

AirRAG: Activating Intrinsic Reasoning for Retrieval Augmented Generation using Tree-based Search

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Abstract

Leveraging the autonomous decision-making capabilities of large language models (LLMs) has demonstrated superior performance in reasoning tasks. However, despite the success of iterative or recursive retrieval-augmented generation (RAG) techniques, these methods are often constrained to a single solution space when confronted with complex problems. In this paper, we propose a novel thinking pattern in RAG that integrates system analysis with efficient reasoning actions, significantly **Activating intrinsic reasoning** capabilities and expanding the solution space of specific tasks via Monte Carlo Tree Search (MCTS), which we refer to as **AirRAG**. Specifically, our approach designs five fundamental reasoning actions, which are expanded to a broad tree-based reasoning space using MCTS. The approach also incorporates self-consistency verification to explore potential reasoning paths and inference scaling law. Additionally, computationally optimal strategies are employed to allocate more inference resources to key actions, thereby enhancing overall performance. Experimental results demonstrate the effectiveness of AirRAG, showing significant performance gains on complex question-answering datasets. Furthermore, AirRAG is flexible and lightweight, making it easy to integrate with other advanced technologies.

1 Introduction

Retrieval-Augmented Generation (RAG) has shown great potential in addressing the issue of generating factually incorrect content, especially in domain-specific or knowledge-intensive tasks (Kandpal et al., 2023). However, as task complexity increases, several new challenges emerge, such as the inability to retrieve sufficient knowledge with a single query and the difficulty of understanding the intricate reasoning logic inherent

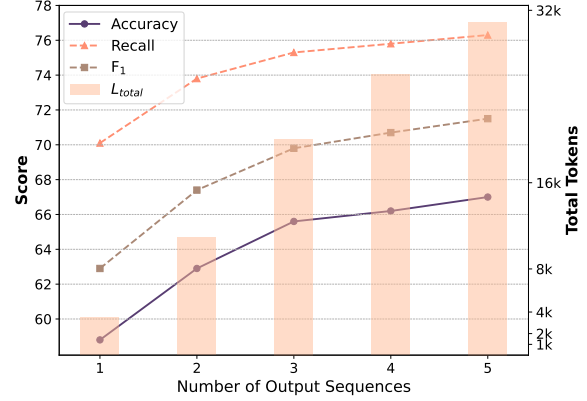


Figure 1: Comparison of average performance across three datasets with varying numbers of output sequences. L_{total} represents the total number of tokens consumed during the reasoning process. AirRAG leverages generation diversity and self-consistency to explore the potential solution space, significantly enhancing overall performance by scaling inference computation.

in the question. To tackle these challenges, it is crucial to harness the reasoning capabilities of large language models (LLMs) to improve RAG performance (Jiang et al., 2023; Jeong et al., 2024; Asai et al., 2024; Yu et al., 2024).

Previous research on complex query scenarios has primarily focused on optimizing the query and retrieval processes to obtain relevant information (Shi et al., 2023; Zhou et al., 2023; Gao et al., 2023; Jiang et al., 2023; Zheng et al., 2024). While these methods improve task efficiency, their performance often depends heavily on manually crafted rules and prompt engineering, limiting flexibility and making it difficult to adapt quickly to different scenarios. Moreover, recursive retrieval is frequently used to improve the depth and relevance of search results in information retrieval tasks. This process continuously updates intermediate queries and results to satisfy dynamic information needs during the complex task-solving process (Jiang et al., 2023; Asai et al., 2024; Yan et al., 2024;

Jeong et al., 2024). Recent approaches leverage the decision-making abilities of LLMs to implement automated iterative retrieval and generation (Yu et al., 2024; Yue et al., 2024).

However, these approaches face two significant issues. First, modular RAG struggles to cover the diverse range of question types, requiring substantial human effort and resulting in inefficiencies. The limited solution space also prevents the full activation of LLMs’ decision-making abilities. Second, the single reasoning paradigm and the chain-like reasoning process often fail to effectively explore the solution space, particularly when reasoning relies on self-exploration. This process is vulnerable to low-quality intermediate reasoning steps and is easily trapped in a narrow solution space. Furthermore, guiding self-exploration becomes challenging when using relatively smaller language models (e.g., *Qwen2.5-14B-Instruct* (Yang et al., 2024)). Therefore, it is necessary to design rational reasoning actions that comprehensively explore a broad and deep solution space.

In response to these challenges, we propose AirRAG, a method that leverages intrinsic reasoning capabilities and expands the solution space using Monte Carlo Tree Search (MCTS). We design five fundamental reasoning actions: system analysis, direct answer, retrieval-answer, query transformation, and summary-answer. These actions can effectively address a wide range of problems in various scenarios, including those that require progressive or parallel queries. Importantly, these actions can be executed efficiently even on relatively smaller language models. Additionally, we introduce MCTS and self-consistency to enable controllable reasoning path generation and efficient inference scaling. To accurately select the answer from multiple reasoning paths, we combine a voting mechanism with a process-supervised reward model. As inference computation increases, our approach demonstrates significant performance improvements as shown in Figure 1. Moreover, AirRAG features a flexible architecture that can easily integrate other advanced methods into the approach as additional action branches. In summary, our main contributions are as follows:

- We design five fundamental reasoning actions that can address most problem types in RAG scenarios, ensuring controllable reasoning processes.
- We introduce MCTS and self-consistency to

effectively expand the solution space for complex tasks. Our approach improves generalization and performance through comprehensive inference scaling and a pluggable architecture.

- We show through experimental results that AirRAG outperforms current iterative or recursive RAG approaches, effectively activating the intrinsic reasoning capabilities of LLMs and expanding the solution space in a controllable manner.

2 Related Work

Retrieval-Augmented Generation (RAG). RAG has demonstrated significant improvements in the performance of LLMs in knowledge-intensive tasks. Compared to vanilla RAG, optimizing the query and retrieval process enhances knowledge correlation and, consequently, improves reasoning performance. Several methods, such as query expansion and transformation, have been proposed to achieve better retrieval results (Zhou et al., 2023; Ma et al., 2023; Gao et al., 2023). However, as task complexity increases, retrieving sufficient knowledge in a single query becomes increasingly difficult. To address this, iterative retrieval techniques have been proposed to gather additional contextual references. For instance, IR-CoT (Trivedi et al., 2023) utilizes chain-of-thought (CoT) to guide the retrieval process, refining the CoT with the retrieved information. Similarly, ITER-RETGEN (Shao et al., 2023) combines retrieval and generation modules to promote a deeper understanding of specific tasks.

