CausalRAG: Integrating Causal Graphs into Retrieval-Augmented Generation

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Abstract

Large language models (LLMs) have revolutionized natural language processing (NLP), particularly through Retrieval-Augmented Generation (RAG), which enhances LLM capabilities by integrating external knowledge. However, traditional RAG systems face critical limitations, including disrupted contextual integrity due to text chunking, and over-reliance on semantic similarity for retrieval. To address these issues, we propose CausalRAG, a novel framework that incorporates causal graphs into the retrieval process. By constructing and tracing causal relationships, CausalRAG preserves contextual continuity and improves retrieval precision, leading to more accurate and interpretable responses. We evaluate CausalRAG against regular RAG and graph-based RAG approaches, demonstrating its superiority across several metrics. Our findings suggest that grounding retrieval in causal reasoning provides a promising approach to knowledge-intensive tasks.

1 Introduction

Large language models (LLMs) have transformed natural language processing (NLP), enabling a wide range of applications (Anthropic, 2024; Google, 2024; OpenAI, 2024). However, their reliance on static, pre-trained knowledge limits their ability to incorporate and reason over dynamically updated external information, particularly in knowledge-intensive domains. Retrieval-Augmented Generation (RAG) addresses this limitation by combining external retrieval with generative modeling to improve contextual understanding and response quality (Lewis et al., 2021).

Recent efforts to improve RAG focus on two fronts: 1) enhancing retrieval efficiency through adaptive and modular frameworks (Gan et al., 2024; Ravuru et al., 2024; Zhang et al., 2024a); and 2) better structuring external knowledge, with graph-based RAGs emerging as a dominant approach

(Edge et al., 2024; Guo et al., 2024; Potts, 2024).

Despite these advancements, existing RAG architectures still face critical limitations that impact retrieval quality and response accuracy, primarily due to three key issues: 1) disruption of contextual integrity caused by the text chunking design; 2) reliance on semantic similarity rather than causal relevance for retrieval; and 3) a lack of accuracy in selecting truly relevant documents.

Through theoretical and empirical analysis, we rethink the limitations of current RAG systems by introducing a novel perspective grounded in context recall and precision metrics. Using this lens, we find that both regular and graph-based RAGs often fail to retrieve causally grounded content or accurately align it with the user query. We identify this fundamental issue as a primary reason why LLMs in RAG frameworks frequently produce seemingly relevant yet shallow responses that lack essential details

To address these gaps, we propose *CausalRAG*, a novel RAG framework that integrates causal graphs to guide retrieval. By identifying cause–effect relationships within external knowledge, *CausalRAG* preserves contextual coherence and improves reasoning fidelity. This leads to **more accurate and causally grounded responses**, while reducing hallucinations and enhancing answer faithfulness.

We evaluate *CausalRAG* across datasets and varying context lengths, comparing it with regular and other competitive graph-based RAGs over multiple metrics. Results demonstrate that *Causal-RAG* achieves superior performance across different contexts. Additionally, we conduct a case study and a parameter analysis to further examine our framework, analyzing and providing insights that contribute to ongoing research in RAG. The contributions of this work are threefold:

 We identify the root limitations of current RAG systems through analytical and empirical studies, revealing why LLMs often produce superficial and under-grounded responses.

- We propose CausalRAG, which improves retrieval and generation by grounding responses in causal structure.
- Our work further mitigates hallucination issues and enhance interpretability, offering new insights into the design of RAG systems.

2 Related Work

2.1 Retrieval-Augmented Generation

RAG enhances LLMs' ability to handle knowledge-intensive tasks by integrating external knowledge retrieval (Lewis et al., 2021). Existing research advances RAG in two main directions: 1) optimizing retrieval flow and interaction; and 2) structuring and utilizing external knowledge—particularly through knowledge graphs—for multi-stage reasoning.

