# D-RAG: Differentiable Retrieval-Augmented Generation for Knowledge Graph Question Answering

**Anonymous ACL submission**

## Abstract

Knowledge Graph Question Answering (KGQA) aims to answer natural language questions based on knowledge graphs. Recent approaches apply the Retrieval-Augmented Generation (RAG) paradigm to incorporate Large Language Models (LLMs) to this task, where a retriever selects a question-related subgraph and an LLM-based generator is then adopted to predict answers based on the retrieved subgraph. However, the subgraph selection process is non-differentiable, preventing end-to-end training of the retriever and the generator, which leads to sub-optimal performance. To overcome this limitation, this paper proposes a Differentiable RAG (D-RAG) approach that jointly optimizes the retriever and the generator for KGQA. Via reformulating the optimization objective as an expectation over a subgraph distribution with respect to answer generation likelihood, D-RAG makes the joint optimization feasible. Specifically, it implements this joint optimization through a differentiable subgraph sampling and prompting module that integrates Gumbel-Softmax reparameterization for sampling and a neural prompt construction process that fuses semantic and structural information. Experimental results on WebQSP and CWQ demonstrate that D-RAG outperforms state-of-the-art approaches.

## 1 Introduction

Knowledge Graph Question Answering (KGQA) aims to automatically answer natural language questions via well-structured facts stored in Knowledge Graphs (KGs). It is an essential task in Natural Language Processing (NLP) and is vital in various applications such as information retrieval and intelligent assistance (Potdar et al., 2025; Liang et al., 2024). However, KGQA poses challenges to existing approaches, as it requires a deep understanding of natural language questions and the ability to perform complex reasoning over KGs. Considering that Large Language Models (LLMs) (DeepSeek, 2025; OpenAI, 2024b; Meta, 2024) have shown strong capabilities in natural language understanding and reasoning, some recent approaches (Peng et al., 2024; Luo et al., 2024a; He et al., 2024) incorporate LLMs into KGQA via the Retrieval-Augmented Generation (RAG) paradigm (Lewis et al., 2020). Specifically, they adopt a retriever to select a question-relevant subgraph from the KG. Then, they serialize the subgraph into the prompt and adopt LLMs as the generator to reason for answers.

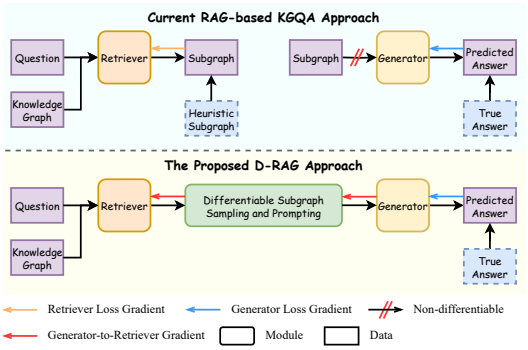


Figure 1: Comparison between the current RAG-based KGQA approaches and the proposed D-RAG approach. The red arrows highlight the end-to-end gradient flow.

Despite the promising performance of these RAG-based KGQA approaches, significant challenges remain in optimizing both the retriever and the generator. As illustrated in Figure 1, current approaches (Luo et al., 2024a; Mavromatis and Karypis, 2024) typically adopt a sequential optimization paradigm, where the retriever is trained using heuristic supervision signals, and the generator is subsequently optimized with the retriever frozen. This sequential optimization leads to sub-optimal performance for the complete system. Specifically, the generator's semantic understanding capabilities

cannot guide the retriever, while the retriever cannot effectively communicate structural knowledge in a way the generator can optimally utilize.

To address above limitations, we propose the **D**ifferentiable **R**etrieval-**A**ugmented **G**eneration (D-RAG) for KGQA. First, we reformulate the optimization objective as a tractable expectation over a subgraph distribution with respect to answer generation likelihood, making the joint optimization tractable. Second, we develop a differentiable subgraph sampling and prompting module that achieves end-to-end training. In the subgraph sampling step, D-RAG transforms discrete subgraph selection into differentiable fact-level sampling using the Gumbel-Softmax reparameterization trick (Jang et al., 2017; Maddison et al., 2017). In the prompt construction step, D-RAG converts the sampled subgraph into LLM-compatible prompts that fuse both semantic and structural information while maintaining gradient flow throughout the entire pipeline. This end-to-end optimization creates a synergistic relationship where the generator's semantic understanding informs retrieval quality, and the retriever provides structurally meaningful information that enhances the generator's reasoning capabilities.

Experimental results on WebQSP and CWQ show that D-RAG outperforms the state-of-the-art approaches by 2.5% and 1.8% on Hits@1, and by 3.4% and 4.4% on the F1 scores, respectively. These improvements stem from the end-to-end optimization strategy, which effectively reduces retrieval noise and enhances answer generation quality.

The main contributions of this work are as follows:

- We propose D-RAG, the first differentiable RAG-based KGQA approach, to the best of our knowledge, that enables end-to-end optimization with gradient flow from the generator to the retriever.
- We reformulate the optimization objective as a tractable expectation over subgraph distributions and develop a differentiable subgraph sampling and prompting module. This module combines Gumbel-Softmax reparameterization for differentiable sampling with neural prompt construction that integrates both semantic and structural information, establishing an effective end-to-end optimization framework for KGQA.
- Comprehensive experiments on two widely used benchmark datasets, i.e., WebQSP and CWQ, demonstrate that D-RAG outperforms state-of-the-art performance, validating the effectiveness of the proposed approach.

## 2 Related Works

### 2.1 Knowledge Graph Question Answering

KGQA approaches can be broadly categorized into Semantic Parsing-based (SP-based) and Information Retrieval-based (IR-based) ones (Lan et al., 2023). While SP-based methods parse questions into formal queries for execution, IR-based methods retrieve relevant subgraphs for answer ranking or generation. D-RAG falls into the latter category.

Traditional IR-based approaches typically learn entity and relation representations for answer ranking using network architectures such as graph neural networks (Sun et al., 2018; He et al., 2021; Zhang et al., 2022), which we categorize as Graph Reasoning methods. The emergence of LLMs has led to RAG-based approaches that leverage LLMs' powerful reasoning capabilities for answer generation. These RAG-based approaches can be divided into two groups: LLM Reasoning methods that primarily rely on LLMs for both subgraph retrieval and answer generation (Luo et al., 2024a; Jiang et al., 2023a; Sun et al., 2024; Ma et al., 2024; Luo et al., 2024b), and Graph-LLM approaches that address LLMs' limitations in processing graph-structured data (Guo et al., 2023; Guan et al., 2025) by incorporating graph-specific techniques during retrieval while using LLMs for reasoning (He et al., 2024; Li et al., 2025; Mavromatis and Karypis, 2024; Liu et al., 2024a).

Despite the promise of these RAG-based approaches, a critical limitation is their lack of end-to-end training capabilities. While SR (Zhang et al., 2022) achieves end-to-end KGQA by constructing tree-structured subgraphs from multi-hop paths, their posterior approximation requires computing answer generation probability for each top-k path independently, which would incur prohibitive computational costs when LLMs serve as the generator.

### 2.2 End-to-End Training in RAG

Most RAG systems follow a pipeline paradigm (Gao et al., 2023), where separate modules for retrieval, prompting, and generation are optimized separately. Several works have explored end-to-end trainable approaches for text

retrieval, including REALM (Guu et al., 2020), EMDR$^2$ (Sachan et al., 2021), VOD (Liévin et al., 2023), and StochasticRAG (Zamani and Bendersky, 2024). However, these text-centric methods cannot be directly applied to KGQA due to the structured nature of graph data and the need for specialized graph retrieval mechanisms.

StochasticRAG (Zamani and Bendersky, 2024) is the most similar one to the proposed approach, as both methods leverage Gumbel tricks for discrete sampling, whether for documents or subgraphs. However, D-RAG differs in two key aspects: (1) StochasticRAG retrieves a fixed number of documents, which is not suitable for KGQA. In contrast, our approach transforms subgraph sampling into independent sampling of facts, allowing for flexible subgraph sizes; (2) Unlike documents that can be directly fed to LLMs, we employ a differentiable prompting step to bridge the gap between graph structures and LLM reasoning.