Activating the reasoning capabilities of LLMs in RAG. In addition to optimizing retrieval, activating the reasoning capabilities of LLMs can significantly improve the efficiency and relevance of the retrieved information. Leveraging the decision-making abilities of LLMs enhances the overall performance (Nakano et al., 2022; Schick et al., 2023). Self-RAG and its variants (Asai et al., 2024; Yan et al., 2024; Jeong et al., 2024) adopt a self-reflection mechanism that iteratively predicts reflection tokens during training, enabling better control during inference. Auto-RAG (Yu et al., 2024) systematically plans retrievals and refines queries to acquire valuable knowledge through multi-turn iterations. IterDRAG (Yue et al., 2024) explores inference scaling strategies in RAG, enhancing LLMs’ ability to effectively acquire and utilize contextual information. Despite the progress made in

these methods, they often struggle to explore the solution space effectively during reasoning. Self-exploration frequently leads to being trapped in a limited solution space, hindered by low-quality reasoning steps even after multiple iterations. This issue is often attributed to the chain reasoning pattern and the difficulty small-scale LLMs face when handling overly complex tasks in a single iteration. **Monte Carlo Tree Search (MCTS)**. To address these challenges, tree-based search algorithms, particularly Monte Carlo Tree Search (MCTS), have emerged as effective tools to expand search spaces and enhance reasoning capabilities (Silver et al., 2017; Chen et al., 2024; Qi et al., 2024; Zhang et al., 2024). MCTS has been shown to extend reasoning by exploring multiple branching queries, thus enabling the exploration of diverse reasoning paths (Yao et al., 2023; Besta et al., 2024). In the mathematical reasoning scenario, Zhang et al. (2024) and Chen et al. (2024) leverage MCTS to achieve more efficient exploration of solution spaces, while Qi et al. (2024) designs rich human-like reasoning actions to improve reasoning trajectories. Furthermore, recent research indicates that inference scaling (Yue et al., 2024) and self-consistency (Wang et al., 2023) can lead to substantial improvements. In this context, our approach samples diverse reasoning paths to achieve both inference scaling and self-consistency verification during the next expansion of the action space.

Unlike existing methods that focus on optimizing query and retrieval processes or leveraging LLMs’ reasoning capabilities through iterative retrieval, AirRAG uniquely integrates MCTS and self-consistency to systematically expand the solution space and ensure the controllability of the reasoning process. Simultaneously, we design five fundamental reasoning actions that effectively address a broader range of question types, particularly in complex tasks. This pluggable architecture also allows for easy integration of current advanced methods, making AirRAG a flexible and powerful solution for RAG scenarios. In the experiment, we thoroughly verify the performance gains brought by the inference scaling law and investigate how to rationally allocate inference resources.

3 Methodology

In order to effectively explore the solution space during reasoning, we propose a controllable tree-based framework of RAG. This framework com-

bines Monte Carlo Tree Search (MCTS) with five distinct reasoning actions, enabling efficient and controlled expansion of the solution space. Meanwhile, we further implement more comprehensive inference scaling strategies based on Yue et al. (2024) and employ pruning techniques along with computationally optimal strategies to strike a balance between effectiveness and efficiency. The whole process is illustrated in Figure 2.

3.1 Define Fundamental Reasoning Actions

Relying solely on the autonomy of LLMs for iterative self-exploration often results in getting trapped in a solution space that is difficult to navigate, especially when dealing with different types of complex questions. IterDRAG (Yue et al., 2024) uses a single action type to generate the next reasoning step, which can lead to ineffective space exploration. The core of MCTS generation lies in the action space, which defines the scope of tree exploration. Therefore, simplifying human cognitive processes in complex reasoning is essential (Jaffe et al., 2023). Inspired by this, we introduce five fundamental human-like reasoning actions to bridge the gap between LLM reasoning and human cognition in RAG scenarios.

- A_1 : *System Analysis* (SAY). This action analyzes the overall structure of the problem, followed by its decomposition or planning. It represents systematic and global thinking before problem-solving.
- A_2 : *Direct Answer* (DA). This action leverages parametric knowledge of LLMs to answer questions directly, without relying on any external knowledge.
- A_3 : *Retrieval-Answer* (RA). This action retrieves related knowledge from the external knowledge base to support subsequent reasoning.
- A_4 : *Query Transformation* (QT). This action transforms human questions in order to improve retrieval performance. It supports various transformations, such as rewriting, step back prompting, follow-up questions and multi-query retrieval.
- A_5 : *Summary-Answer* (SA). This action combines intermediate reasoning steps, answers and the initial questions to generate the final answer.