Optimizing retrieval flow and interaction. The first stream focuses on refining retrieval dynamics to improve output quality. Several methods introduce pre-, mid-, and post-retrieval enhancements to reduce redundancy and computation (Wang et al., 2024). Modular RAG architectures enable iterative retrieval-generation loops for more adaptive workflows. For instance, CAiRE-COVID (Su et al., 2020) demonstrated multi-document summarization with iterative retrieval, and others extended this to multi-hop QA (Feng et al., 2023). Recent work like METRAG (Gan et al., 2024) leverages LLM supervision for utility-driven retrieval, while RAFT (Zhang et al., 2024a) trains models to disregard distractor documents through chain-of-thought reasoning.

Structuring and utilizing external knowledge for multi-stage reasoning. The second stream focuses on representing and leveraging external knowledge—often via knowledge graphs—to support multi-level reasoning. GraphRAG (Edge et al., 2024) represents documents as nodes and edges and summarizes subgraph communities for retrieval. LightRAG (Guo et al., 2024) introduces dual-level retrieval and supports graph dynamic updates, while Lazy GraphRAG (Potts, 2024) further improves efficiency by delaying heavy computations until query time.

More recent multi-stage RAGs formalize hierarchical reasoning across multiple stages. PolyRAG (Chen et al., 2025) uses a knowledge pyramid for coarse-to-fine retrieval. KG²RAG (Zhu et al., 2025) guides RAG with KG-guided chunk expansion process to enhance factual grounding and control. GenTKGQA (Gao et al., 2024) performs twostage retrieval and generation over temporal subgraphs. HippoRAG2 (Gutiérrez et al., 2025) integrates PageRank ranking with deeper passage reasoning for better answer quality. However, most of these approaches focus primarily on matching and ranking information within the knowledge graph, with limited attention to the causal intent behind the user's query. A key challenge in RAG remains ensuring that retrieved information is not only relevant but also coherently aligned with the user's underlying reasoning needs and the generation objective (Gupta et al., 2024).

2.2 Causal Graphs and RAG

Causal graph integration has emerged as a promising way to improve retrieval and reasoning. Causal structures support more interpretable and reliable outputs by modeling underlying dependencies (Ma, 2024). Prior work in this area primarily focuses on causal discovery using RAG and LLMs. For instance, LLM-assisted BFS has been used to accelerate full causal graph discovery (Jiralerspong et al., 2024), while Corr2Cause evaluates LLMs' ability to infer causation from correlation (Jin et al., 2024).

Despite these advancements, most studies focus on utilizing RAG or LLMs for causal discovery or causal effect estimation (Ma, 2024; Kıcıman et al., 2024), whereas the direct integration of causal graphs into RAG architectures remains largely unexplored. Our work aims to be a pioneer in this direction. A few existing studies have touched upon this concept but differ in scope. One integrates causality within the transformer architecture itself (Chen et al., 2024), and another uses causal graphs only in pre-retrieval stages without deeper exploration (Samarajeewa et al., 2024). GraphRAG (Edge et al., 2024), while influential for its use of community detection and graph summarization, does not incorporate causality—nor do many recent multi-stage graph-based RAG frameworks.

In the following sections, we first analyze the limitations of regular and graph-based RAGs using a new recall–precision lens. We then introduce a causal graph structure to address these gaps.

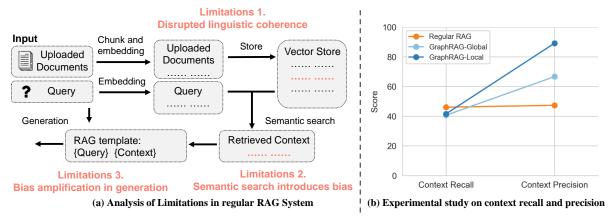


Figure 1: Analytical and experimental studies reveal limitations in regular RAG and GraphRAG. (a) identifies three key retrieval and generation issues in regular RAG; (b) evaluates RAG via context precision and recall, showing regular RAG excels in recall but lacks precision. GraphRAG improves precision but trades off some recall.