## 3 Preliminary

**Knowledge Graph Question Answering.** In this paper, the knowledge graph is composed of multiple facts, where each fact $\tau = (h, r, t)$ represents a triple consisting of a head entity $h$, a relation $r$, and a tail entity $t$. Formally, the KG can be represented as $\mathcal{G} = \{(h, r, t)|h, t \in \mathcal{E}, r \in \mathcal{R}\}$, where $\mathcal{E}$ denotes the set of all entities and $\mathcal{R}$ represents the set of all relation types, with each entity and relation type typically corresponding to a natural language form. Given a knowledge graph $\mathcal{G}$, the KGQA task takes a natural language question $q$ as input and outputs an answer $a$ corresponding to one or more entities in $\mathcal{G}$. The ultimate goal is to maximize the likelihood of the correct answer, which can be formulated as $\mathbb{E}_{(q,\, a)}\left[\log p(a|q, \mathcal{G})\right]$.

**RAG-based KGQA.** The RAG paradigm for KGQA involves two independent modules: a retriever $R_\beta$ that identifies the question-relevant subgraph $g_{sub}$ with probability $p_\beta(g_{sub}|\mathcal{G}, q)$, and a generator $G_\gamma$ that generates the answer $a$ with probability $p_\gamma(a|g_{sub}, q)$. $\beta$ and $\gamma$ denote the parameters of the retriever and the generator, respectively.

The overall answer generation probability can be formulated as:

$$p_\theta(a|q, \mathcal{G}) = \sum_{g_{sub} \subseteq \mathcal{G}} p_\gamma(a|q, g_{sub}) p_\beta(g_{sub}|q, \mathcal{G}), \tag{1}$$

where $\theta$ denotes all parameters in the above two modules.

## 4 The Proposed D-RAG Approach

This section presents **D**ifferentiable **R**etrieval-**A**ugmented-**G**eneration (D-RAG), as illustrated in Figure 2. Our approach integrates a graph neural network (GNN)-based retriever and an LLM-based generator through a differentiable subgraph sampling and prompting module, enabling end-to-end training. Below, we detail these modules and the training strategy.

### 4.1 GNN-based Retriever

The GNN-based retriever encodes the knowledge graph to identify question-relevant facts. Given a question and a knowledge graph, it outputs fact representations that serve multiple purposes in D-RAG.

**Fact Representation.** For each fact $\tau_i$ in the knowledge graph, we construct a representation by concatenating its constituent elements:

$$\mathbf{F}_i = [\mathbf{h}_i \parallel \mathbf{r}_i \parallel \mathbf{t}_i] \in \mathbb{R}^{D_{\text{GNN}}}, \tag{2}$$

where $\mathbf{h}_i$, $\mathbf{r}_i$, and $\mathbf{t}_i$ are representations of the head entity, relation, and tail entity, respectively, derived from a GNN module based on ReaRev (Mavromatis and Karypis, 2022).

From these fact representations, we compute the selection probability for each fact using a linear layer followed by a sigmoid function: $p(\tau_i) = \sigma(\mathbf{W}\mathbf{F}_i + \mathbf{b})$, where $\mathbf{W}$ and $\mathbf{b}$ are learnable parameters.

**Subgraph Selection Probability Factorization.** For subgraph sampling, computing the exact probability of a specific subgraph is combinatorially complex. Therefore, we employ a factorization approach that decomposes the subgraph selection probability into independent binary selectionss for each fact:

$$p(g_{sub}) = \prod_{\tau_i \in g_{sub}} p(\tau_i) \prod_{\tau_j \notin g_{sub}} (1 - p(\tau_j)). \tag{3}$$

Detailed derivations of this factorization and specifications of the GNN architecture are provided in Appendix A and B, respectively.

### 4.2 LLM-based Generator

The LLM-based generator predicts answers to questions based on the information contained in the retrieved subgraph. It processes the input through

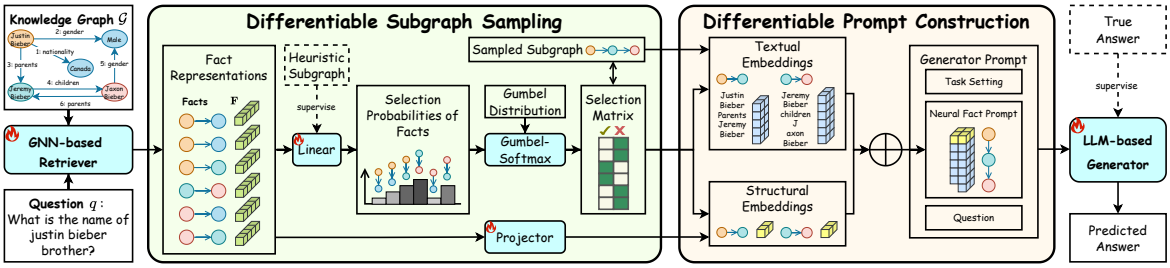


Figure 2: The proposed D-RAG consists of four steps: 1) The GNN-based retriever processes the knowledge graph to obtain fact representations; 2) The differentiable subgraph assigns selection probabilities to facts and uses Gumbel-Softmax reparameterization trick to sample a subgraph; 3) The differentiable prompt construction transforms the sampled subgraph into a neural fact prompt that combines semantic and structural information; 4) The LLM-based generator predicts the final answer.

autoregressive decoding to generate answers:

$$p_\gamma(a|g_{sub}, q) = \prod_{i=1}^{L_a} p_\gamma(a_i|a_{<i}, g_{sub}, q), \quad (4)$$

where $L_a$ is the token length of the ground-truth answer.

The generator receives input comprising three components as shown in Figure 2: the task setting, the question, and the neural fact prompt derived from the retrieved subgraph. These are combined in a structured template:

```
Answer the question based
on the provided facts.
Question: <question>
Provided facts: <fact1><fact2> ...
Answer:
```

Answers are formatted as a bar-separated list: `<Ans1>|<Ans2>|...|<AnsN>`. Complete prompt examples are provided in Appendix C.

### 4.3 Differentiable Subgraph Sampling and Prompting

D-RAG constructs differentiable bridges across the retriever-generator interface through two designs: (1) reformulating the optimization objective into a tractable form, and (2) implementing differentiable operations for both subgraph sampling and prompt construction. This end-to-end approach enables joint optimization where the retriever learns to identify graph patterns that enhance the generator's reasoning capabilities.

#### 4.3.1 Differentiable Formulation

The optimization objective of maximizing Equation 1 involves a summation with combinatorial complexity, making it generally intractable. We address this by optimizing its evidence lower bound (ELBO) (Hoffman et al., 2013), formulated as:

$$\begin{aligned}\log p_\theta(a|q,\mathcal{G}) &= \mathbb{E}_{g_{sub}\sim r}\left[\log \frac{p_\theta(a, g_{sub}|q,\mathcal{G})}{r(g_{sub})}\right] \\ &+ D_{KL}(r(g_{sub}) \,||\, p_\theta(g_{sub}|a,q,\mathcal{G})) \\ &\geq \mathbb{E}_{g_{sub}\sim r}\left[\log \frac{p_\theta(a, g_{sub}|q,\mathcal{G})}{r(g_{sub})}\right], \end{aligned} \quad (5)$$

where $r(g_{sub})$ represents the variational distribution of the subgraph, and the inequality holds because the Kullback-Leibler divergence is non-negative. By specifying the variational distribution $r(g_{sub})$ as the retriever's distribution $p_\beta(g_{\text{sub}}|q,\mathcal{G})$, the ELBO simplifies to:

$$\begin{aligned}\log p_\theta(a|q,\mathcal{G}) &\geq \mathbb{E}_{g_{sub}\sim p_\beta}\left[\log \frac{p_\theta(a, g_{sub}|q,\mathcal{G})}{p_\beta(g_{sub}|q,\mathcal{G})}\right] \\ &= \mathbb{E}_{g_{sub}\sim p_\beta}\left[\log \frac{p_\gamma(a|g_{sub},q)p_\beta(g_{sub}|q,\mathcal{G})}{p_\beta(g_{sub}|q,\mathcal{G})}\right] \\ &= \mathbb{E}_{g_{sub}\sim p_\beta}\left[\log p_\gamma(a|g_{sub},q)\right], \end{aligned} \quad (6)$$

where $p_\beta$ is modeled by the GNN-based retriever and $p_\gamma$ by the LLM-based generator. This formulation transforms the original combinatorial objective into a tractable expectation over subgraph distributions. To optimize this expectation through gradient-based methods, two critical challenges need to be addressed: (1) implementing differentiable operations for discrete subgraph sampling from distribution $p_\beta$, and (2) constructing differentiable prompts that allow gradients to flow through the generator $p_\gamma$.