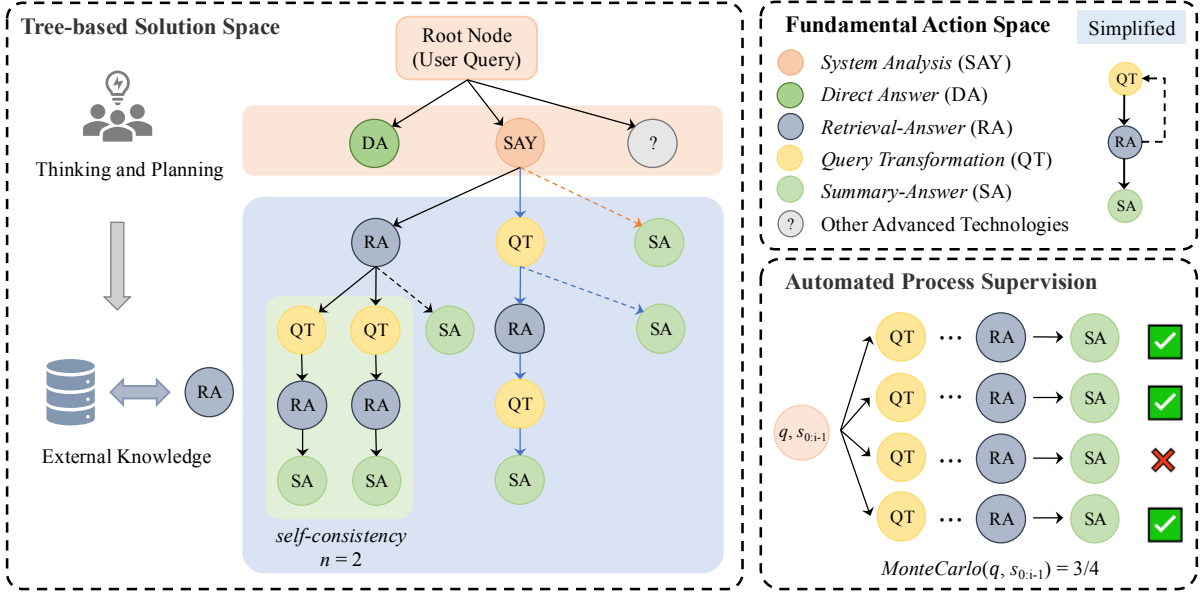


Figure 2: The schematic diagram of our proposed AirRAG. AirRAG implements a paradigm that combines system thinking with step-by-step reasoning. In the inference phase, we introduce MCTS and self-consistency to scaling computation, which significantly outperforms other strong baselines.

The above five actions define a highly diverse action space $\{A_1, A_2, A_3, A_4, A_5\}$. In the first step, the initial state is denoted as s_0 and then MCTS selects the action a_1 and a_2 to prompt the LLM to generate the next reasoning steps in parallel. Subsequent actions are performed sequentially to expand the reasoning path. It is important to note that there are sequential dependencies between different actions. For example, A_1 and A_2 can only be executed after the root question. Additionally, we incorporate the diverse sampling of self-consistency (Wang et al., 2023) for each action to expand the reasoning paths. Specifically, an action is more likely to generate the correct reasoning step if we sample multiple times in the current state. Finally, we can obtain multiple generated reasoning trajectories, such as $[s_0 \oplus s_{1:n}]$. To further improve inference efficiency, we choose the action $\{A_3, A_4, A_5\}$ as a simplified action space, referred to as *AirRAG-Lite*, which achieves a better balance between efficiency and effectiveness.

3.2 Perform Reasoning Processes via MCTS

3.2.1 Solution Generation

Based on the action space defined above, we introduce MCTS to generate candidate reasoning trajectories. The initial root node, s_0 , represents the question without any reasoning steps. The policy is directly modeled by a language model as $\pi(a|s) = \text{LM}(a|s)$, and the state transition func-

tion combines preceding reasoning steps with current actions, i.e., $s_i = \text{Concat}(s_{0:i-1}, a_j)$. During each MCTS rollout, we execute multiple steps, including *selection*, *expansion*, *simulations*, and *backpropagation*. Multiple rollouts are performed to expand the solution space. To balance the exploration and exploitation, we adopt the well-known Upper Confidence Bounds applied to Trees (UCT) (Kocsis and Szepesvári, 2006) for node selection as follows:

$$\text{UCT}(s, p) = \frac{Q(s, a)}{N(s)} + w \sqrt{\frac{\log N_p(s)}{N(s)}}, \quad (1)$$

where $Q(s, a)$ is the reward value for node s and is updated through backpropagation. $N(s)$ denotes the number of visits to s , p is the parent node of s , and w is the weight to balance exploration and exploitation.

When the search reaches a terminal node, defined either by a terminal state or a predetermined maximum tree depth d , we obtain a trajectory from the root to the terminal node. All trajectories from the rollout iterations are collected as candidate solutions. Section 3.3 explains how we select the optimal answer node from these trajectories.

3.2.2 Inference Scaling

Numerous studies have demonstrated that scaling inference computation can significantly improve the performance of LLMs without additional training (Snell et al., 2024; Yue et al., 2024). Based on

the above methods, we explore strategies to leverage inference computation scaling in AirRAG. One straightforward strategy is extending the *effective context length* (short for L_{\max}) during the document retrieval phase, allowing more related documents to supplement the knowledge base. Additionally, we perform multiple *rollouts* to thoroughly explore the solution space relying on the tree-based search. Adjusting *the number of output sequences* (n) generated during certain actions enables self-consistency verification and further inference scaling. These strategies provide flexibility for scaling inference computation in RAG, empowering LLMs to address complex knowledge-intensive queries more effectively.

To improve efficiency and minimize redundant computations, we implement an early pruning strategy for state nodes and reasoning paths. Deduplication is applied to the output sequence states generated by each action, ensuring the diversity of the subsequent path. Furthermore, if multiple rollouts select the same state sequence, only one valid reasoning path is retained.

3.2.3 Flexible Architecture

Our tree-based architecture provides the flexibility to integrate other advanced approaches. We reproduce the IterDRAG method based on the prompt design by Yue et al. (2024). Meanwhile, inspired by its iterative implementation, we simplify the fundamental action space to $\{A_3, A_4, A_5\}$, enabling a faster implementation while still achieving relatively good results. These methods serve as an exploratory extension of our approach and can be activated or deactivated as needed.

3.3 Select the Optimal Answer Node

For common mathematical reasoning tasks, a simple consistency-based method can efficiently select the most precise reasoning path. For example, the most frequent number extracted from multiple candidate solutions in MATH (Hendrycks et al., 2021) can be chosen as the final answer. However, extracting precise answers and performing effective aggregation becomes more challenging for knowledge-intensive tasks. To address this, we design two self-consistency verification methods for such problems. *Jaccard similarity* and *text embeddings* are two different approaches used in natural language processing to measure the similarity between texts. We apply these methods to cluster text

answers and compute answer scores as follows:

$$\text{jcdScore}_i = \frac{1}{N} \sum_{j=1}^N \frac{|A_i \cap A_j|}{|A_i \cup A_j|}, \quad (2)$$

$$\text{embScore}_i = \frac{1}{N} \sum_{j=1}^N \cos(E_i, E_j), \quad (3)$$

where N is the number of valid answer nodes, A_i is the word-level set of answer text i , and E_i denotes the embedding vector of answer text i .

In addition, we further investigate the *self-refine* and process-supervision *reward model* to identify the most accurate reasoning trajectory. Self-refinement uses the A_5 (Summary-Answer) action to refine the final answer from all candidate answer nodes. The reward modeling process consists of two steps: data synthesis and instruction tuning.