3 Why Regular RAG Fails in Providing Accurate Responses

In this section, through both analytical and experimental investigations, we identify three fundamental limitations of regular RAG and rethink its design by examining its three core elements—user query, retrieved context, and response—through a novel perspective based on precision and recall.

3.1 Limitations of Regular RAG

The first limitation arises from RAG's common practice of chunking texts into minimal units (as illustrated in Figure 1a). This process disrupts the natural linguistic and logical connections in the original text. These connections are crucial for maintaining contextual integrity, and if they are lost, an alternative mechanism must be implemented to restore them.

The second limitation lies in the semantic search process. RAG typically retrieves the semantically closest documents from a vector database based on query similarity. However, in many cases, critical information necessary for answering a query is not semantically similar but rather causally relevant. A classic example is the relationship between diapers and beer—while they are not semantically related, they may exhibit a causal connection in real worlds. This limitation suggests that RAG's reliance on semantic similarity may lead to the retrieval of contextually irrelevant but superficially related information.

The third limitation is that even when RAG retrieves a relevant context, this does not necessarily guarantee an accurate response. To formalize this issue, we used two key metrics: *context recall* and

context precision, defined as follows:

Context Recall =
$$\frac{\sum_{i=1}^{N} \mathbb{I}(C_i \in R)}{|R|}$$
 (1)

Here R is the reference set of all relevant references. C_i is the i^{th} retrieved reference. $\mathbb{I}(C_i \in R)$ is an indicator function that returns 1 if C_i belongs to the reference set R, otherwise 0. It should always return 1 if no hallucination occurs in the LLM.

Context Precision =
$$\frac{\sum_{i=1}^{N} \mathbb{I}_{\mathbb{Q}}(C_i \in R)}{\sum_{i=1}^{N} \mathbb{I}(C_i \in R)}$$
(2)

Here $\mathbb{I}_{\mathbb{Q}}(C_i \in R)$ is an indicator function that returns 1 if the context retrieved is causally related to the user's query, otherwise 0.

Recall-precision perspective. Context recall measures the extent to which relevant contextual information can be retrieved from external knowledge given a query. In practice, increasing the number of retrieved documents typically improves recall in RAG systems. However, this semantic search-based approach often sacrifices precision—the proportion of retrieved content that is truly correct and directly relevant to the user query. For example, when asking, "How does this article define AI?", regular RAG tends to retrieve all cited definitions that are semantically similar, even though only the author's own definition is actually pertinent. This illustrates a core limitation of relying on semantic similarity rather than causal relevance: the retrieval of content that appears related but is logically irrelevant. More critically, low

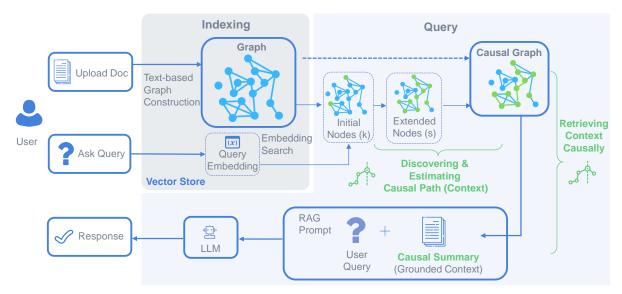


Figure 2: Overview of *CausalRAG*'s architecture. Documents are indexed as graphs, and queries retrieve causally related nodes. A causal summary is generated and combined with the query to ensure grounded responses.

retrieval precision introduces systematic bias, diluting the accuracy and reliability of the retrieved context.

In summary, while RAG can recall numerous answers from reference materials, the proportion of correct context remains low, ultimately reducing its precision. This recall-precision perspective provides a new lens to see the limitations of RAG frameworks.

