Search Wisely: Mitigating Sub-optimal Agentic Searches By Reducing Uncertainty

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Abstract

Agentic Retrieval-Augmented Generation (RAG) systems enhance Large Language Models (LLMs) by enabling dynamic, multi-step reasoning and information retrieval. However, these systems often exhibit sub-optimal search behaviors like over-search (retrieving redundant information) and under-search (failing to retrieve necessary information), which hinder efficiency and reliability. This work formally defines and quantifies these behaviors, revealing their prevalence across multiple QA datasets and agentic RAG systems (e.g., one model could have avoided searching in 27.7% of its search steps). Furthermore, we demonstrate a crucial link between these inefficiencies and the models' uncertainty regarding their own knowledge boundaries, where response accuracy correlates with model's uncertainty in its search decisions. To address this, we propose β-GRPO, a reinforcement learning-based training method that incorporates confidence threshold to reward high-certainty search decisions. Experiments on seven QA benchmarks show that β-GRPO enable a 3B model with better agentic RAG ability, outperforming other strong baselines with a 4% higher average exact match score[1].

1 Introduction

Recent advances in Large Language Models (LLMs) have propelled their use in information-intensive tasks such as question answering and knowledge synthesis, especially when paired with retrieval capabilities (Wang et al., 2025b). Agentic Retrieval-Augmented Generation (RAG) frameworks (Jin et al., 2025a; Song et al., 2025a; Chen et al., 2025) push this further by empowering LLMs to perform multi-step reasoning (Li et al., 2025) and dynamically decide when and what to retrieve (Guan et al., 2025), closely emulating sophisticated human research processes. However, despite these advancements, current agentic RAG systems often struggle with efficiency and reliability due to sub-optimal search behaviors (Shen et al., 2024; Qian et al., 2025; Wang et al., 2025a). In particular, two major challenges: 1) over-search, where the model retrieves information it already knows , and 2) under-search, where it fails to seek external knowledge when necessary, have been identified as critical obstacles that degrade performance.

In this work, we conduct a thorough quantitative analysis to identify and measure the prevalence of over-search and under-search. Our experiments on several multi-hop QA datasets (2WikiMultiHopQA (Ho et al., 2020), Bamboogle (Press et al., 2023), HotpotQA (Yang et al., 2018), and MuSiQue (Trivedi et al., 2022)) using contemporary LLMs like R1-Searcher (Song et al., 2025a) and Search-R1 (Jin et al., 2025a) reveal significant instances of sub-optimal search. We also further explore the connection between these behaviors and a model's awareness of its knowledge boundaries, finding that candidate responses generated with higher certainty about the necessity of a search query tend to achieve better accuracy.

To address this, we introduce β-GRPO, a variant of GRPO (Shao et al., 2024) where the confidence of search calls are modeled as the minimal token probability of the search queries produced by the model and a confidence threshold is incorporated into the reward function, only encouraging generations with high-certainty search calls leading to correct answer. Through extensive experiments on seven QA benchmarks, we show that β-GRPO enables a 3B model with better agentic RAG ability compared to strong baselines with a 4% higher average exact match score and 1.21% fewer over-searches and 7.33% fewer under-searches.

2 Identifying Sub-optimal Search

To investigate the prevalence of over-search and under-search, we conduct three experiments with

[1]We will release all our codes and data upon acceptance.

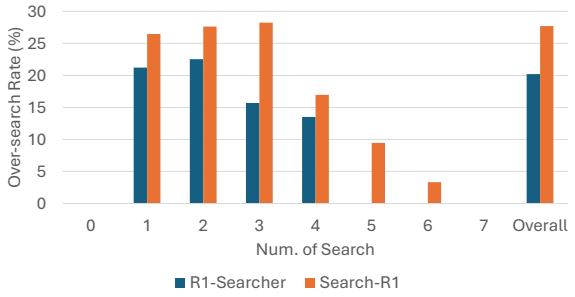

Figure 1: Percentage for all search steps that can be answered without performing searches of R1-Searcher and Search-R1 on 4 datasets combined, with respect to the number of searches of each test sample.