- **Data synthesis:** We leverage MCTS to perform multiple rollouts on partial training sets. Based on known ground truth, we sample positive and negative reasoning trajectories and use Monte Carlo estimation to evaluate intermediate state scores.
- **Instruction tuning:** Synthetic samples are used to fine-tune a relatively small LLM, such as *Qwen2.5-14B-Instruct*.

4 Experiments

In this section, we conducted experiments on complex QA benchmarks by answering the following research questions.

- **RQ1:** Does AirRAG outperform state-of-the-art baselines?
- **RQ2:** How does AirRAG perform when it comes to comprehensive inference scaling?
- **RQ3:** What is the performance benefit of AirRAG in optimizing the allocation of inference computation?
- **RQ4:** How does AirRAG perform for various verification methods for multiple candidate rollouts?
- **RQ5:** What is the intuitive performance of AirRAG in the reasoning process?

4.1 Experimental Settings

4.1.1 Datasets

To evaluate the effectiveness of AirRAG, we conduct experiments on various question-answering (QA) tasks, including both open-domain QA and multi-hop QA. The complex multi-hop QA datasets consist of HotpotQA (Yang et al., 2018), MuSiQue (Trivedi et al., 2022) and 2WikiMultiHopQA (2Wiki) (Ho et al., 2020). Other single-hop QA datasets include Natural Questions (NQ) (Kwiatkowski et al., 2019), TriviaQA (Joshi et al., 2017), PopQA (Mallen et al., 2023) and WebQA (Berant et al., 2013).

4.1.2 Implementation Details

We use the hyperparameters reported for the existing models whenever available. Implementation details are available in the Appendix A.

4.1.3 Baselines and Metrics

To investigate the enhancement effects of thinking and planning on complex RAG tasks, we compare it with vanilla RAG, which performs only a single retrieval and generation process. We evaluate the naive generators of *Qwen2.5-14B-Instruct* (Yang et al., 2024) and *Llama-3-8B-Instruct* (Grattafiori et al., 2024). In the retrieval phase, we employ *multilingual-e5-base* (Wang et al., 2024) as the retriever. The prompt of vanilla RAG are shown in the Appendix C. For iterative retrieval, we compare AirRAG with Iter-RetGen (Shao et al., 2023), Self-RAG (Asai et al., 2024), Auto-RAG (Yu et al., 2024), and IterDRAG (Yue et al., 2024). To further explore RAG performance and inference computation scaling, we focus on a comparison with IterDRAG for a given budget on inference computation. For evaluation metrics, we report Exact Match (EM), F1 score (F1) and Accuracy (Acc) between the generated summary and gold answer, where accuracy measures whether the gold answer is covered in the generated answer.

4.2 Main Results (RQ1)

We first evaluate the performance of AirRAG on various complex QA datasets. Table 1 compares its accuracy and F1 with strong baselines under the given inference computation budget, which is implemented based on *Qwen2.5-14B-Instruct* and one million document database. The optimal performance exhibits consistent gains as L_{\max} expands, which is termed as the *inference scaling laws* for RAG (Yue et al., 2024). We integrate the remaining

methods for a given maximum computational budget into our approach, dubbed as *AirRAG-Blender*. The best results are obtained by using only the SA action to refine the final answer from all candidates, as shown in Table 1. This also demonstrates the flexibility of our approach architecture. In addition, to verify the robustness and generalization of AirRAG, Table 5 shows the performance on more diverse LLMs and datasets. For a fair comparison, we utilize the widely used Wikipedia dump from December 2018 (Karpukhin et al., 2020) as the retrieval corpus. We observe consistent improvements over vanilla RAG and existing iterative methods (more than 10% on average). The significant boost over IterDRAG and Auto-RAG suggests that AirRAG explores more effective reasoning paths through the human-like thinking paradigm and tree-based search.

4.3 Inference Scaling for RAG (RQ2)

Inference computation scaling can enable LLMs to improve their output performance (Snell et al., 2024). Self-consistency can also improve the robustness of the reasoning process (Wang et al., 2023). Therefore, we carry out a comprehensive experimental analysis on the inference computation scaling. Based on tree-based search and RAG scenario, there are multiple ways to optimize the use of inference computation resources. Specifically, we can adjust both the number of retrieved documents in a single retrieval and the effective context length in all iterations. The average performance of three datasets exhibits consistent gains in Figure 3. In subsequent experiments, unless otherwise specified, the data presented represent the average performance across the HotpotQA, MuSiQue, and 2Wiki datasets. In particular, the initial computation scaling brings significant performance improvements. In addition, the number of output sequences and rollouts in MCTS can expand the solution space and explore potential reasoning paths. As shown in Figure 1, the average performance increases with the number of output sequences per action, demonstrating the effectiveness of self-consistency. We also investigate the number of effective reasoning paths under different rollouts in Figure 4. Similarly, the performance improvement caused by the increase of effective reasoning paths in the early stage is relatively high. Similarly, the increase in early reasoning paths leads to relatively higher performance gains. We provide additional dataset-specific results in Appendix B.

L_{\max}	Method	HotpotQA		MuSiQue		2Wiki		Average	
		F1	Acc	F1	Acc	F1	Acc	F1	Acc
8k	ZeroShot QA	42.5	41.3	13.5	12.1	48.2	47.3	34.7	33.6
	Vanilla RAG	70.3	65.4	23.0	17.7	55.8	53.4	49.7	45.5
	IterDRAG*	74.3	69.1	26.7	19.4	60.5	57.6	53.8	48.7
	AirRAG-Lite	80.6	75.4	35.4	28.9	75.3	73.1	63.8	59.1
	AirRAG	79.6	75.2	41.0	35.0	76.0	74.2	65.6	61.5
32k	AirRAG-Blender	81.1	79.8	41.6	36.4	82.2	81.7	68.3	66.0
	Vanilla RAG	77.1	72.0	29.0	22.9	60.9	58.1	55.7	51.0
	IterDRAG*	77.7	71.6	30.8	22.3	63.0	60.2	57.1	51.4
	AirRAG-Lite	82.4	76.9	36.7	30.1	78.8	76.8	66.0	61.3
	AirRAG	82.5	77.4	43.2	36.3	80.4	78.9	68.7	64.2
128k	AirRAG-Blender	82.9	80.6	43.3	37.6	83.4	83.0	69.9	67.1
	IterDRAG*	76.8	71.0	31.7	24.8	65.5	62.4	58.0	52.7
	AirRAG-Lite	82.5	77.1	35.7	30.4	78.3	76.0	65.5	62.2
	AirRAG	83.3	78.0	43.5	36.5	82.3	80.5	69.7	65.0
	AirRAG-Blender	83.7	81.4	43.9	38.5	84.4	84.2	70.6	68.0

Table 1: Overall evaluation results on the test sets of three datasets. * indicates the results reproduced by us. L_{\max} denotes the maximum number of input tokens across all rollouts. The best results for each L_{\max} are in **bold**. The number of both rollouts and output sequences is set to 1.