#### 4.3.2 Differentiable Subgraph Sampling

Sampling a subgraph results a selection matrix $\mathbf{Z} = [\mathbf{z}_1; \mathbf{z}_2; \ldots; \mathbf{z}_{N_f}] \in \{0,1\}^{N_f \times 2}$, where $N_f$

is the total number of facts in the knowledge graph and each row $\mathbf{z}_i$ indicates whether the $i$-th fact is selected ($[1, 0]$) or not ($[0, 1]$). Given $\mathbf{Z}$, the sampled subgraph is represented as $g_{sub} = \{\tau_i | \mathbf{z}_i = [1, 0]\}$.

To make this subgraph sampling process differentiable, we adopt the Gumbel-Softmax reparameterization trick (Jang et al., 2017; Maddison et al., 2017). For each fact $\tau_i$, the retriever outputs a Bernoulli parameter $p_i = p_\beta(\tau_i)$, representing its selection probability. We apply the Gumbel-Softmax trick:

$$\mathbf{z}_i^{\text{soft}} = \text{softmax}\begin{pmatrix} (\log p_i + \eta_{i1}) \,/\, t \\ (\log(1 - p_i) + \eta_{i2}) \,/\, t \end{pmatrix}^T, \tag{7}$$

where $\eta_{i1}, \eta_{i2}$ are independent Gumbel(0,1) noise samples and $t$ is the temperature coefficient.

The final binary selection indicator $\mathbf{z}_i$ is obtained through:

$$\mathbf{z}_i = \text{onehot}(\text{argmax}(\mathbf{z}_i^{\text{soft}})) + \mathbf{z}_i^{\text{soft}} - \text{SG}(\mathbf{z}_i^{\text{soft}}), \tag{8}$$

where SG denotes the stop-gradient operation. This formulation combines discrete selection in the forward pass with differentiability in the backward pass.

With this reparameterization, our training objective becomes:

$$\mathbb{E}_{\boldsymbol{\eta} \sim p(\boldsymbol{\eta})} \left[ \log p_\gamma(a | g_{sub}, q) \right], \tag{9}$$

which transforms the expectation from a complex parameterized distribution to sampling from a fixed distribution, enabling gradient flow through the discrete sampling process.

#### 4.3.3 Differentiable Prompt Construction

After sampling the subgraph, we transform it into a neural prompt that preserves both semantic and structural information while maintaining end-to-end differentiability.

For semantic information, each fact is converted into natural language using the template `<head name>, <relation name>, <tail name>` and then tokenized and encoded into embeddings $\mathbf{V}_i \in \mathbb{R}^{L_i \times D_{\text{LLM}}}$, where $L_i$ is the token length and $D_{\text{LLM}}$ is the LLM embedding dimension. We multiply each embedding $\mathbf{V}_i$ by the corresponding selection indicator $\mathbf{z}_{i1}$ from matrix $\mathbf{Z}$, effectively retaining only the embeddings of selected facts.

For structural information, we utilize the fact representations $\mathbf{F} = [\mathbf{F}_1; \mathbf{F}_2; \ldots; \mathbf{F}_{N_f}] \in \mathbb{R}^{N_f \times D_{\text{GNN}}}$ learned by the GNN retriever (defined in Equation 2). These representations capture each fact's position and relevance within the knowledge graph. A two-layer MLP projects these representations to align with the LLM embedding space: $\mathbf{F}' = \text{Projector}(\mathbf{F}) \in \mathbb{R}^{N_f \times D_{\text{LLM}}}$. Similarly, we select only the structural embeddings $\mathbf{F}'_i$ corresponding to facts where $\mathbf{z}_{i1} = 1$.

For each selected fact $\tau_i$, we concatenate its semantic embedding $\mathbf{V}_i$ with its structural embedding $\mathbf{F}'_i$ to form an enriched representation. These combined embeddings are then concatenated to create the complete neural fact prompt $\mathbf{V}_\mathbf{F}$ for the LLM-based generator.

Our approach enables gradient flow from the LLM loss $L$ back to the retriever parameters $\beta$ through dual pathways:

$$\frac{\partial L}{\partial \beta} = \underbrace{\frac{\partial L}{\partial \mathbf{V}_\mathbf{F}} \frac{\partial \mathbf{V}_\mathbf{F}}{\partial \mathbf{Z}} \frac{\partial \mathbf{Z}}{\partial \beta}}_{\text{Semantic pathway}} + \underbrace{\frac{\partial L}{\partial \mathbf{V}_\mathbf{F}} \frac{\partial \mathbf{V}_\mathbf{F}}{\partial \mathbf{F}'} \frac{\partial \mathbf{F}'}{\partial \beta}}_{\text{Structural pathway}}, \tag{10}$$

where the first term represents gradient flow through the discrete selection process, and the second term captures flow through the fact representations.

For multi-hop reasoning, facts are arranged by their selection probabilities, helping preserve potential logical sequences within the sampled subgraph.

### 4.4 Training Strategy and Inference

With the differentiable subgraph sampling and prompting module proposed above, D-RAG supports end-to-end training. To accelerate convergence, we adopt a two-phase training strategy.

In the first phase, the GNN-based retriever is pre-trained using heuristically constructed subgraphs as guidance:

$$L_1 = D_{KL}(p_{heur}(g_{sub}) \,||\, p_\beta(g_{sub})), \tag{11}$$

where $p_{heur}$ represents the heuristic subgraph distribution (typically in one-hot form), and $p_\beta$ is the retriever's predicted distribution.

In the second phase, the retriever and generator are trained jointly with the generation loss:

$$L_2 = -\mathbb{E}_{\boldsymbol{\eta} \sim p(\boldsymbol{\eta})} \left[ \log p_\gamma(a | \mathbf{V}_\mathbf{F}, q) \right], \tag{12}$$

where $\mathbf{V}_\mathbf{F}$ is the neural fact prompt constructed from the sampled subgraph $g_{sub}$ as described in the previous section. Importantly, $\mathbf{V}_\mathbf{F}$ depends on both the Gumbel noise $\boldsymbol{\eta}$ and the retriever parameters $\beta$.

To balance the significantly different gradient magnitudes between the retriever pre-training and

generation objectives, we apply a direct gradient normalization approach:

$$L_{\text{joint}} = \lambda \frac{L_1}{||\nabla_\beta L_1||} + (1-\lambda)\frac{L_2}{||\nabla_\beta L_2||}, \quad (13)$$

where $\lambda$ is a balancing hyperparameter and $||\nabla_\beta L_i||$ represents the norm of gradients with respect to the retriever parameters.

During inference, we employ a hybrid strategy that first selects the top-k facts with highest selection probabilities, then filters out facts below a probability threshold to remove irrelevant information.

# 5 Experiments

## 5.1 Experiment Settings

**Datasets.** The experimental evaluation was conducted on two benchmark datasets: WebQSP (Yih et al., 2016) and CWQ (Talmor and Berant, 2018), both built upon the Freebase (Bollacker et al., 2008) knowledge graph. These datasets represent classical benchmarks for complex logical reasoning in KGQA. WebQSP contains relatively straightforward questions that typically require 1-2 hop reasoning chains, and CWQ presents more challenging scenarios involving 3-4 hop reasoning chains. Detailed specifications of the datasets are provided in Appendix D.

**Baselines.** D-RAG is compared with 15 baselines across three categories: 1) Graph reasoning methods that leverage graph structure for scoring-based answer inference; 2) LLM reasoning methods that perform reasoning with LLMs without utilizing graph structure during retrieval; and 3) Graph-LLM methods that maintain dedicated graph-based retrieval and leverage LLMs for reasoning. The details of each baseline are described in Appendix E.

**Evaluation Metrics.** Following previous works (Luo et al., 2024a; Sun et al., 2024), D-RAG employs Hits@1 and F1 metrics for evaluation on WebQSP and CWQ. The evaluation process first parses LLM-generated answers into a list for comparison with the ground truth answers. The Hits@1 metric measures whether any correct answer appears in the model's response, representing a basic retrieval capability. In contrast, F1 provides a more rigorous and comprehensive assessment by balancing precision and recall, thus better reflecting the model's overall answer quality. Further details are provided in Appendix F.

**Implementations.** D-RAG employs the ReaRev (Mavromatis and Karypis, 2022) model as the GNN and utilizes the Llama3-8B-Instruct (Meta, 2024) as the LLM. Based on entities linked to the knowledge graph, heuristic subgraphs are extracted via SPARQL query parsing. A heuristic subgraph is a set of facts that conform to the intrinsic logic of the SPARQL query, typically forming a tree structure. Full implementation details are provided in Appendix G.