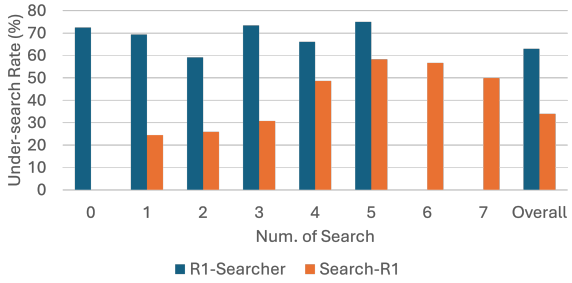

Figure 2: Error rate for all non-search steps of R1-Searcher and Search-R1 on 4 datasets combined, with respect to the number of searches of each test sample.

the test sets of four widely recognized multihop QA datasets: 2WikiMultiHopQA (Ho et al., 2020), Bamboogle (Press et al., 2023), HotpotQA (Yang et al., 2018), and MuSiQue (Trivedi et al., 2022). We mainly investigate two recent LLMs that interact with search engines: R1-Searcher (Song et al., 2025b) and Search-R1 (Jin et al., 2025b). We adopt the version trained based on Qwen2.5-7B (Qwen et al., 2025) for a fair comparison.

2.1 Step-wise Analysis

To directly measure whether a search step was truly necessary, we separate all outputs into individual steps and identify if each of them matches with the definition of over-search and under-search. For over-search rate measurement, we prompted the model to answer sub-queries from all the steps with search behavior using only their internal knowledge and the preceding context. For under-search rate measurement, we examine steps without searching and evaluate the correctness of the generated information. A detailed explanation of the analysis pipeline is provided in Appendix A.2.

Capability to Answer from Memory The results in Figure 1 show that a significant portion of search actions were instances of over-search. R1-Searcher could have answered correctly without searching in 20.2% of its search steps overall, while Search-R1 could have done so in 27.7% of its search steps. This highlights a substantial room for efficiency improvement. Figure 1 also shows the over-search rate for each subset of test samples grouped by the total number of search steps an agent used to solve an entire problem instance. The results per each subset indicates that over-search is a persistent issue irrespective of the overall search complexity adopted by the model for a given problem. Despite the step-wise analysis, we also conduct an analysis on comparing the number of searches versus the pre-given number of hops from the dataset in Appendix A.3, which also supports our conclusion.

Error Rate in Non-Search Steps Figure 2 analyzes the error rate in non-search steps, which can be seen as the rate of under-search. Both models exhibited high error rates (R1-Searcher: 63%, Search-R1: 33.98%) in non-search steps, suggesting a strong tendency towards under-search leading to incorrect reasoning or hallucination. For R1-Searcher, this error rate was particularly high with fewer total searches (over 72% if no searches were made). For Search-R1, errors in non-search steps remained notable even when performing many searches overall (e.g., 48.70% for 4-search problems), possibly due to decision complexity in later stages. (See Figure 2 for detailed error rates by search step count).

2.2 Sub-optimal Search & Knowledge Boundary

The observed tendencies towards over-search and under-search, combined with our definition, suggest a core deficiency in how agentic RAG models perceive knowledge boundaries—the limits of what they know versus what they need to find out. To illustrate the link between better knowledge boundary awareness and improved outcomes, we analyze the performance of 4 Qwen2.5-3B based Search-R1 models (including PPO and GRPO trained, Base and Instruct variants). We generate 5 candidate responses for each question and group these responses based on each output's **minimum probabilities within all the search query tokens** as the indication of certainty on knowledge boundary.