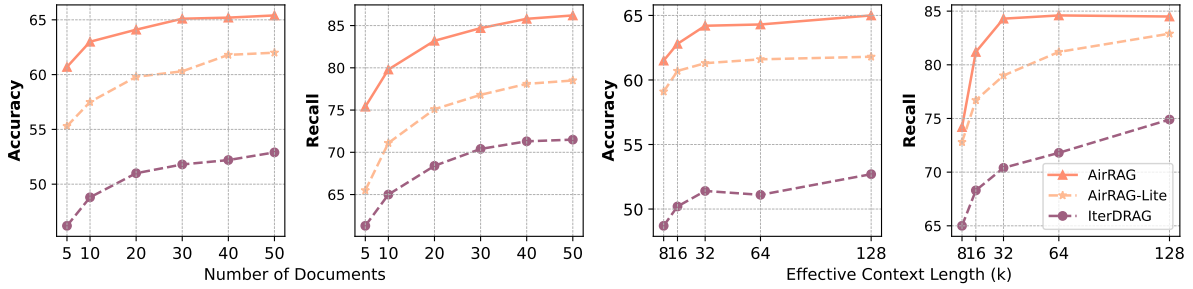


Figure 3: Impact of the retrieved document number scaling (Left) and the maximum context length scaling (Right) on model performance (averaged Accuracy and Recall of three datasets). All methods show consistent performance improvements as the effective inference computation scales.

Method	Average	
	F1	Acc
Vanilla RAG	47.0	43.2
IterDRAG	49.8	45.9
AirRAG		
+ $n_{\text{all}}=1$	62.9	58.8
+ $n_{\text{all}}=3$	63.4	62.1
+ $n_{a_1, a_4}=3, n_{a_2, a_3, a_5}=1$	63.2	62.0
+ $n_{a_1, a_4}=3, n_{a_2, a_3, a_5}=1, q_{\text{div}}=1.0$	65.1	63.9

Table 2: Performance comparison with different computationally optimal strategies. n_{a_i} denotes the number of output sequences of the reasoning action a_i in a single extension. q_{div} indicates that setting top- p to 1.0 and temperature to 1.0 for query-related actions, i.e. SAY and QT, increases the diversity of reasoning. The default sampling parameters top- p , top- k and temperature are set to 0.8, 50 and 0.7 respectively. Rational sampling strategies and inference scaling further improve performance across multiple datasets.

4.4 Ablation Studies

Effect of Computationally Optimal Strategies (RQ3). Extensive experiments show that the outputs of certain actions (e.g., RA, DA and SA) are almost consistent when performing multiple generations. Therefore, we only increase the number of output sequences (short for n) for the remaining actions (e.g., SAY and QT), which reduces invalid inference computation while maintaining good results. This also reflects that this kind of reasoning action, which effectively activates the creativity of LLMs, requires more diversified sampling strategies. We adjust the sampling parameters (top- $p=1.0$ and temperature=1.0) to improve the diversity of the model output. The complete experimental results in Table 2 show that the diversity of key actions can significantly improve performance.

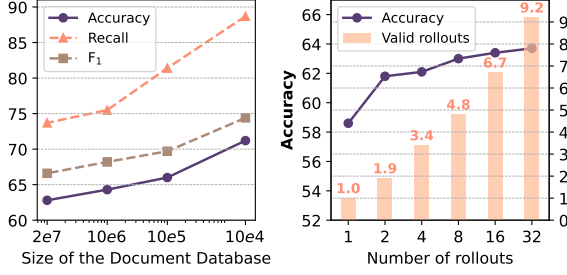


Figure 4: **Left:** Performance comparison under different size of document database. A streamlined database can maintain a better performance. **Right:** Performance comparison in increasing the number of valid rollouts. Sampling a higher number of diverse reasoning paths consistently improves accuracy.

From the aforementioned experiments, it is observed that the recall and accuracy of model are linearly correlated. Intuitively, the size of document database is also related to the recall score. By reducing the scale of the document database, we find a gradual improvement in model performance (shown in Figure 4). This observation provides experimental evidence for effective database partitioning in practical application.

Effect of Verification Methods (RQ4). The larger search space also generates more candidate reasoning trajectories. Therefore, how to select the optimal trajectory is crucial for the final performance. We compare multiple verification methods with the average scores of all candidates in Figure 5. These two self-consistency verification methods are always slightly better than the average score, but they are not nearly as good as the SA and QwenRM methods. The SA method uses the LLM to further refine the final answer from all candidate rollouts, which is simple and effective. Finally, the reward model achieves the most competitive results due to the introduction of supervised information on key intermediate reasoning steps in the training process. However, collecting process-supervised training samples requires high computational costs and high-quality raw data. In the practical application scenario, we can choose the appropriate method while balancing efficiency and effectiveness.