## 5.2 Main Results

To evaluate the overall effectiveness of D-RAG, we compare it with state-of-the-art baselines on KGQA tasks. Table 1 presents the results, where "-" indicates the corresponding method does not report results for that metric.

The D-RAG approach achieves state-of-the-art performance across both datasets among comparable methods. Specifically, on the WebQSP dataset, D-RAG achieves a **2.5%** improvement in Hits@1 over the best-performing baseline SubgraphRAG, and outperforms DECAF by **3.4%** in the F1 score. Although some baselines like RoG achieve competitive Hits@1 (85.7%), their F1 scores (70.8%) lag substantially behind, suggesting they may retrieve some correct answers but with lower precision.

For the more complex CWQ dataset, the proposed approach demonstrates a **1.8%** advantage in Hits@1 compared to the best-performing ToG approach, and surpasses GNN-RAG by **4.4%** in the F1 score. Notably, methods like SubgraphRAG suffer from a significant performance drop on CWQ (F1 decreases from 70.6% to 47.2%). In contrast, D-RAG maintains consistently superior performance across datasets of varying complexity, achieving the highest scores on both basic retrieval capability (Hits@1) and the more comprehensive measure of answer quality (F1).

A recent work, GCR (Luo et al., 2024b), using the proprietary GPT4-o-mini (OpenAI, 2024a), achieves substantially lower F1 scores than our D-RAG approach: 6.4% lower on WebQSP (74.1% vs. 80.5%) and 2.1% lower on CWQ (61.7% vs. 63.8%). While GCR reports higher Hits@1 scores with GPT4-o-mini (92.2% on WebQSP and 75.8% on CWQ), its performance drops significantly when using comparable open-source models. With Qwen-2-7B (Yang et al., 2024), which has similar parameter size to D-RAG, GCR's Hits@1 on WebQSP falls to 86.3%, 2.8% below our approach. These results reveal that while propri-

| Type | Method | WebQSP | | CWQ | |
|---|---|---|---|---|---|
| | | Hits@1 | F1 | Hits@1 | F1 |
| **Graph Reasoning** | Graftnet (Sun et al., 2018) | 66.4 | - | 32.8 | - |
| | NSM (He et al., 2021) | 68.7 | 62.8 | 47.6 | 42.4 |
| | SR+NSM (Zhang et al., 2022) | 68.9 | 64.1 | 50.2 | 47.1 |
| | ReaRev (Mavromatis and Karypis, 2022) | 76.4 | 70.9 | 52.9 | - |
| | UniKGQA (Jiang et al., 2023b) | 75.1 | 70.2 | 50.7 | 48.0 |
| | NuTrea (Choi et al., 2023) | 77.4 | 72.7 | 53.6 | 49.5 |
| **LLM Reasoning** | Llama3-8B (Meta, 2024) | 59.8 | 45.7 | 30.8 | 27.6 |
| | StructGPT (Jiang et al., 2023a) | 72.6 | - | - | - |
| | DECAF (DPR + FiD-large) (Yu et al., 2023) | 80.7 | 77.1 | 67.0 | - |
| | ToG (GPT4) (Sun et al., 2024) | 82.6 | - | 68.5 | - |
| | RoG (joint) (Luo et al., 2024a) | 85.7 | 70.8 | 62.6 | 56.2 |
| **Graph-LLM** | G-Retriever (He et al., 2024) | 70.1 | - | - | - |
| | EtD (ChatGPT) (Liu et al., 2024a) | 82.5 | - | 62.0 | - |
| | GNN-RAG (Mavromatis and Karypis, 2024) | 85.7 | 71.3 | 66.8 | 59.4 |
| | SubgraphRAG (Llama3.1-8B) (Li et al., 2025) | 86.6 | 70.6 | 57.0 | 47.2 |
| | D-RAG | **89.1** | **80.5** | **70.3** | **63.8** |

Table 1: Performance comparison with different baselines on WebQSP and CWQ.

etary models may excel at Hits@1 through internal knowledge, they still struggle with retrieval precision that impacts F1 scores. D-RAG mitigates this limitation, achieving higher F1 scores using only open-source models.

### 5.3 Ablation Study

To evaluate the effectiveness of end-to-end optimization between the retriever and the generator, our ablation experiments compare D-RAG with four training method variants: 1) *REINFORCE*, which optimizes both modules jointly using the REINFORCE algorithm (Williams, 1992) with variance reduction; 2) *Dynamic Cascade*, where both modules are trained simultaneously with the generator using real-time retriever outputs, but without gradient backpropagation from the generator to the retriever; 3) *Static Cascade*, where the generator is optimized using outputs from the frozen retriever; 4) *Isolation*, where the generator is trained using heuristic subgraphs as input, completely decoupling the two modules. Further details are available in Appendix H.

**Impact on Overall Performance.** Table 2 presents the performance comparison across different training methods on WebQSP and CWQ. We report both "Full Dataset" performance across the entire test set and "Retrieved Subset" metrics for cases where at least one relevant fact is retrieved.

The results reveal that D-RAG consistently outperforms all variants in most metrics across both datasets, with particularly substantial F1 score improvements. On retrieval success cases, D-RAG achieves up to 6.4% and 8.5% higher F1 scores than the best variant on WebQSP and CWQ respectively, demonstrating that end-to-end optimization enables more effective utilization of retrieved facts.

*Dynamic Cascade* shows modest improvements over *Static Cascade*, confirming the benefit of continuously updating the retriever during training. While *REINFORCE* generally outperforms *Static Cascade*, it still falls short of D-RAG's performance, suggesting direct gradient propagation is more effective than reward-based optimization. The *Isolation* variant maintains reasonable Hits@1 performance but exhibits significant drops in F1 scores due to the training-inference gap between clean training subgraphs and noisy inference retrieval.

**Impact on Retrieval Performance.** Figure 3 reveals two advantages of D-RAG's retriever optimization. First, D-RAG consistently achieves the highest retriever F1 scores after joint training begins, demonstrating that gradient propagation from the generator effectively refines retrieval quality. Second, D-RAG shows a more significant down-

| Training Method | WebQSP | | | | CWQ | | | |
|---|---|---|---|---|---|---|---|---|
| | Full Dataset | | Retrieved Subset | | Full Dataset | | Retrieved Subset | |
| | Hits@1 | F1 | Hits@1 | F1 | Hits@1 | F1 | Hits@1 | F1 |
| D-RAG | **89.1** | **80.5** | **94.0** | **86.2** | **70.3** | **63.8** | 81.7 | **75.6** |
| REINFORCE | 85.1 | 72.9 | 90.4 | 78.9 | 61.7 | 55.4 | 73.0 | 66.7 |
| D-RAG w/o e2e | | | | | | | | |
| Dynamic Cascade | 85.3 | 74.0 | 90.4 | 79.8 | 61.9 | 55.9 | 73.5 | 67.1 |
| Static Cascade | 84.8 | 73.0 | 90.7 | 79.4 | 60.6 | 54.3 | 73.2 | 66.6 |
| Isolation | 82.7 | 53.2 | 91.1 | 59.6 | 63.1 | 30.0 | **85.1** | 40.0 |

Table 2: Ablation study comparing overall performance across different training methods.

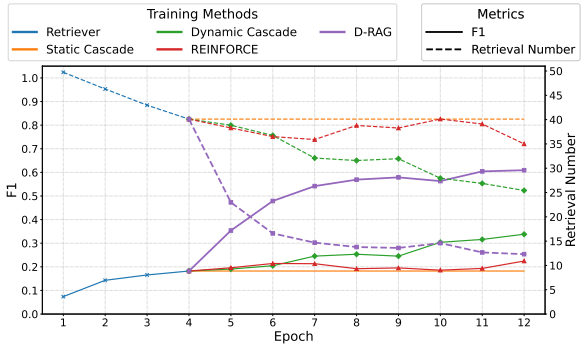


Figure 3: Evolution of retriever F1 (solid lines) and retrieval number (dashed lines) across training epochs on WebQSP. Epochs 1-4 represent retriever-only pretraining, followed by joint training with different methods. Top-50 facts with selection probability >0.5 were used for retrieval evaluation.