As shown in Table 1, candidate responses generated with lower intrinsic uncertainty generally lead to higher final accuracy (as high as 6% on Bam-

Model Config	Prob. Group	2Wiki	Bamboogle	HotpotQA	Musique
Base + PPO	Max	**0.184**	0.096	**0.152**	0.038
	Min	0.168	0.096	0.114	0.038
Base + GRPO	Max	**0.249**	0.112	**0.327**	**0.085**
	Min	0.234	0.104	0.289	0.056
Instruct + PPO	Max	**0.333**	0.250	0.262	**0.138**
	Min	0.297	0.250	0.262	0.116
Instruct + GRPO	Max	0.402	**0.125**	**0.343**	0.116
	Min	0.402	0.063	0.302	0.116

Table 1: Cover EM scores on multi-hop QA datasets, comparing groups of responses with higher vs. lower uncertainty (derived from average of minimum probability of search query tokens) on knowledge boundary. Bold indicates instances where the Max Prob. group achieved a strictly better performance.

boogle and 3.8% on HotpotQA), across different training methods and base models. This suggests that when the model exhibits higher confidence (lower uncertainty) in its generation path, it is more likely to be on a correct trajectory. Therefore, improving an agent's ability to accurately gauge its internal knowledge state—effectively sharpening its knowledge boundary detection and reducing undue uncertainty—is a crucial step towards mitigating both over-search and under-search, thereby enhancing the overall efficiency and reliability of agentic RAG systems. Our approach is motivated by this principle, aiming to train agents to better assess and reduce uncertainty at each search decision.

3 Approach

Current RL powered agentic RAG methods (Jin et al., 2025a; Song et al., 2025a; Chen et al., 2025) do not explicitly model the knowledge self-awareness during the training process, resulting in generations with low confidence, which are not desired and shown to easily contain wrong answer compared to generations with higher confidence (Table 1). To this end, we propose a simple yet effective variant of GRPO (Shao et al., 2024), β-GRPO, which leverages the uncertainty of the search query spans for more effective rewarding and training.

Agentic RAG with RL (Search-R1 (Jin et al., 2025a)) Given a question, we prompt the policy model to explicitly reason enclosed within `<think></think>` tags about whether to use an off-the-shelf search tool, and, if so, to generate a search query within `<search></search>` tags. The search tool then returns relevant documents inside `<information></information>` tags. Once obtaining new information, the policy model can either continue searching for additional information or provide a final answer within `<answer></answer>` tags. The instruction given to the policy model could be found in Appendix A.4. If the final answer match the groundtruth, the response will be given a reward 1, otherwise 0. And the policy are updated via policy gradient methods like GRPO (Shao et al., 2024).

β-GRPO Motivated by the observation that rollouts with low-confidence search calls are more likely to be incorrect, we incorporate model confidence into the RL reward process. Specifically, for each rollout containing search calls (enclosed within `<search></search>` tags), we extract the probabilities of the search tokens including the tags and use the minimum probability among them as a measure of the model confidence for the search calls within a rollout (Jiang et al., 2023). We then set a confidence threshold β: only rollouts with the confidence of search calls (if exist) above β and correct answers receive a reward of 1, otherwise 0.

4 Experiments

Datasets We follow Search-R1 (Jin et al., 2025a) using a mixture of the NQ (Kwiatkowski et al., 2019) and HotpotQA (Yang et al., 2018) training sets for model training. For evaluation, we consider seven QA benchmarks, including general QA datasets, NQ, TriviaQA (Joshi et al., 2017), and PopQA (Mallen et al., 2023), as well as multi-hop QA datasets: HotpotQA, 2WikiMultiHopQA (Ho et al., 2020), Bamboogle (Press et al., 2023), and MuSiQue (Trivedi et al., 2022). Exact match (EM) is used as our main evaluation metric.

Baselines We compare our method with several baselines: methods that do not use a retriever including direct prompting, Chain-of-Thought (CoT) (Wei et al., 2022) prompting, supervised fine-tuning (SFT) (Chung et al., 2022), and reinforcement learning-based fine-tuning (R1) (DeepSeek-AI et al., 2025); methods that use a retriever but do not perform agentic retrieval, such as Retrieval-Augmented Generation (RAG) (Lewis et al., 2020) and IRCoT (Trivedi et al., 2023); and finally, agentic retrieval methods, including Search-o1 (Li et al., 2025) and Search-R1 (Jin et al., 2025a).