4.5 Qualitative Analysis (RQ5)

To make it easier to understand why our proposed AirRAG works, we present a qualitative analysis in MuSiQue. Existing iterative methods are often trapped in a single solution space when confronted with complex tasks. As illustrated in Figure 13,

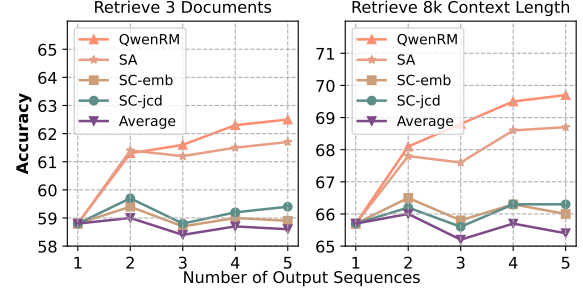


Figure 5: Performance comparison of different verification methods. "QwenRM" is short for reward model trained on the Qwen model. "SA" is the reasoning action of summary and answer. "SC-emb/jcd" are two self-consistency verification methods based on text embeddings and jaccard similarity. "Average" is the average score over all candidate rollouts. The single retrieval process is set to retrieve three documents or fixed 8k context.

these iterative methods exhibit a key limitation that insufficient or ambiguous retrieval context can lead to repetitive follow-up queries until it reaches the predefined maximum depth of iterations. This inefficient iteration results in high computational cost and incorrect answer. In contrast, our proposed AirRAG designs efficient reasoning actions to activate the intrinsic reasoning capabilities of LLMs. As shown in Figure 14, the SAY action decomposes the original query into a more rational sequence of sub-queries, and then the combination of RA and QT ensures the accuracy of the intermediate reasoning step. We eventually leverage the efficient reasoning trajectory to obtain the correct answer.

5 Conclusions

In this paper, we propose AirRAG, a novel RAG approach to activate intrinsic reasoning capabilities of LLMs. AirRAG designs an efficient action space for the controllable reasoning generation. We also introduce Monte Carlo Tree Search to expand the solution space. Meanwhile, by employing the tree-based search and self-consistency verification, we explore potential reasoning paths and achieve comprehensive inference computation scaling in RAG. In addition, computationally optimal strategies are used to apply more computation to key actions, leading to further performance improvements. Experimental results on diverse QA datasets demonstrate the significant superiority of AirRAG over other methods designed for complex RAG scenarios. Furthermore, AirRAG can be integrated with other advanced methods with great flexibility.

Limitations

Although our model achieves competitive performance in various RAG tasks, there are some methods and limitations that can be improved. The current optimal computation allocation strategy is derived from sufficient experiments. We can consider designing an automated policy model to implement the trade-off between computational cost and performance. Despite great efforts in the inference scaling of RAG, the experimental analysis may be limited due to the massive computational cost of tree-based search approaches. We will explore more complex reasoning tasks to verify the robustness and effectiveness of our approach. In addition, the large search space also brings more noise information, so we will further investigate the reward model or strategy to explore a better reasoning path.

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A Implementation Details

For evaluation, we randomly select 1,000 samples from the whole validation sets of each dataset as our final test set, with a fixed random seed 0. To better understand the complexity of multi-hop reasoning in these datasets, we analyze the hop distribution of the HotpotQA, MuSiQue, and 2Wiki-MultiHopQA test sets in Figure 6. The statistics show that there is a high proportion of complex reasoning queries with 3 hops or more (about 30%, 50%, 25%). HotpotQA lacks explicit hop annotations, so we instead count the number of supporting facts. MuSiQue has a significantly higher proportion of 3-hop and 4-hop queries compared to the other datasets, indicating great reasoning complexity. This observation is further corroborated by our experimental results in Table 1 and Figure 7. The performance of our approach on MuSiQue is much lower than those of the other two datasets.

In the retrieval process, we employ the *multilingual-e5-base* (Wang et al., 2024) as the retriever and use the widely used Wikipedia dump from December 2018 as the retrieval corpus (Karpukhin et al., 2020) which comprises over 21 million passages. For generation, the default sampling parameters $\text{top-}p$, $\text{top-}k$ and temperature are set to 0.8, 50 and 0.7 respectively. Evaluation metrics include Exact Match (EM), F1 score (F1), and Accuracy (Acc), where accuracy indicates whether the ground truth is a substring of the final generated answer. For reward model training, we sample 8,000 question-answer pairs from each dataset and generate more than 156,000 reasoning paths using our proposed AirRAG (rollouts=32, $n=4$, $q_{div}=1.0$). In inference scaling experiments, we sample maximum computation budgets L_{\max} (e.g., 8k, 16k, 32k, 64k and 128k tokens). The L_{\max} (maximum effective context length) denotes the maximum number of input tokens across all rollouts following (Yue et al., 2024). The predetermined maximum tree depth d is set to 10, specifically indicating that the SAY and SA actions are executed once, while the RA-QT or QT-RA actions have a maximum of 4 iterations.

B Additional Experiment Results

We report the average performance of our approach on three datasets with the support of the *Qwen2.5-72B-Instruct* model in Table 3 and 4. The experimental results show that the performance is further improved (+4.6%, +6.1%, +6.9% in average accu-

racy) over 14B model. Meanwhile, we observe that the performance of our AirRAG based on the 14B model surpasses other methods using a 72B model. Furthermore, we present detailed inference scaling results for each dataset individually, as shown in Figure 7 and Figure 8.

Method	Qwen2.5-72B		Qwen2.5-14B	
	F1	Acc	F1	Acc
Vanilla RAG	51.6	46.9	47.0	43.2
IterDRAG	53.4	48.5	49.8	45.9
AirRAG	69.6	68.5	65.1	63.9

Table 3: Performance comparison between *Qwen2.5-14B-Instruct* and *Qwen2.5-72B-Instruct*. Three documents are retrieved in a single RA action. Rollouts and n are set to 32 and 3 respectively.

L_{\max}	Method	Qwen2.5-72B		Qwen2.5-14B	
		F1	Acc	F1	Acc
8k	ZeroShot QA	38.8	37.6	34.7	33.6
	Vanilla RAG	56.2	51.8	49.7	45.5
	IterDRAG*	57.0	52.2	53.8	48.7
	AirRAG-Lite	70.9	66.6	63.8	59.1
	AirRAG	72.4	67.6	65.6	61.5
	AirRAG-Blender	73.2	70.0	68.3	66.0
16k	Vanilla RAG	56.8	52.5	53.5	49.2
	IterDRAG*	58.3	53.9	55.3	50.2
	AirRAG-Lite	73.2	68.8	65.2	60.7
	AirRAG	74.2	69.7	67.2	62.8
	AirRAG-Blender	75.3	71.0	69.3	66.5

Table 4: Overall average evaluation results between *Qwen2.5-14B-Instruct* and *Qwen2.5-72B-Instruct* over three datasets. L_{\max} denotes the maximum number of input tokens across all rollouts or iterations. Both rollouts and n are set to 1.