3.2 Rethinking Graph-based RAGs

Applying this perspective, we can better understand why Graph-based RAGs serve as improved variants of RAG. By summarizing and ranking the importance of graph information before retrieval, they largely enhance the quality of retrieved context, thereby improving context precision. However, it only partially addresses the identified limitations, as its summarization process does not entirely filter out irrelevant information. More importantly, its reliance on subgraph summarization for retrieval may adversely impact recall by omitting less graph-central but still causally relevant context. To further examine these trade-offs, we conducted an experimental study to empirically validate these analytical insights.

Experimental study. Figure 1(b) reports experimental results for Regular RAG and both variants of GraphRAG. The graph-based approaches markedly improve context precision, reflecting the additional reranking and subgraph-summary steps in their retrieval pipelines. This gain comes with a

modest reduction in context recall, indicating that some relevant passages are pruned during summarization. These scores were obtained with the Ragas evaluation framework (Es et al., 2023); more comprehensive experiments and implementation details are shown in Section 5.

By combining our recall–precision-based analytical insights with empirical findings, we highlight the inherent limitations of both standard RAG and its graph-based extensions. Specifically, we show that relying on semantic similarity and subgraph summarization—rather than causal relationships—introduces trade-offs that often result in superficial and less accurate generation. We also present a case study in Section 5.3, which explicitly compares the retrieval processes across different RAG frameworks. In the following section, we introduce our proposed framework, *CausalRAG*, developed to address these limitations through causally grounded retrieval.

4 Methodology

In this section, we introduce our proposed framework—*CausalRAG*—which integrates RAG with causality to overcome the limitations of existing RAG systems. Overall, *CausalRAG* constructs a text-based graph from uploaded documents and discovers causal paths among nodes to guide retrieval (Figure 2). By embedding the user query, matching relevant nodes, and expanding them along causally linked paths, the system generates a causal summary that serves as the retrieval context. This

approach enables the framework to preserve contextual coherence and retrieve more targeted and causally relevant evidence. We now describe each step of the framework in detail.

4.1 Indexing

At the outset, upon receiving the user's uploaded documents and query, the system first indexes both inputs into a vector database. For the documents, we employ a text-based graph construction method that transforms unstructured text into a structured graph comprising nodes and edges. Specifically, we follow the approach proposed in LangChain (Chase, 2022), where an LLM parses the text to identify key entities or concepts as nodes and infers relationships between them as edges. Though this is a widely adopted approach in RAG research, we further validate the resulting graphs using expert knowledge, as discussed in the case study (Section 5.3). Once the graph is constructed, it is embedded and stored in the vector database, enabling efficient similarity-based retrieval. The user query is also embedded at this stage, preparing the system for subsequent matching. Importantly, this indexing process is performed offline and independently of query time, ensuring fast and scalable inference.

4.2 Discovering and Estimating Causal Paths

At query time, we first match the user query to graph nodes using embedding distance and select the top-k closest nodes. The parameter k controls the retrieval breadth: higher values return more context but increase computational cost. We then expand these nodes along graph edges by a step size s, which allows the framework to preserve causally and relationally connections within the text, allowing CausalRAG to retrieve more context while maintaining high recall. The parameter s determines the expansion depth and diversity of retrieved information.

Once the relevant nodes and edges are collected, we employ an LLM to identify and estimate causal paths within them, constructing a refined causal graph and generating the causal summary report (see LLM prompts in Appendix A). LLMs have demonstrated superiority in discerning and analyzing causal relationships (Zhang et al., 2024b; Zhou et al., 2024) and this step ensures that *CausalRAG* prioritizes causally relevant information, improving precision. The resulting causal graph serves two purposes: (1) capturing long-range cause–effect

dependencies often missed by semantic retrieval, particularly in longer texts; and (2) filtering out superficially related but causally irrelevant content, reducing hallucinations and improving faithfulness.

4.3 Retrieving Context Causally

After tracing and identifying key causal paths in the causal summary, we feed the result into the next stage and combine it with the user's query (see LLM prompts in Appendix A). The causal summary prioritizes nodes that directly support the query, ensuring coherence and factual consistency while filtering out spurious information. This step reduces the risk of retrieving misleading yet superficially similar contexts. Finally, the combined prompt—including the causal summary—is used for generation, enabling *CausalRAG* to reason over major causal relationships rather than merely aggregating loosely related text spans.