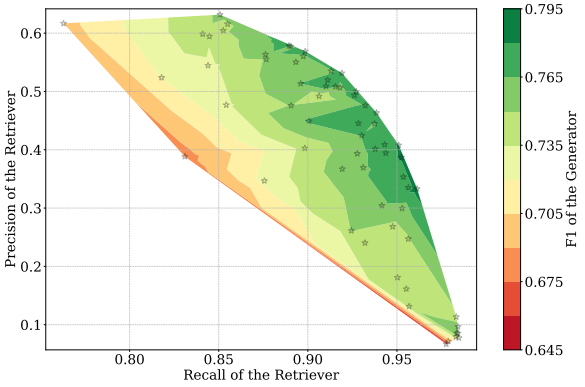


Figure 4: Impact of retriever quality on generator performance (WebQSP dataset). Heatmap shows generator F1 scores (color intensity) as a function of retriever recall (x-axis) and precision (y-axis). Each point represents a model configuration with different retrieval configurations using various probability thresholds (0.01-0.9) applied to the top-100 retrieved facts.

ward trend in retrieved fact count compared to others, which is meaningful progress toward the actual average of 6.4 relevant facts per WebQSP question (corresponding to the heuristic subgraph), demonstrating superior noise reduction capability.

### 5.4 Relationship Between Retrieval and Generation Performance

To understand how different aspects of retrieval quality affect generation performance, we examined various retrieval configurations and their impact on generator performance. As shown in Figure 4, both retrieval recall and precision significantly impact generator performance. Models in the lower-right region (high recall but low precision) perform worse than those with balanced metrics, indicating that retrieving many relevant facts without filtering irrelevant ones leads to suboptimal results. Similarly, models in the upper-left region (high precision but low recall) underperform due to insufficient fact coverage.

To further evaluate the effectiveness and efficiency of D-RAG, we perform additional experiments, including more overall performance analysis, detail analysis, efficiency analysis, and case study in Appendix I.

## Conclusion

In this paper, we presented D-RAG, a novel differentiable approach for KGQA that enables end-to-end optimization between the retriever and the generator. D-RAG achieves this through reformulating the optimization and a differentiable implementation of subgraph sampling and prompt construction, Experimental results demonstrate that D-RAG outperforms state-of-the-art methods with substantial improvements, with the joint optimization significantly reducing noise in the retrieved subgraph while showing that both precision and recall in retrieval impact generator performance.

## Limitations

Despite the effectiveness of D-RAG, we acknowledge several limitations of our current approach. First, our approach relies on entity linking results without considering potential errors in this preprocessing step. Second, our end-to-end optimization approach is limited to open-source language models and cannot be directly applied to closed-source API-based models.

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# A Probability Factorization Analysis

In this section, we first prove the validity of Equation 3, followed by a discussion on the rationale behind fact-wise factorization.

The factorization of subgraph probability represents an approximation of the complex probability distribution, with an underlying assumption that the selection of each fact is independent. Consider a knowledge graph with $N_f$ facts, where each fact has two possible states (selected or not selected), resulting in $2^{N_f}$ possible subgraphs. The sum of probabilities over all possible subgraphs can be expressed as:

$$\sum_{g_{sub}} p(g_{sub}) \tag{885}$$

$$= \sum_{g_{sub}} \prod_{\tau_i \in g_{sub}} p(\tau_i) \prod_{\tau_j \notin g_{sub}} (1 - p(\tau_j)) \tag{886}$$

$$= \sum_{\tau_1} \sum_{\tau_2} \cdots \sum_{\tau_{N_f}} \prod_{i=1}^{N_f} p(\tau_i)^{\mathbb{I}(\tau_i)} (1 - p(\tau_i))^{1-\mathbb{I}(\tau_i)} \tag{887}$$

$$= \prod_{i=1}^{N_f} \sum_{\mathbb{I}(\tau_i) \in \{0,1\}} p(\tau_i)^{\mathbb{I}(\tau_i)} (1 - p(\tau_i))^{1-\mathbb{I}(\tau_i)} \tag{888}$$

$$= \prod_{i=1}^{N_f} (p(\tau_i) + (1 - p(\tau_i))) = 1, \tag{889}$$

where the third row follows from the fact that summing over all subgraphs is equivalent to considering both possibilities (selected or not selected) for each fact independently. $\mathbb{I}(\tau_i)$ is an indicator function that equals 1 when fact $\tau_i$ is included in the subgraph and 0 otherwise. The final result of 1 validates the probability formulation in Equation 3.

Beyond fact-wise factorization, node-level and path-wise granularities are also common choices for probability decomposition. Path-wise granularities, however, face combinatorial complexity challenges, which explains why direct modeling of subgraph probability is computationally intractable. Node-wise granularity, on the other hand, disregards relation information between entities and fails to handle multi-edge scenarios. These limitations motivate our choice of fact-wise factorization. To address the potential dependencies between fact selections that may be overlooked by the independence assumption implicit in factorization, we employ a GNN-based retriever. The inherent capability of GNNs to capture graph structural information

helps mitigate the independence assumption, as the internal parameters of GNN can effectively encode the correlations between facts.

## B Specific design of GNN-based Retriever

### B.1 Module

For the GNN-based retriever, D-RAG adopts ReaRev (Mavromatis and Karypis, 2022) as the core architecture, which consists of three primary modules:

- The Instruction Module employs Sentence-BERT (Reimers and Gurevych, 2019) as its Language Model (LM) encoder to transform queries into instructions;
- The Graph Reasoning Module initializes and updates node representations through message passing, considering the relationship between instructions and nodes;
- The Instruction Update Module refines instructions based on the node representations and predicted terminal node distributions.

In our implementation, the node encoder corresponds to the output of the Graph Reasoning Module, and the relation encoder refers to the LM encoder and MLP projection components used in the node initialization process.

### B.2 Loss design of GNN-based Retriever

As shown in Equation 11 of the main text, the loss function $L_1$ for training the GNN-based retriever is formulated as:

$$\begin{aligned} &D_{KL}(p_{heur}(g_{sub})|p_\beta(g_{sub})) \\ &= -\sum_{\tau \in g_{sub}} \log p_\beta(\tau) = L_{\text{BCE}}. \end{aligned} \tag{14}$$

This can be implemented using PyTorch's BCE (Binary Cross Entropy) weighted loss [1]. Inspired by the work of (Lin et al., 2024), to address the sparsity of positive examples in knowledge graph link classification tasks, we further incorporate a rank loss:

$$L_{\text{rank}} = -\frac{1}{N_+ N_-} \sum_{i=1}^{N_+} \sum_{j=1}^{N_-} \log \sigma(p(\tau_i) - p(\tau_j)), \tag{15}$$

[1] https://pytorch.org/docs/stable/generated/torch.nn.BCEWithLogitsLoss.html

where $N_+$ and $N_-$ denote the number of positive and negative examples, respectively, $\tau_i$ represents a positive example, $\tau_j$ represents a negative example, and $\sigma(\cdot)$ is the sigmoid function. This ranking loss generates larger gradients on sparse samples, effectively complementing the BCE loss and enhancing the model's classification capability.

The total loss of the GNN-based retriever is a weighted combination of these two losses:

$$L_1 = \rho L_{\text{BCE}} + (1 - \rho) L_{\text{Rank}}, \tag{16}$$

where we empirically set $\rho = 0.7$ to balance between the BCE loss and the ranking loss.

## C Prompts

Figure 5 illustrates the full input prompt received by the LLM-based generator, which consists of three components: task setting, question, and subgraph. The subgraph is shown in typewriter font, representing the neural fact prompt in D-RAG.

In the subgraph part, each line corresponds to a distinct fact that will be converted to embedding form before being input to the LLM. The `<S-Embedding>` marker at the beginning of each line represents the structural embedding mentioned in the proposed approach. The textual content following this marker contains the semantic information of each fact. Together, these elements constitute the neural fact prompt that enables the model to effectively integrate knowledge during generation.

## D Datasets

D-RAG evaluates on two benchmark KGQA datasets: WebQuestionSP (WebQSP) (Yih et al., 2016) and Complex WebQuestions (CWQ) (Talmor and Berant, 2018). Following previous works (Luo et al., 2024a; He et al., 2021), the same train and test splits are adopted for fair comparison. The datasets are analyzed from two perspectives: basic statistics and reasoning complexity.

The overall statistics of both datasets are summarized in Table 3, including the number of samples in training, validation and test sets.