C Prompt Examples

Given a user input query, our proposed AirRAG, as shown in Figure 2, first attempts the *direct answer* (DA) action without prompts and performs *system analysis* (SAY) using the prompt in Figure 9. Subsequently, AirRAG performs *retrieval and answer* (RA) with the prompt in Figure 11, or *query transformation* (QT) to generate refined queries for better retrieval and answer. This process of RA-QT or QT-RA can continuously iterate until no new sub-queries arise or the maximum iteration depth is reached. Finally, the *summary answer* (SA) in Figure 11 utilizes all the information and conclusions from intermediate steps to refine the final answer.

Method	NQ	TriviaQA	PopQA	WebQA	HotpotQA	2Wiki
	EM	EM	F1	EM	F1	F1
Vanilla RAG	35.1	58.8	36.7	15.7	35.3	21.0
Self-RAG	36.4	38.2	32.7	21.9	29.6	25.1
Iter-RetGen	36.8	60.1	37.9	18.2	38.3	21.6
Auto-RAG	37.9	60.9	47.8	25.1	44.9	48.9
AirRAG	53.6	63.2	51.8	52.6	67.6	66.3

Table 5: Performance comparison on six benchmarks, where *Llama3-8B-Instruct* is used as the generator LLM. Partial experimental results are quoted from Jin et al. (2024) and Yu et al. (2024). The best results are in **bold**. The number of both rollouts and output sequences is set to 1. The number of documents for a single retrieval is set to 5. Our proposed AirRAG significantly outperform the others.

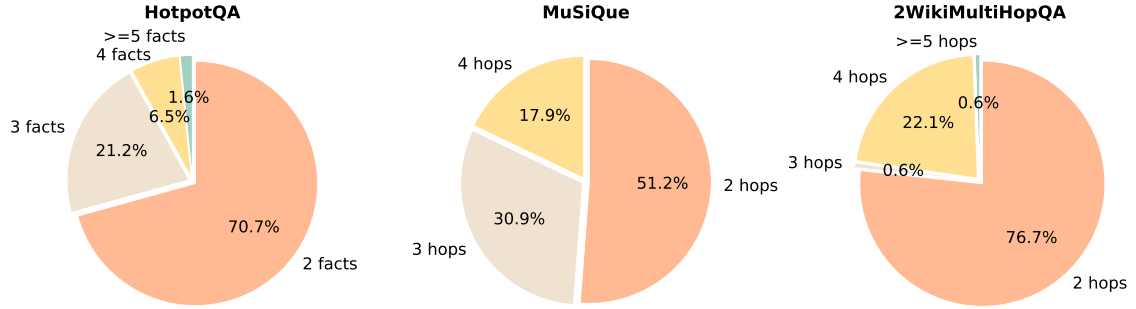


Figure 6: Overview of the distribution of query complexity over three multi-hop QA datasets.

D Case Study

We select a sample from the complex multi-hop dataset MuSiQue to analyse in detail, as shown in Figures 13 and 14.

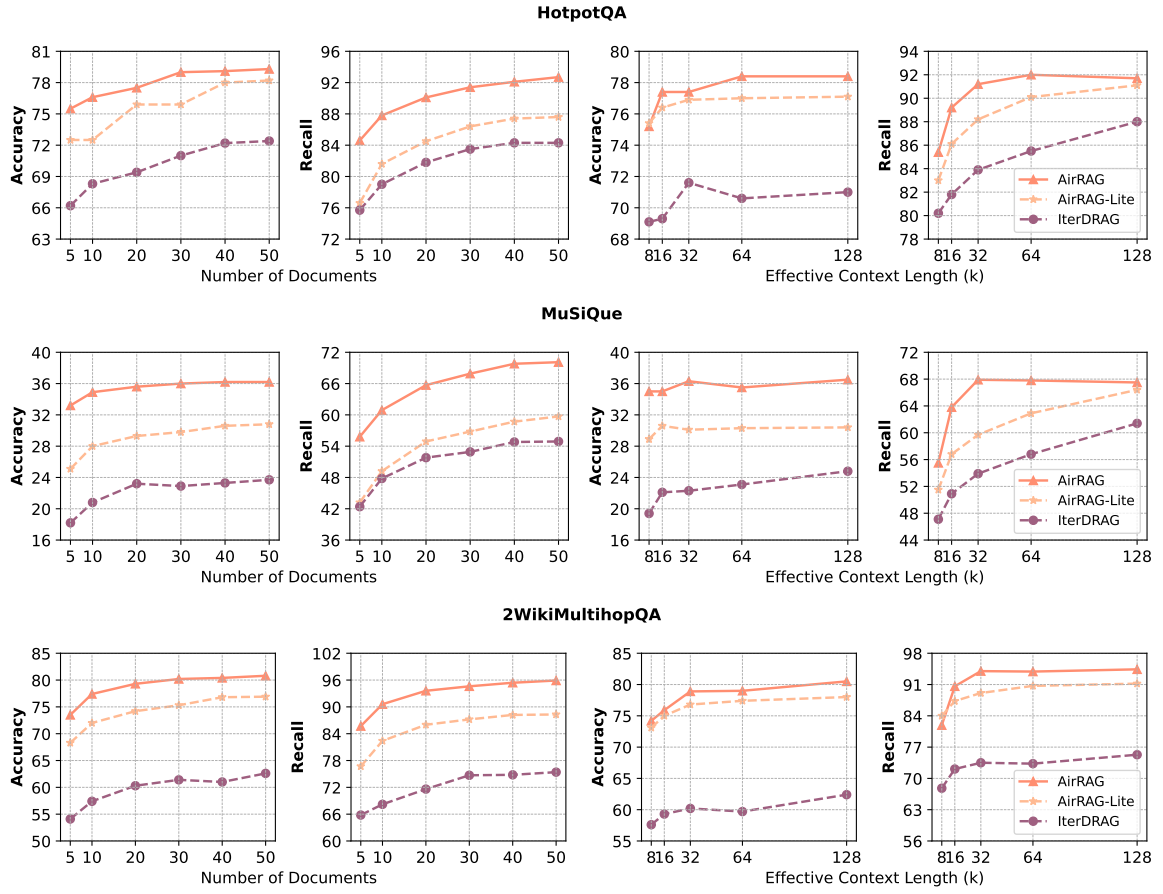


Figure 7: Impact of the retrieved document number scaling and the maximum context length scaling over three datasets.