5 Experiment

To evaluate the effectiveness of *CausalRAG*, we conduct a series of experiments comparing it with regular RAG and other competitive graph-based RAGs across multiple performance metrics to ensure a comprehensive assessment. In addition, we present a case study that explicitly compares the retrieval processes of different RAG variants, and a parameter study to further examine the behavior and performance of *CausalRAG*.

5.1 Experimental Setup

Baselines. We evaluate five RAG variants: Regular RAG (Lewis et al., 2021), GraphRAG with both local and global search (Edge et al., 2024), HippoRAG2 (Gutiérrez et al., 2025), and our proposed CausalRAG. Regular RAG serves as a standard baseline, relying solely on semantic similarity for retrieval. GraphRAG is a widely recognized framework that leverages graph community summaries, and we include both of its modes: the local version retrieves from raw document graphs and is wellsuited for passage-level queries, while the global version summarizes graph communities to support broader context understanding. HippoRAG2 is a recent and competitive method that enhances retrieval by selecting seed nodes and ranking filtered triples for generation.

Datasets. While many open-domain QA benchmark datasets exist, most are designed for explicit fact retrieval (e.g., "When was Google founded?"

Life Sciences	Computing & Math	Social Sciences	Physics	Other	Total Tokens
13.27%	14.29%	21.43%	14.29%	36.73%	21,285

Table 1: Statistics of the dataset domain distribution and token lengths.

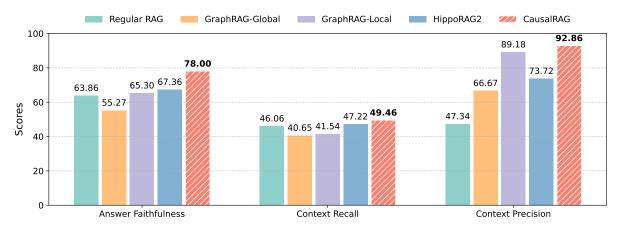


Figure 3: Performance comparison of *CausalRAG*, regular RAG, and other graph-based RAGs across three key metrics: answer faithfulness, context recall, and context precision.

"1998") and target classic NLP tasks. These datasets often fall short in evaluating discourse-level understanding, such as querying the underlying ideas, logic, or narrative within a document—tasks that better reflect real-world needs. Although some reading comprehension datasets exist (Rajpurkar et al., 2018), their answers are typically short entities and designed for NLP models rather than RAG systems.

To more effectively evaluate RAGs in knowledge-intensive tasks, recent research calls for datasets that require higher-level discourse understanding, such as those based on podcasts, news articles, or Wikipedia (Edge et al., 2024; Gutiérrez et al., 2025). Following this direction, we use academic papers sampled from the OpenAlex dataset (Priem et al., 2022a). Dataset statistics are provided in Table 1. For each document, we use an LLM to generate n=5 grounded questions, ensuring they are explicitly answerable (see Appendix B for examples).

Metrics & implementation details. We use the Ragas evaluation framework (Es et al., 2023) to assess all models on three metrics: answer faithfulness, context precision, and context recall. The definitions of context precision and context recall are provided in the previous section. Answer faithfulness measures factual consistency on a scale from 0 to 100, with higher scores indicating closer alignment with reference documents. We use GPT-40-mini as the base LLM for all frameworks. We set the parameters k = s = 3 for CausalRAG, and

use the same k value for GraphRAG's community-based retrieval, Regular RAG's document retrieval, and HippoRAG2's triple-based retrieval to ensure a fair comparison.

5.2 Performance Comparison

Figure 3 presents the main experimental results comparing five RAG frameworks across three evaluation metrics: answer faithfulness, context recall, and context precision. The results reveal distinct patterns in how different retrieval strategies affect generation quality. Below, we summarize the key findings and underlying trade-offs.