Based on our preliminary experiments, we found that training the policy model from scratch using our confidence-based rewards prevents it from learning effective search behavior. Therefore, we use Qwen2.5-3B (Qwen et al., 2025) and initialize it with the parameters from Search-R1. Then

Methods	General QA			Multi-Hop QA				
	NQ†	TriviaQA⋆	PopQA⋆	HotpotQA†	2wiki⋆	Musique⋆	Bamboogle⋆	Average
Direct Prompting	0.106	0.288	0.108	0.149	0.244	0.020	0.024	0.134
CoT Prompting	0.023	0.032	0.005	0.021	0.021	0.002	0.000	0.015
IRCoT	0.111	0.312	0.200	0.164	0.171	0.067	0.240	0.181
Search-o1	0.238	0.472	0.262	0.221	0.218	0.054	**0.320**	0.255
RAG	0.348	0.544	0.387	0.255	0.226	0.047	0.080	0.270
SFT	0.249	0.292	0.104	0.186	0.248	0.044	0.112	0.176
R1	0.226	0.455	0.173	0.201	0.268	0.055	0.224	0.229
Search-R1	0.406	0.587	0.435	0.284	0.273	0.049	0.088	0.303
Search-R1-GRPO	0.432	0.578	0.413	0.294	0.271	0.067	0.112	0.309
Search-R1-β-GRPO (ours)	**0.468**	**0.625**	**0.449**	**0.334**	**0.304**	**0.086**	0.144	**0.344**

Table 2: Main results. The best performance is set in bold. †/⋆ represents in-domain/out-domain datasets.

Search-R1-GRPO	Search-R1-β-GRPO (ours)
Question: In what Country is Sul America Esporte Clube in? **Generation**: <think> The question asks for the country hosting Sul America Esporte Clube, a team in the brazilian C1 and C2 league, thus the direct reasoning is likely to be Brazilian football team residing in Brazil.	**Question**: In what Country is Sul America Esporte Clube in? **Generation**: <search> in what Country is Sul America Esporte Clube in </search> <information> Doc 1: ... Doc 2: ... Doc 3: ... </information> <answer> Brazil </answer> (Confidence: 0.99)

Table 3: Case Study. The retrieved documents are omitted for clarity.

we continue training using GRPO with different reward functions: one using the original answer-based reward (Search-R1-GRPO), and the other using our proposed confidence-based reward (Search-R1-β-GRPO). We set the value of β as 0.4 according to the analysis in Section 5. Detailed training configurations could be found in Appendix A.5.

Results As shown in Table 2, agentic search with RL training (Search-R1*) significantly outperforms other baselines, indicating that incorporating search through autonomous reasoning and RL training is more effective than non-agentic or prompting methods. Our model, Search-R1-β-GRPO, achieves the highest overall average EM score across the datasets. Figure 3 in Appendix A.5 shows the training rewards for Search-R1-GRPO and Search-R1-β-GRPO. We observe that the rewards for Search-R1-GRPO fluctuate and do not show clear improvement over training steps. In contrast, Search-R1-β-GRPO achieves higher and more stable rewards. This improved performance suggests that our proposed reward assignment based on the confidence of search calls within a rollout is effective.

5 Analysis

Ablation on β & Case Study Following Jiang et al. (2023), we experiment with three confidence threshold values: 0.2, 0.4, and 0.6. The average EM scores are 0.341, 0.344 and 0.336 with a threshold of 0.4 yields the best result. Moreover, we find 115 test cases from the multi-hop QA datasets where Search-R1-β-GRPO produces a correct answer with higher confidence, while Search-R1-GRPO gives an incorrect answer. These cases clearly benefit from the increased model confidence enabled by the proposed β-GRPO. An example is shown in Table 3: Search-R1-GRPO lacks confidence and fails to provide a definite answer, whereas Search-R1-β-GRPO generates a confident search query and produces the correct answer.