Table 4 shows the distribution of reasoning hops required for answering questions, indicating the logical complexity of questions in each dataset. The hop counting method analyzes the path length from topic entities to answer entities in SPARQL queries. For WebQSP, hop counts are determined precisely as most questions involve single topic entities with equal path lengths from

**Complete Generator Prompt**

**Answer the question based on the provided facts.**
**Question:** what does jamaican people speak
**Provided facts:**

```
<S-Embedding> Jamaica, location.country.official_language, Jamaican English
<S-Embedding> Jamaica, location.country.languages_spoken, Jamaican English
<S-Embedding> Jamaica, location.country.languages_spoken, Jamaican Creole English Language
<S-Embedding> Jamaica, location.country.currency_used, Jamaican dollar
<S-Embedding> Jamaica, location.country.form_of_government, Democracy
<S-Embedding> Jamaica, location.country.form_of_government, Parliamentary system
<S-Embedding> Jamaica, base.locations.countries.continent, North America
<S-Embedding> Jamaica, location.country.form_of_government, Constitutional monarchy
<S-Embedding> Grenada, location.country.official_language, English Language
<S-Embedding> Bermuda, location.country.official_language, English Language
<S-Embedding> Belize, location.country.official_language, English Language
<S-Embedding> Turks and Caicos Islands, location.country.official_language, English Language
<S-Embedding> Bahamas, location.country.official_language, English Language
<S-Embedding> Cayman Islands, location.country.official_language, English Language
<S-Embedding> Puerto Rico, location.country.official_language, English Language
<S-Embedding> Grenada, location.country.languages_spoken, English Language
<S-Embedding> Bermuda, location.country.languages_spoken, English Language
<S-Embedding> Costa Rica, location.country.languages_spoken, Jamaican Creole English Language
<S-Embedding> , location.country.languages_spoken, English Language
<S-Embedding> Turks and Caicos Islands, location.country.languages_spoken, English Language
```

**Answer:**

Figure 5: The complete input prompt for the LLM-based generator, incorporating 20 facts.

topic to answer entities. For CWQ, we compute fuzzy hop counts due to frequent multi-topic scenarios. When SPARQL queries represent constrained graphs rather than simple reasoning chains, we take the maximum path length among all topic-to-answer paths as the final hop count.

| Datasets | #Train | #Validate | #Test |
|---|---|---|---|
| WebQSP | 2826 | 246 | 1,628 |
| CWQ | 27,639 | 3519 | 3531 |

Table 3: Statistics of the datasets.

| Datasets | 1-hop | 2-hop | 3-hop | ≥4-hop |
|---|---|---|---|---|
| WebQSP | 62.00% | 37.66% | 0.17% | 0.17% |
| CWQ | 24.66% | 64.78% | 7.50% | 3.06% |

Table 4: Statistics of reasoning hop distribution in WebQSP and CWQ.

## E Baselines

The D-RAG approach is compared with the 15 baselines grouped into three categories: 1) Graph reasoning methods; 2) LLM reasoning methods; and 3) Graph-LLM methods. The details of each baseline are described as follows:

**Graph Reasoning Methods.**

- Graftnet (Sun et al., 2018) performs question answering by propagating features through a heterogeneous graph that fuses knowledge bases and text documents.
- NSM (He et al., 2021) leverages language models' bidirectional reasoning capabilities for multi-hop question answering.
- SR+NSM (Zhang et al., 2022) introduces a trainable path-wise subgraph retriever that decouples retrieval from reasoning.
- ReaRev (Mavromatis and Karypis, 2022) adaptively refines reasoning instructions using knowledge graph context and executes them through a BFS-guided neural network.
- UniKGQA (Jiang et al., 2023b) unifies retrieval and reasoning stages in KGQA through a shared PLM-based architecture and joint pretraining strategy.
- NuTrea (Choi et al., 2023) utilizes tree search-based message passing to explore future paths with RF-IEF node embeddings that capture global KG context.

**LLM Reasoning Methods.**

- Llama3-8B (Meta, 2024) performs direct reasoning without fact retrieval by leveraging its pre-trained knowledge.
- StructGPT (Jiang et al., 2023a) enhances LLM reasoning by iteratively collecting evidence from structured data through specialized interfaces before performing reasoning steps.
- DECAF (DPR + FiD-large) (Yu et al., 2023) improves KB question answering by combining logical form generation with direct answer prediction, while simplifying the process through text-based retrieval.
- ToG (GPT4) (Sun et al., 2024) enables LLMs to perform traceable reasoning by iteratively exploring knowledge graphs through beam search.
- RoG (joint) (Luo et al., 2024a) enhances LLM reasoning by leveraging KG structure to generate faithful reasoning chains through a planning-retrieval-reasoning framework.

**Graph-LLM Methods.**

- G-Retriever (He et al., 2024) enables conversational graph interaction by combining GNNs, LLMs, and RAG through Prize-Collecting Steiner Tree optimization.
- EtD (ChatGPT) (Liu et al., 2024a) combines GNNs for efficient knowledge exploration with frozen LLMs for final answer determination, creating a resource-efficient framework for KGQA.
- GNN-RAG (Mavromatis and Karypis, 2024) combines GNNs for subgraph reasoning and path extraction with LLMs for natural language understanding in a RAG framework.
- SubgraphRAG (Llama3.1-8B) (Li et al., 2025) enhances KG-based RAG by implementing efficient subgraph retrieval with flexible size control and directional structural encoding.

## F Discussion on Evaluation Metrics

The evaluation procedure varies across different methods. While node prediction and graph query approaches produce direct answers requiring no additional processing, LLM-based methods often generate responses containing multiple predicted answers. This characteristic of LLMs explains why many recent works (Mavromatis and Karypis, 2024; Li et al., 2025; Luo et al., 2024b) prefer the term Hit over Hits@1, as the evaluation focuses on the presence of correct answers within the complete generated response rather than strictly the first answer.

It is important to note that the above discussion pertains to the overall performance of KGQA systems in terms of answer generation. Throughout this paper, we also report retrieval performance using F1, recall, and precision metrics. These retrieval metrics are calculated by comparing the facts in the retrieved subgraph with those in the heuristic subgraph, which serves as a reference standard. A key consideration is that KGQA benchmarks do not provide ground truth subgraph annotations. The heuristic subgraphs are constructed by parsing SPARQL queries associated with each question, detailed in Appendix G. This parsing ensures that the heuristic subgraphs fully align with the multi-hop reasoning required by the questions, making them relatively reliable reference standards for evaluating retrieval performance.

## G Implementation Details

**Preprocessing.** Consistent with prior work (Mavromatis and Karypis, 2022; Luo et al., 2024a), we assume that the entities mentioned in the questions (referred to as topic entities) have already been linked to the knowledge graph through entity linking (Yih et al., 2015). After identifying entities in the questions, we construct a heuristic subgraph for each question by parsing the SPARQL query. For each SPARQL query, we focus on the logic chain from the topic entity to the answer entity, identifying paths that connect the topic entity to the answer through specific logical chains. All facts along these paths collectively form the heuristic subgraph used in the proposed approach.

**Inference.** During inference, we employ a hybrid strategy that first selects the top-k facts with highest selection probabilities, then filters out facts below a probability threshold to remove irrelevant information. For both WebQSP and CWQ datasets, we set $k = 100$ (due to context length constraints) and use a probability threshold of 0.01, which is determined through grid search on the WebQSP

validation set.

**Optimization and Hyperparameters.** We train separate models for CWQ and WebQSP datasets. The training process follows a two-stage approach: GNN pre-training followed by joint training. During the first training phase (retriever pre-training), we train the model for 10 epochs. In the second training phase (joint training), we train for 18 epochs.

For model optimization, we apply different strategies to the GNN and LLM components. The GNN undergoes full parameter fine-tuning with a learning rate of 5e-5, while the LLM is fine-tuned using LoRA with a learning rate of 1e-5. The LoRA hyperparameters are configured as: lora_r=8, lora_alpha=16, and dropout=0.05, specifically targeting the q_proj and v_proj modules. We employ the AdamW optimizer with a weight decay of 0.001, a batch size of 16, and a cosine learning rate scheduler.

Regarding the hyperparameters in our formulations, we set the Gumbel-Softmax temperature coefficient to 0.5 and the loss balancing parameter $\lambda$ to 0.9. All experiments are conducted on 2 NVIDIA A800-80GB GPUs.

## H Details of Ablation Study

As mentioned in Section 4.4, we initially pre-train the retriever using heuristic subgraph labels to prevent it from retrieving completely irrelevant subgraphs. All training method variants describes below, including our proposed D-RAG, are trained based on this pre-trained retriever. Here we elaborate on the four training method variants:

1. *REINFORCE*: We implements the REINFORCE algorithm with variance reduction techniques to jointly optimize both the retriever and the generator. Two reward functions are considered: (i) the negative of the generator's answer loss, and (ii) the recall of retrieved subgraphs compared to heuristic subgraphs. As we observes no significant difference between these reward formulations, the results reported in the main paper correspond to the recall reward.