Causality delivers the most balanced and accurate retrieval. The model incorporating causal reasoning achieves the highest performance across all three metrics, with a context–precision score of 92.86 and a faithfulness score of 78.00, while maintaining competitive recall (49.46). By grounding retrieval in explicit causal paths, it filters out semantically similar but logically irrelevant content, thereby reducing superficial answers and improving the alignment and coherence between the retrieved context and the user query.

Graph-level structuring improves precision but introduces a recall—coverage trade-off. GraphRAG's two operating modes illustrate this tension. Local search, which queries the raw knowledge graph, yields strong precision (89.18) but discards many supporting passages, dropping recall to 41.54. Global search restores some of

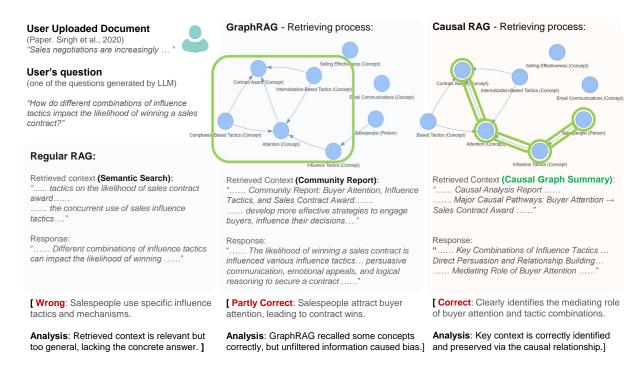


Figure 4: Case Study – A user uploads a long paper and asks a related question. This figure compares Regular RAG, GraphRAG, and *CausalRAG* by analyzing their retrieval processes. It highlights the drawbacks of semantic and graph-based retrieval and shows how causal reasoning in CausalRAG leads to more robust and precise results.

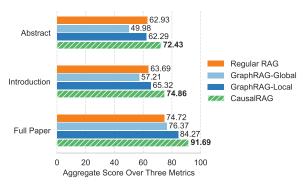


Figure 5: Case Study – A follow-up experiment evaluates the RAGs in the previous case using three versions of the same paper. Graph-based methods improve with length, while *CausalRAG* remains consistently robust.

that missing evidence by summarizing community subgraphs, yet the broader scope simultaneously re-introduces off-topic material, pulling precision down to 66.67 and faithfulness below 55.3. These results corroborate (Edge et al., 2024)'s observation that finer-grained community answers excel at factual grounding, whereas higher-level summaries aid breadth but dilute specificity.

Entity-centric multi-stage KGs narrow the gap but still overlook discourse context. HippoRAG2 augments Personalized PageRank with LLM-filtered triples and passage nodes, boosting precision to 73.72 and faithfulness to 67.36 without sacrificing recall relative to Regular RAG. Nevertheless, its reliance on entity extraction leaves many context-rich sentences unlinked to the query, a limitation they noted as concept—context trade-off and need for deeper contextualization(Gutiérrez et al., 2025). By contrast, *CausalRAG*'s path-based expansion integrates both entities and their causal explanations, yielding a retrieval set that is simultaneously broader in coverage and more tightly aligned with the question, thereby establishing a new possibility for knowledge-intensive RAG tasks.

5.3 Case Study

Qualitative exemplar. Figure 4 traces the end-to-end behaviour of the three systems on a single question drawn from a marketing paper: "How do different combinations of influence tactics impact the likelihood of winning a sales con*tract?*" The semantic baseline retrieves passages that mention "influence tactics" but stop short of establishing how those tactics translate into contract wins; its answer therefore echoes the query without providing the missing mechanism. Graph-based retrieval narrows the search space by clustering entities such as buyer attention and sales contract award, yet the community summary also injects peripheral phrases, leading the model to an over-generalised explanation that only partially matches the ground truth. By contrast, the causality-driven pipeline first aligns the query with a causal pathway—Influence Tactics \rightarrow Buyer Attention \rightarrow Contract Award. Because that pathway is preserved through retrieval and summarisation, the generated answer pinpoints the mediating role of buyer attention and specifies which tactic pairs are most effective, fully satisfying expert judgment.