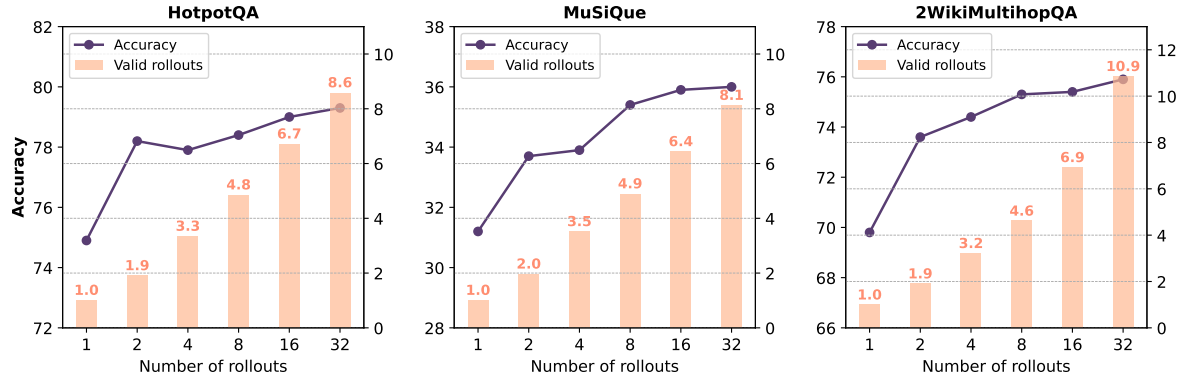


Figure 8: Performance comparison on the number of different effective rollouts over three datasets. Sampling more diverse reasoning paths consistently improves accuracy.

Example prompt for SAY reasoning action

Given the user query, you may rephrase it for better clarity, summarize it at a higher level, or decompose it into multiple sub-queries to facilitate more effective information retrieval and response generation. If no modification is necessary, return "None". Otherwise, list sub-queries, each on a new line.

<Here are some examples.>

Query: {question}

Output:

Figure 9: Example prompt for SAY reasoning action.

Example prompt for QT reasoning action

Given the context provided, please determine whether rephrasing, summarization, or decomposition into sub-queries is necessary to enhance the accuracy and efficiency of information retrieval and response generation. If no modification is required, return "None". Subsequent queries should be listed individually.

<Here are some examples.>

Main Query: {question}

History: {history}

This Query: {this_question}

Figure 10: Example prompt for QT reasoning action.

Example Prompt for RA actions

You are an expert in question answering. I am going to give you some contexts with may or may not be relevant to the question. Answer the question according to the contexts.

{contexts}

Question: {question}

Figure 11: Example Prompt for RA actions.

Example prompt for SA reasoning action

You are an expert in question answering. Given the context, sub-queries and responses, output a correct and concise answer to User Query.
<Here are some examples.>
User Query: {question}
{history}
Contexts: {contexts}
Final Answer:

Figure 12: Example prompt for SA reasoning action.

The iterative methods often traps in a solution space

Context: <Retrieved documents>
Question: What is the mouth of watercourse for the body of water where Bartram's Covered Bridge is located?
Follow up: Which body of water is Bartram's Covered Bridge located on?
Follow up: | Intermediate answer: | So the final answer is:

Output: Follow up: Which body of water is Bartram's Covered Bridge located on?

(Note: The context does not specify which body of water Bartram's Covered Bridge is located on, but it does mention that the bridge carries Goshen Road over Crum Creek. Therefore, we **need to confirm that Crum Creek is the body of water in question before proceeding to find the mouth of the watercourse.**)

...
... (It enters an endless cycle of iteration until it reaches predefined maximum depth.)

Gold Answer: Delaware River

Process Annotation: Q1: Bartram's Covered Bridge » crosses

A1: Crum Creek

Q2: Q1 » mouth of the watercourse

A2: Delaware River

The iterative self-exploration often traps in a solution space with low-quality reasoning steps even after many attempts.

Figure 13: Incorrect reasoning path of iterative RAG methods. Ambiguity or missing information in the intermediate steps leads in duplicate sub-query.

The simple and effective action space of AirRAG leads to the correct reasoning trajectory

Question: What is the mouth of watercourse for the body of water where Bartram's Covered Bridge is located?

Action1: SAY

Input: What is the mouth of watercourse for the body of water where Bartram's Covered Bridge is located?

Output: **Where is Bartram's Covered Bridge located?**

What is the mouth of the watercourse for the body of water near Bartram's Covered Bridge?

Action2: RA

Input: <Retrieved documents> Where is Bartram's Covered Bridge located?

Output: Bartram's Covered Bridge is located on the border between Delaware County and Chester County, Pennsylvania, carrying Goshen Road over Crum Creek.

Action3: QT

Input: What is the mouth of the watercourse for the body of water near Bartram's Covered Bridge?

Output: **What is the mouth of Crum Creek?**

Action4: RA

Input: <Retrieved documents> What is the mouth of Crum Creek?

Output: Based on the provided contexts, there are two different locations referred to as Crum Creek, and they flow into different bodies of water:

1. The Crum Creek in Delaware County and Chester County, Pennsylvania, flows into the Delaware River in Eddystone, Pennsylvania.

2. The Crum Creek (also called Cathatachua Creek) in East Creek, New York, flows into the Mohawk River.

Since the question does not specify which Crum Creek is being referred to, both answers are possible. However, if we consider the first context as the primary reference, the mouth of Crum Creek is the Delaware River in Eddystone, Pennsylvania.

Action5: SA

Input: <Retrieved documents> <Sub-queries with answers>

Output: The mouth of the watercourse for the body of water where Bartram's Covered Bridge is located, **Crum Creek**, is the **Delaware River** in Eddystone, Pennsylvania.

Gold Answer: Delaware River.

AirRAG obtains the correct answer by performing five reasoning actions efficiently.

Figure 14: Effective reasoning rollout of AirRAG. The fundamental action space and tree-based search provides greater compatibility and flexibility, which avoids being trapped in a single solution space by a low-quality intermediate step for chain-like reasoning paradigm.