2. *Dynamic Cascade*: In this approach, both modules are trained simultaneously with the generator using real-time outputs from the retriever during training. However, gradient backpropagation from the generator to the retriever is blocked, meaning the retriever is only optimized using heuristic subgraph labels.

3. *Static Cascade*: The generator is optimized using outputs from the initial fixed retriever (after pre-training). The retriever remains frozen throughout this process and is trained only with heuristic subgraph labels.

4. *Isolation*: The generator is trained using heuristic subgraphs as input, completely decoupling the two modules. Both the retriever and the generator are essentially trained independently.

Table 5 summarizes the key differences between these training methods. The key distinction between D-RAG and the *REINFORCE* variant lies in the granularity of supervision: D-RAG employs fine-grained supervision through direct end-to-end gradient-based optimization, allowing it to analyze the influence of each individual fact on answer generation, while *REINFORCE* uses policy gradient methods that provide only coarse-grained, holistic supervision regarding the quality of the retrieved subgraph information.

## I Additional Expreiment Results

### I.1 Performance Comparison Under Different Situation

In this section, we provide a detailed analysis of the performance results presented in Table 6, which compares our proposed D-RAG method against several baseline training methods as described in Section 5.3.

From Table 6, we can draw three important observations:

**1) D-RAG's Comprehensive Effectiveness:** D-RAG consistently outperforms alternative training methods across almost all metrics and complexity levels. This superiority extends to both generation metrics (Hits@1 and F1) and retrieval metrics (Recall and Precision), demonstrating the holistic effectiveness of the proposed approach.

**2) Recall Necessity but Insufficiency:** High recall is necessary but not sufficient for strong generation performance. or 3-hop questions, the difference in recall between D-RAG and Dynamic Cascade is 6.9 percentage points (89.8% vs. 82.9%), yet the gap in generation F1 is significantly larger

| Training Method | Retriever Supervision | Generator Input | G → R gradient |
|---|---|---|---|
| D-RAG | Retrieval label + Answer label | Real-time retriever output | ✓ |
| REINFORCE | Retrieval label + Reward label | Real-time retriever output | ✓ |
| Dynamic Cascade | Retrieval label | Real-time retriever output | × |
| Static Cascade | Retrieval label | Fixed pre-trained retriever output | × |
| Isolation | Retrieval label | Heuristic subgraph | × |

Table 5: Comparison of different training methods highlighting differences in retriever supervision signals, generator inputs, and whether gradients flow from generator to retriever (G → R) during joint training.

| Training Method | Generation Hits@1 | | | | Generation F1 | | | |
|---|---|---|---|---|---|---|---|---|
| | 1-hop | 2-hop | 3-hop | 4-hop | 1-hop | 2-hop | 3-hop | 4-hop |
| D-RAG | **74.4** | **81.3** | **79.8** | **58.0** | **69.0** | **76.2** | **74.5** | **55.6** |
| REINFORCE | 63.7 | 73.4 | 65.9 | 45.7 | 59.6 | 67.4 | 59.4 | 45.7 |
| Dynamic Cascade | 66.1 | 74.0 | 65.9 | 39.5 | 62.4 | 67.8 | 59.2 | 39.5 |
| Static Cascade | 64.4 | 71.1 | 64.3 | 43.2 | 60.4 | 64.9 | 57.9 | 42.7 |
| Training Method | Retrieval Recall | | | | Retrieval Precision | | | |
| | 1-hop | 2-hop | 3-hop | 4-hop | 1-hop | 2-hop | 3-hop | 4-hop |
| D-RAG | **92.6** | **95.5** | **89.8** | **91.2** | **6.9** | **20.2** | **23.1** | 13.9 |
| REINFORCE | 89.1 | 90.7 | 81.1 | 80.7 | 4.0 | 9.0 | 13.0 | 14.1 |
| Dynamic Cascade | 89.4 | 91.6 | 82.9 | 82.5 | 4.3 | 10.9 | 14.7 | **15.1** |
| Static Cascade | 86.7 | 85.5 | 78.1 | 78.7 | 3.9 | 9.2 | 13.6 | 14.1 |

Table 6: Performance comparison of D-RAG against different training methods on the CWQ dataset. Results show both overall performance (Hits@1 and F1) and retrieval performance (Recall and Precision) across different complexity levels (1-4 hops).

at 15.3% (74.5% vs. 59.2%). This suggests that retrieval precision and effective utilization of retrieved documents also play crucial roles in generation quality.

**3) Widening Retrieval-Generation Gap:** As question complexity increases, the gap between retrieval performance and generation performance widens. For 4-hop questions, despite D-RAG maintaining high recall (91.2%), its generation Hits@1 drops to 58.0% - a gap of 33.2%. In comparison, for 1-hop questions, this gap is much smaller (92.6% recall vs. 74.4% Hits@1, a difference of 18.2%).

### I.2 Detail Analysis

Due to computational constraints, all experiments in this detail analysis were conducted with joint training limited to 8 epochs, whereas the main experimental results reported in previous sections used 18 training epochs. This difference in training duration may account for some performance discrepancies between these detailed analyses and our primary results.

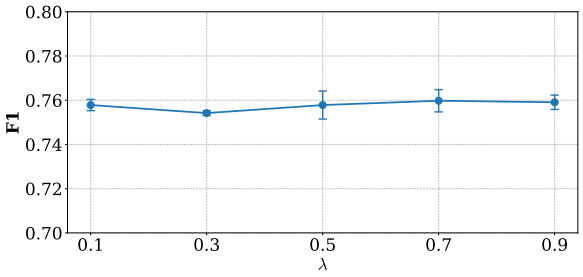



Figure 6: Impact of loss balancing hyperparameter $\lambda$ on overall performance for WebQSP Dataset. The plot shows the overall F1 scores (y-axis) achieved with different values of $\lambda$ (x-axis) in the joint loss function 13. Error bars represent standard deviations across three experimental runs.

**Robustness to Loss Balancing Hyperparameter.** Figure 6 examines the effect of the loss balancing hyperparameter $\lambda$ on the overall performance, where $\lambda$ controls the weighting between retriever and generator losses as defined in Equation 13.

The experimental results demonstrate remarkable stability across the entire range of $\lambda$ values

(0.1 to 0.9). This consistent performance indicates that the system is largely insensitive to the specific weighting between retriever and generator components. This robustness can be primarily attributed to the gradient normalization mechanism employed in our loss formulation, which effectively prevents either component from dominating the optimization process regardless of the $\lambda$ value. Future work could explore more sophisticated gradient balancing techniques such as GradNorm (Chen et al., 2018), which builds upon gradient normalization by introducing adaptive weighting strategies that automatically adjust task weights during training based on learning dynamics.

| Fact Order | Training Method | |
|---|---|---|
| | D-RAG | Dynamic Cascade |
| ascent | $76.11 \pm 0.09$ | $75.04 \pm 0.38$ |
| descent | $76.33 \pm 0.22$ | $74.94 \pm 0.10$ |
| random | $76.66 \pm 0.34$ | $73.77 \pm 0.77$ |

Table 7: The F1 scores across different fact ordering strategies and training methods. The table compares the performance (F1 score ± standard deviation) of D-RAG and Dynamic Cascade training methods under three fact ordering strategies.

**Impact of Fact Ordering on Overall Performance.** Since the order of input facts can influence LLM generation (Liu et al., 2024b), we compare three ordering strategies: 1) *Ascent*: Facts are arranged in ascending order of selection probabilities; 2) *Descent*: The reverse of ascent, with facts ordered from high to low probabilities; 3) *Random*: Facts are shuffled randomly during both training and inference.

Table 7 evaluates the influence of fact ordering on overall performance for both D-RAG and *Dynamic Cascade* in Section 5.3. The results reveal two key findings. First, D-RAG demonstrates remarkable robustness across all ordering strategies. This stability suggests that D-RAG effectively learns to process fact sequences regardless of their presentation order, an advantageous property for real-world applications where optimal fact ordering may not be predetermined or existed.