Length-controlled follow-up. To test whether these qualitative differences persist when context grows, we replicate the experiment on three versions of the same paper—abstract (250 tokens), introduction (1k), and full text (16k)—and score each system on the composite of faithfulness, precision, and recall (Figure 5). Graph-level methods benefit from additional material: their aggregate score climbs from 49.98/62.29 on the abstract to 76.37/84.27 on the full paper, confirming that community-based indexing scales gracefully with document length. Yet the causality-oriented approach remains consistently ahead, posting 72.43 on the abstract, 74.86 on the introduction, and 91.69 on the full text. This steadiness indicates that causal expansion recovers the right evidence even when local term overlap is sparse (short documents) and still filters noise when semantic matches proliferate (long documents).

Emerging pattern. Taken together, the case study and its quantitative extension suggest a general rule: graph structure raises precision by adding relational cues, but explicit causal alignment is required to preserve both precision and recall across scales. Semantic search alone misses latent mechanisms; graph aggregation alone retains residual noise. Embedding causal constraints into retrieval therefore offers a principled path to robust performance on knowledge-intensive tasks, regardless of document length or query granularity.

5.4 Parameter Study

We also tested the impact of different parameter combinations of k and s on CausalRAG (as shown in Figure 6). Using the average of our evaluation metrics, we observe a consistent trend: the performance of CausalRAG improves as k and s increase. Specifically, the performance rises from 0.534 at k=s=1 to 0.824 at k=s=5, aligning with intuitive expectations.

Notably, the improvement is more pronounced when increasing k from 1 to 3, suggesting that retrieving additional context enhances reasoning

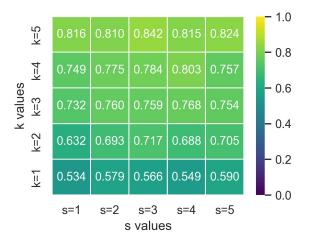


Figure 6: Parameter study showing how different parameter choices (k and s) affect model performance.

quality. However, when $k \geq 4$, performance gains become less significant, indicating possible saturation due to information redundancy. Similarly, while increasing s generally leads to better results, its effect diminishes at higher values of k, where retrieval is already extensive.

These results suggest an optimal trade-off between performance and computational efficiency. While the highest values (k=5,s=5) yield the best results, moderate settings such as k=3,s=3 still achieve competitive performance with lower retrieval costs. Future work could explore adaptive strategies to adjust these parameters dynamically based on query complexity.

5.5 Conclusion and Future Work

We introduced *CausalRAG*, a novel framework that integrates causal reasoning into retrieval-augmented generation to address core limitations of existing RAG systems. By leveraging causality, *CausalRAG* retrieves context that is not only relevant but also causally grounded—enhancing generation quality, reducing hallucinations, and improving answer fidelity.

Future work may extend *CausalRAG* in several directions. A key area is testing scalability in long-context scenarios, which requires constructing and processing numerous high-dimensional graphs, each derived from large-scale documents spanning millions of tokens. While current practices often merge documents into a single graph or use smaller graphs due to data quality and computational constraints, this direction is critical for understanding RAG scalability. In addition to improving performance, evaluating efficiency and generation latency remains important for practical deployment.

Limitations

While *CausalRAG* improves retrieval effectiveness through causal reasoning, it has certain limitations. First, the approach relies on the internal knowledge of LLMs to construct graphs and identify causal relationships. Although both capabilities have been actively studied, emerging domain-specific knowledge—such as in medicine or law—may still constrain its effectiveness in specialized contexts. Second, identifying causal paths during inference also requires additional LLM calls, introducing extra computational costs that may limit the performance in real-world deployments.

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Appendix

A LLM Prompts Used

The full prompts used in the *CausalRAG* framework for causal discovery and causal summarization (Figure 7), as illustrated in Figure 2. The prompts are adapted from Edge et al. (2024).

