints or determine which specific weight components are pivotal. The lack of clarity extends to the decision of which parts of the weights should be merged. Second, the Bayesian Optimization approach, employing the Gaussian process, necessitates evaluating performance in each iteration on a held-out set to adjust the optimal merging weight. Consequently, using Gaussian processes for optimal merging weight search is more resourceintensive compared to merging methods like uniform soup. Third, in our experiments, we only use checkpoints from Baichuan 7B and DeepSeek 7B, and we also notice that some researchers or projects, like Groeneveld et al. (2024) (OLMo) and Biderman et al. (2023) (Pythia), also release intermediate checkpoints when pretraining their LLMs.

These considerations highlight that while our method shows promising direction, it does so with a recognition of its inherent limitations and the need for further refinement. Our ultimate goal is to illuminate the "black box" of checkpoint merging, providing a clearer understanding of the intricate dynamics at play and paving the way for more resource-efficient optimization strategies in LLM pretraining.

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A Appendix for Pilot Experiments

A.1 Performance on CMMLU Dataset

In this section, we describe the performance of merging checkpoints on the CMMLU dataset.

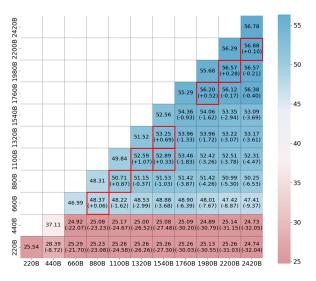


Figure 6: The performance of conducting pairwise checkpoint merging via greedy soup in CMMLU.

In accordance with the research question outlined in pilot experiments, we extended our analysis to the CMMLU dataset to corroborate the findings from the C-Eval dataset. Utilizing the same methodology, we evaluated all possible pairwise merging, totaling 55 combinations (C_{11}^2). Employing the greedy soup strategy as outlined by Wortsman et al. (2022), checkpoints are sequentially incorporated into the soup if they demonstrate an improvement in accuracy on the development data.

The analysis yields observations that are consistent with those obtained from the C-Eval dataset, reinforcing the generality of our findings. Specifically, we observe that:

(1) Adjacent checkpoint merging yields superior performance: Echoing the C-Eval dataset's findings, merging two checkpoints from consecutive training phases in the CMMLU dataset generally led to performance enhancements over individual checkpoints. Notably, merging Baichuan2-1980B with Baichuan2-2200B achieved an accuracy of 56.57% on the CMMLU dataset, surpassing the 56.29% accuracy of Baichuan2-2200B when assessed independently. This not only highlights the effectiveness of adjacent checkpoint merging but also indicates a significant improvement over the final checkpoint, Baichuan-2420B (with an accuracy of 56.78%), by elevating the test accuracy by 0.10%. (2) Merging distant checkpoints leads

Dataset	Baichuan2-220B	Baichuan2-440B	Uniform Soup	Greedy Soup	Fisher	RegMean
C-Eval	23.89	34.12	24.10	34.12	26.68	26.37
CMMLU	25.54	37.11	25.78	37.11	27.46	25.23
MMLU	23.85	33.29	23.1	33.29	23.15	23.33
GSM8K	6.82	9.10	8.04	9.10	8.16	5.46

Table 5: The results of merging Baichuan2-220B with Baichuan2-440B across various benchmark datasets.

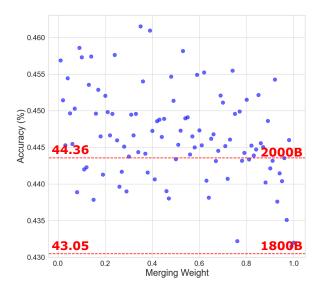


Figure 7: Merging DeepSeek checkpoints 1800B and 2000B reveals equal performance, with 69% of weights improving beyond the superior base model.

to performance deterioration: In line with the C-Eval dataset observations, merging significantly disparate checkpoints, such as Baichuan2-220B with Baichuan2-2200B, resulted in a notable performance decline, with accuracy dropping to 25.26% on the CMMLU dataset. This outcome closely mirrors the performance of the lesser-trained checkpoint, Baichuan2-220B, which has an accuracy of 25.54%, underscoring the negative impact of merging widely separated checkpoints.

The CMMLU dataset findings reinforce the C-Eval dataset's results, highlighting the critical importance of strategic checkpoint merging for enhanced model performance across diverse datasets.

A.2 Performance on DeepSeek

In our initial experiments, we delve into the possibility of boosting performance through strategic checkpoint merging within the Baichuan pretrained model, focusing on the checkpoint pairs 1540B and 1760B, along with 2200B and 2420B, in the advanced stages of pretraining. This exploration aims to uncover patterns of improvement that could be applied across different models. How-

ever, our analysis has not extended to other models like DeepSeek. To bridge this gap, we undertake a detailed examination of DeepSeek by evaluating the merging of checkpoints 1800B and 2000B, assessing 100 merging weight points distributed evenly within the [0, 1] interval. Our objective is to ascertain if the trend of performance enhancement through merging observed in Baichuan is also evident in other pre-trained models, specifically through the lens of weight combination efficacy.

The pivotal question guiding our research is: Do similar patterns of performance improvement emerge in other pre-trained models, such as DeepSeek, when applying strategic checkpoint merging, as observed in the Baichuan model?

Our research confirms this hypothesis, revealing that: Specifically, an impressive 70% of the tested merging weight combinations for DeepSeek's checkpoints 1800B and 2000B result in performance enhancements.

This finding indicates that the strategy of merging checkpoints to enhance performance is not unique to the Baichuan model but is also applicable to other pre-trained models like DeepSeek. The consistency of this pattern across different models highlights the potential of checkpoint merging as a universally effective method for optimizing pre-trained model performance during their later training phases.

B Additional Tables

B.1 All the results of Baichuan2-220B with Baichuan2-440B across various benchmark datasets.

As outlined in our pilot experiments, performing weight merging on checkpoints of LLMs during the early stages of pre-training leads to a degradation in performance. In the Table 5, we present our experimental results on weight merging between Baichuan2-220B and Baichuan2-440B models. We use Uniform Soup, Greedy Soup, Fisher, and RegMean to conduct merging and measure

the post merging performance. Without exception, none of the outcomes show performance surpassing that of the superior base model (Baichuan2-440B). This evidence suggests that conducting checkpoint merging in the early pre-training phase is not a viable strategy.