In contrast, the Dynamic Cascade method shows greater sensitivity to fact ordering, with performance declining noticeably under random ordering (73.77%) compared to more structured approaches (ascent: 75.04%, descent: 74.94%). This indicates that consistent, deterministic ordering strategies generally outperform random fact arrangements.

| Training Method | Time (minutes) |
|---|---|
| D-RAG | $74.43 \pm 0.43$ |
| Dynamic Cascade | $68.92 \pm 1.28$ |
| Static Cascade | $69.66 \pm 0.42$ |

Table 8: Training time per epoch on CWQ with 5,000 random samples. Time variations ($\pm$) indicate the standard deviation across multiple epochs.

### I.3 Training Efficiency Analysis

Table 8 presents the training time per epoch for different training methods on the CWQ dataset using 5,000 random samples.

D-RAG shows a modest increase in training time compared to others, requiring 8.0% more time than *Dynamic Cascade* and 6.9% more than *Static Cascade*. This additional overhead primarily comes from computing gradient norms during loss calculation and the extra backpropagation computations required for end-to-end training.

Interestingly, *Dynamic Cascade* achieves faster training times than *Static Cascade* despite the additional computation needed for retriever updates. As shown in Figure 3, *Dynamic Cascade* retrieves fewer facts than *Static Cascade*, suggesting that the computational benefits from retrieving fewer facts outweigh the cost of training the retriever.

Similarly, the relatively small time difference between D-RAG and the cascade variants can be largely attributed to D-RAG's ability to retrieve fewer and more relevant facts as training progresses (as shown in Figure 3).

### I.4 Case Study

To illustrate the advantages of D-RAG, we select representative examples from both WebQSP and CWQ datasets, covering a range of reasoning complexity (1-hop to 3-hop) and answer cardinality (single and multiple answers). Table 9 and 10 present these case studies with visualizations of the retrieved subgraphs and generated answers across different training methods.

The retrieved subgraphs in different cases reveal D-RAG's superior retrieval characteristics compared to other methods. D-RAG consistently produces more focused subgraphs with significantly reduced noise and maintains high recall of relevant facts. This selective retrieval aligns with our goal of providing LLMs with concise yet comprehensive information, as excessive irrelevant facts can

distract the generation process and insufficient coverage may miss critical reasoning chains. In the WebQSP example "who inspired Obama" (Table 9, 1-hop), we observe that *Static Cascade* retrieves a sparse and incomplete subgraph leading to an incorrect answer, D-RAG successfully identifies and preserves all three correct answers with minimal extraneous facts.

The 3-hop example from CWQ—"What county is the city that includes the Houston City Council as a part of their government located in?"—particularly highlights D-RAG's effectiveness in complex reasoning scenarios. This question requires following a challenging reasoning chain: `Houston City Council <- governmental body <- governing officials -> county -> Montgomery County`. *Static Cascade* fails to retrieve the complete reasoning chain, resulting in an incorrect answer ("Texas"), and *Dynamic Cascade* suffers from excessive noise that impedes identifying the correct reasoning chain. In contrast, D-RAG effectively prunes irrelevant facts and preserving the critical reasoning chains, enabling the generator to correctly identify "Montgomery County". These cases empirically validate the proposed approach, demonstrating how end-to-end optimization produces cleaner, more focused subgraphs that contain essential reasoning chains and minimize noise. Based on these high-quality subgraphs, the KGQA system generates accurate answers, underscoring the practical benefits of D-RAG in real-world knowledge-based question answering scenarios.

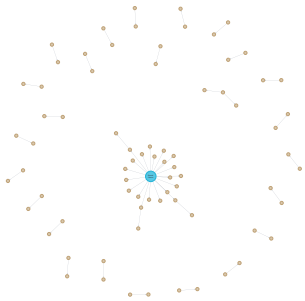
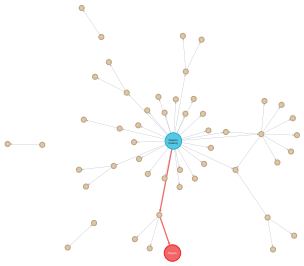
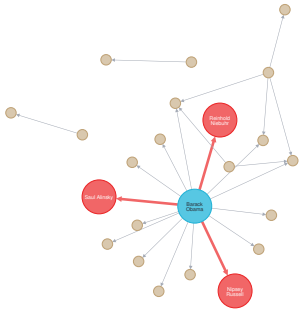
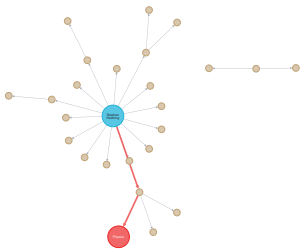
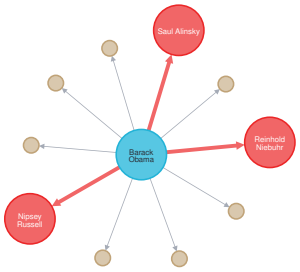
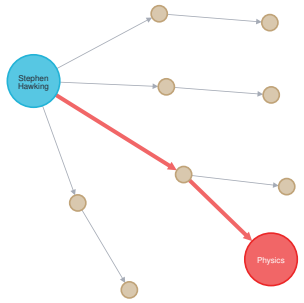
| | 1-hop Example | 2-hop Example |
|---|---|---|
| Question | who inspired obama | what did stephen hawking study |
| True Answers | Reinhold Niebuhr \| Nipsey Russell \| Saul Alinsky | Physics |
| Heuristic Subgraph from SPARQL |  |  |
| Static Cascade (Subgraph) |  |  |
| Static Cascade (Answers) | Martin Luther King Jr. | Astrophysicist \| Cosmologist\| Physicist... |
| Dynamic Cascade (Subgraph) |  |  |
| Dynamic Cascade (Answers) | Saul Alinsky | Cosmologist \| Physicist \| Astrophysicist... |
| D-RAG (Subgraph) |  |  |
| D-RAG (Answers) | Reinhold Niebuhr \| Nipsey Russell \| Saul Alinsky | Physics |

Table 9: Case studies on WebQSP dataset. Comparison of retrieved subgraphs and generated answers across different methods on 1-hop and 2-hop questions. Blue nodes represent question entities, red nodes represent answer entities, and yellow nodes are intermediate entities.

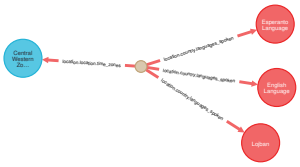
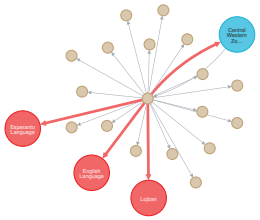
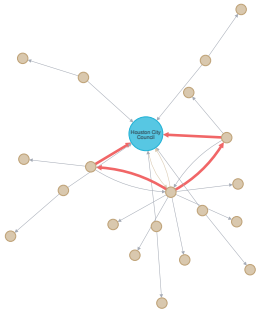
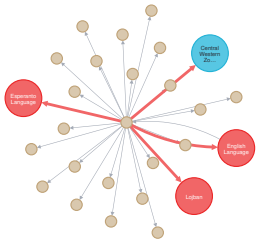
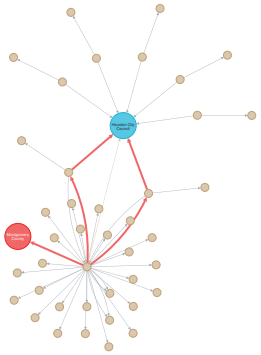
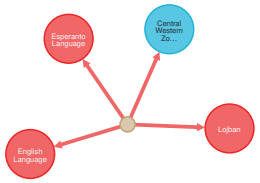
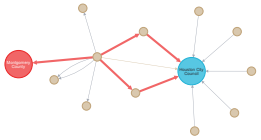
| | 2-hop Example | 3-hop Example |
|---|---|---|
| Question | What languiages are spoken by residents of the Central Western Time Zone? | What county is the city that includes the Houston City Council as a part of their government located in? |
| True Answers | Esperanto Language \| Lojban \| English Language | Montgomery County |
| Heuristic Subgraph from SPARQL |  |  |
| Static Cascade (Subgraph) |  |  |
| Static Cascade (Answers) | English Language | Texas |
| Dynamic Cascade (Subgraph) |  |  |
| Dynamic Cascade (Answers) | English Language | Harris County |
| D-RAG (Subgraph) |  |  |
| D-RAG (Answers) | Esperanto Language \| Lojban \| English Language | Montgomery County |

Table 10: Case studies on CWQ dataset. Comparison of retrieved subgraphs and generated answers across different methods on 2-hop and 3-hop questions. Blue nodes represent question entities, red nodes represent answer entities, and yellow nodes are intermediate entities.