B OpenAlex Dataset Example

This is an exmaple (see Table 2) in the dataset (Priem et al., 2022b) along with generated questions.

Dataset	OpenAlex (Priem et al., 2022b) Atomic Physics			
Discipline				
Author	Thom H. Dunning (1989)			
Text	In the past, basis sets for correlated molecular calculations were largely taken from single-configuration calculations. Recently, Almlöf, Taylor, and co-workers showed that atomic natural orbitals (ANOs) provide an excellent description of correlation effects. Here we report a careful oxygen-atom study establishing that compact primitive Gaussian functions effectively describe correlation when their exponents are optimized. Tests on oxygen-containing molecules indicate these functions perform as well as the ANO sets of Almlöf and Taylor. Guided by the oxygen results, basis sets were developed for all first-row atoms (B–Ne) and hydrogen. Incremental energy lowerings due to correlating functions fall into distinct groups, leading to the concept of consistent sets. The most accurate set, [5s 4p 3d 2f 1g], consistently yields 99% of the correlation energy obtained with the next larger set, even though the latter contains 50% more primitives and twice as many polarization functions. For boron, this set recovers 94–97% of the total (HF+1+2) correlation energy.			
Questions				
	1. What recent findings support the use of atomic natural orbitals in molecular calculations?			
	2. How do compact primitive Gaussian functions contribute to describing correlation effects in oxygen?			
	3. Why is exponent optimization important in Gaussian-based calculations?			
	4. How do the new first-row basis sets compare in energy lowering from correlation effects?			
	5. What accuracy (%) is achieved for boron with the most compact set, and how does this relate to the number of polarization functions?			

Table 2: Example document metadata, full-text excerpt, and evaluation questions used in our study.

---Role--- Causal Discovery Prompt

You are a smart assistant that helps a human analyst to perform **causal discovery** and **impact assessment**. Your task is to analyze a **Network Data** and generate a professional report summarizing the causal effect and key insights.

--- Goal ---

Write a **structured, professional causality analysis report** that:

- **Identifies** key entities and their roles in the causality
- **Explains** the observed causal relationships and their potential impact
- **Assesses** the strength and credibility of causal claims based on available data

---Network Data---

{graph_data}

--- Report Format ---

1. Introduction

Briefly introduce the context and purpose of this causal analysis.

2. Key Entities and Their Roles

Provide an overview of the most important entities in the causal network and their relevance.

3. Major Causal Pathways

Describe the primary causal chains observed, emphasizing key cause-and-effect relationships.

4. Confidence and Evidence Strength

Assess the reliability of the causal claims, mentioning supporting data where available.

5. Implications and Recommendations

Discuss the potential impact of these causal relationships and suggest possible actions.

Write a **structured, analytical, and professional** report.

Causal Summary Prompt

---Role---

You are a helpful assistant responding to questions about data in the tables provided. You are also specializing in **causal reasoning and impact assessment**. Your task is to generate a structured response based on an extracted causal summary.

---Goal---

Generate a response of the target length and format that responds to the user's question, summarize all the Causal Summary from multiple analysts who focused on different parts of the dataset.

If you don't know the answer or if the provided reports do not contain sufficient information to provide an answer, just say so. Do not make anything up.

The final response should remove all irrelevant information from the analysts' reports and merge the cleaned information into a comprehensive answer that provides explanations of all the key points and implications appropriate for the response length and format.

The response shall preserve the original meaning and use of modal verbs such as "shall", "may" or "will".

The response should also preserve all the data references previously included in the analysts' reports, but do not mention the roles of multiple analysts in the analysis process.

--- Causal Summary---

{causal_summary}

--- Target Response Length and Format---

{response_type}

---User Query---

{auerv}

Add sections and commentary to the response as appropriate for the length and format. Style the response in markdown.

Figure 7: LLM prompts for causal discovery and causal summary