Under-searches & Over-searches We also measure the rate of over-search and under-search of our Search-R1-β-GRPO and the baseline Search-R1-GRPO trained based on Qwen2.5-3B with the methods in Section 2.1. Compared with Search-R1-GRPO, which has overall 21.10% over-search rate and 42.04% under-search rate%, our Search-R1-β-GRPO achieves 19.89% over-search rate and 34.71% under-search rate, which are lower than the baseline method. This shows that our method effectively reduces both types of sub-optimal searches.

6 Conclusion

In this work, we formally define and quantify sub-optimal search behaviors, over-search and under-search, in agentic RAG systems, revealing their prevalence and impact. By introducing β-GRPO, a confidence-aware policy gradient method, we enable a 3B model with better agentic RAG ability than strong baselines.

7 Limitations

We formally define and quantify sub-optimal search behaviors in agentic RAG systems and propose β-GRPO to train agentic RAG models with improved self-knowledge awareness. However, we acknowledge that sub-optimal search behaviors, over-search and under-search, are persistent challenges that require further investigation, especially in more open-ended tasks like deep research (Alzubi et al., 2025). Additionally, due to limited computational resources, we are unable to train larger models and leave it for future work.

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A Appendix

A.1 Formal Definition of Under-search & Over-search

Formally, let an LLM agent's interaction for a question be a sequence of steps $T = \{s_1, s_2, \ldots, s_N\}$. Each step s_t comprises a reasoning component r_t. If the model decides to retrieve information, the retrieval step $s_t^R = (r_t, q_t, c_t)$ includes a search sub-query q_t and the retrieved context $c_t = search(q_t)$. The sub-answer a_t for this step s_t^R is typically derived using c_t and reflected in r_{t+1}. If the model does not retrieve, the non-retrieval step $s_t^{NR} = (r_t)$ relies on the existing context $\{s_1, s_2, \ldots, s_{t-1}\}$ and the model's internal knowledge M to derive a_t reflected in r_t. Let a_t^* be the ground-truth answer step s_t. Over-search occurs if a retrieval step s_t^R's answer a_t could have been derived from M and $\{s_1, s_2, \ldots, s_{t-1}\}$ only. Under-search occurs if a non-retrieval step s_t^{NR} leads to $a_t \neq a_t^*$.

A.2 Detailed Step-wise Analysis Procedure

To empirically measure the rates of over-search and under-search, we conducted a detailed step-wise analysis of the agent's decision-making process. The interactions of the agent are logged as a sequence of steps, where each step can involve internal reasoning (thinking), querying a search tool, processing retrieved context, and generating an answer. We define specific procedures to identify and quantify each type of sub-optimal search behavior:

1. **Step Extraction:** We parse the agent's interaction log following the definition in Appendix A.1. Each distinct thinking process is a decision point and considered a step, typically delineated by <step> and </step> tags (or a similar structured logging format). A "search step" is identified as any step where all three relevant operations—think (the model's reasoning), search (the search query issued), context (the information retrieved). A "non-search step" typically only consists of thinking. In this work specifically, the Step Extraction is done by prompting QwQ-32B (Qwen et al., 2025) as we discover that reasoning LLM typically perform better on such task.

2. **Extraction of Partial Input:** For each identified search step, we reconstruct the input that would have been available to the model before it decided to search. This is achieved by taking the complete output generated by the agent from the beginning of the interaction up to and including the content of the think field of the current search step.

3. **Querying with Internal Knowledge for Over-search Analysis:** For over-search rate measurement, the extracted partial output is then appended with a specific instructional prompt: "I will use my own knowledge to answer this query and provide my answer to this query enclosed in <query_answer> </query_answer> tags." This combined text serves as a new input to the original RL-tuned model (e.g., Search-R1-β-GRPO and Search-R1-GRPO), which is tasked with generating an answer without performing any new search. The over-search rate is then measured by computing the percentage of steps that provide equivalent answer (determined by QwQ-32B in our analysis) for both with and without searching, among all "search steps".

4. **Generation of Reference Answer for Under-search Analysis:** For each identified non-search step, the original query or sub-query that the agent was attempting to answer at that point is presented to a more powerful, state-of-the-art language model (e.g., ChatGPT-4o (OpenAI et al., 2024)) with recent knowledge cutoff date. This model generates a "reference answer," which is assumed to be of high quality. The reference answer obtained is compared with the actual answer generated by the agent for that non-search step. The under-search rate is calculated as the proportion of non-search steps where the agent's answer does not match (determined by QwQ-32B in our analysis) the reference answer, quantifying how often the agent fails to search when doing so would have likely led to a more accurate or complete answer.

A.3 Search Frequency vs. Optimal Hops

One indicator of potential over-search is when the number of search queries generated by an agent exceeds the optimal number of reasoning hops required to answer a question. A significantly higher search count often points to redundant information gathering. For this experiment, we only use the test set from Bamboogle (Press et al., 2023) and MuSiQue (Trivedi et al., 2022) as they are the only two datasets providing pre-defined number of hops for each test sample.

Model	Dataset	Search vs. Hops	Correct (%)	Incorrect (%)	Sum (%)
R1-Searcher	Musique	Less	2.8	19	21.8
		Match	21.8	45.8	67.6
		More	1.8	8.8	10.6
R1-Searcher	Bamboogle	Less	0	0	0
		Match	40.8	52.8	93.6
		More	3.2	3.2	6.4
Search-R1	Musique	Less	1.8	7	8.8
		Match	12.4	27.6	40
		More	8.8	42.4	51.2
Search-R1	Bamboogle	Less	0.8	1.6	2.4
		Match	28.8	28	56.8
		More	12	28.8	40.8

Table 4: Comparison of the number of searches generated vs. annotated hops on Bamboogle and Musique datasets. "More" indicates potential over-search as number of searchers exceeds pre-defined optimal hops. "Less" may indicate a potential under-search.

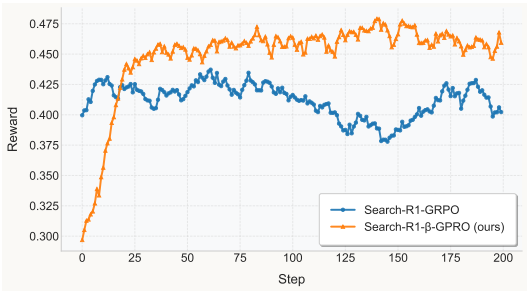

Figure 3: Training Rewards for Search-R1-GRPO and Search-R1-β-GRPO.

R1-Searcher exhibits a tendency to perform more searches than hops in 10.6% of Musique cases and 6.4% of Bamboogle cases. Search-R1 shows a more pronounced tendency, with 51.2% (Musique) and 40.8% (Bamboogle) of cases issuing more searches than annotated hops. This result suggests that models trained with different methods do not inherently solve over-search and might even exacerbate it under certain configurations if not properly guided. While "Less" searches than hops might indicate efficient reasoning or under-search, the "More" category strongly suggests instances of over-searching.

A.4 Instruction

> Answer the given question. You must conduct reasoning inside <think> and </think> first every time you get new information. After reasoning, if you find you lack some knowledge, you can call a search engine by <search> query </search>, and it will return the top searched results between <information> and </information>. You can search as many times as you want. If you find no further external knowledge needed, you can directly provide the answer inside <answer> and </answer> without detailed illustrations. For example, <answer> Beijing </answer>. Question: question.

A.5 Training Configuration & Rewards

We train Search-R1-GPRO and Search-R1-β-GPRO for 200 steps, with a learning rate of 1e-6 and batch size of 512. For a question, we produce 5 generations with temperature of 1 to form a GPRO group. For the search engine, for fair comparison, we also use 2018 Wikipedia dump (Karpukhin et al., 2020) as the knowledge source and E5 (Wang et al., 2022) as the retriever as Search-R1 and for each search query, top-3 documents are returned. Our training are conducted on two A100 GPUs.