Re-Invoke: Tool Invocation Rewriting for Zero-Shot Tool Retrieval

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Abstract

Recent advances in large language models (LLMs) have enabled autonomous agents with complex reasoning and task-fulfillment capabilities using a wide range of tools. However, effectively identifying the most relevant tools for a given task becomes a key bottleneck as the toolset size grows, hindering reliable tool utilization. To address this, we introduce Re-Invoke, an unsupervised tool retrieval method designed to scale effectively to large toolsets without training. Specifically, we first generate a diverse set of synthetic queries that comprehensively cover different aspects of the query space associated with each tool document during the tool indexing phase. Second, we leverage LLM's query understanding capabilities to extract key tool-related context and underlying intents from user queries during the inference phase. Finally, we employ a novel multi-view similarity ranking strategy based on intents to pinpoint the most relevant tools for each query. Our evaluation demonstrates that Re-Invoke significantly outperforms state-of-the-art alternatives in both single-tool and multi-tool scenarios, all within a fully unsupervised setting. Notably, on the ToolE datasets, we achieve a 20% relative improvement in nDCG@5 for single-tool retrieval and a 39% improvement for multi-tool retrieval.

1 Introduction

Recently, large language models (LLMs) have demonstrated impressive capabilities on a variety of complex tasks, including math, reasoning and coding [\(OpenAI,](#page-9-0) [2023c;](#page-9-0) [Anil et al.,](#page-8-0) [2023;](#page-8-0) [Google,](#page-9-1) [2023b\)](#page-9-1). They can even surpass average human performance on standardized exams such as college entrance tests, law school admission, and math competitions [\(Zhong et al.,](#page-10-0) [2024\)](#page-10-0). However, LLMs are pre-trained on a static corpus, limiting their

Figure 1: An example of low-performance retrieval methods failing to identify the actual user intents "improve French language skills" due to the context "planning a trip to France". It selects similar, but incorrect travel assistant tool instead of the ground-truth language learning tool from the given pool of tools.

adaptability to the rapidly evolving real world, and frequent fine-tuning [\(Wei et al.,](#page-10-1) [2021\)](#page-10-1) is computationally expensive.

In contrast, humans leverage a vast array of tools to interact with the external world, using search engines for information retrieval, maps for navigation, calculators for algebraic tasks, and so on. Augmenting LLMs with external tools, rather than relying solely on their internal knowledge, could unlock their potential to tackle even more challenging problems. This insight has driven recent interests in both academic research [\(Parisi et al.,](#page-9-2) [2022;](#page-9-2) [Schick et al.,](#page-10-2) [2023;](#page-10-2) [Lu et al.,](#page-9-3) [2023;](#page-9-3) [Cai et al.,](#page-8-1) [2023;](#page-8-1) [Patil et al.,](#page-9-4) [2023;](#page-9-4) [Hsieh et al.,](#page-9-5) [2023;](#page-9-5) [Qin](#page-10-3) [et al.,](#page-10-3) [2023\)](#page-10-3) and industrial applications. Examples include ChatGPT plugins [\(OpenAI,](#page-9-6) [2023a\)](#page-9-6), with supported third-party APIs, and Bard extensions [\(Google,](#page-9-7) [2023a\)](#page-9-7) connecting to Google APIs and services.

Common approaches to integrate tools with LLMs often rely on supervised methods to generate tool calling functions [\(Schick et al.,](#page-10-2) [2023;](#page-10-2) [Patil](#page-9-4) [et al.,](#page-9-4) [2023;](#page-9-4) [Parisi et al.,](#page-9-2) [2022;](#page-9-2) [Qin et al.,](#page-10-3) [2023;](#page-10-3) [Hao](#page-9-8) [et al.,](#page-9-8) [2023\)](#page-9-8) or in-context learning by providing the tool documents and few-shot demonstrations [\(Xu](#page-10-4)

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[et al.,](#page-10-4) [2023;](#page-10-4) [Lu et al.,](#page-9-3) [2023;](#page-9-3) [Hsieh et al.,](#page-9-5) [2023\)](#page-9-5). However, these methods face practical challenges when scaling to a large number of tools on complex tasks: (a) *Input Token Length Limitations*: LLMs have inherent input token length limitations, making it infeasible to include a comprehensive list of tools within a single prompt. Moreover, LLMs can struggle to effectively process relevant information from lengthy input contexts [\(Liu et al.,](#page-9-9) [2024\)](#page-9-9). (b) *Evolving Tool Pool*: LLMs are often paired with a tool retriever trained on labeled query-tool pairs. However, the ideal LLM toolkit should be vast and dynamic, with tools undergoing frequent updates. Providing and maintaining labels for such an extensive and evolving toolset is impractical. Continuous retraining would also require extensive production maintenance. (c) *Ambiguous User Intents*: User contexts in the queries could obfuscate the underlying intents and failure to identify the intents could lead to calling the wrong tools (See Fig. [1\)](#page-0-1). Retrieving the relevant tools to address all the intents described in the user query remains a challenging task.

To address these unique challenges, we introduce Re-Invoke, a novel unsupervised retrieval method to enable effective retrievals even when user intent is multifaceted or tool document is lacking. To the best of our knowledge, Re-Invoke is the first fully unsupervised approach to tackle multitool retrieval use cases. It leverages LLMs for both tool document enrichment and user intent extraction, thereby enhancing tool retrieval performance across various use cases. Our approach consistently and significantly improves upon state-of-theart alternatives, achieving a 20% relative improvement in nDCG@5 on single-tool retrieval tasks and 39% improvement on multi-tool retrieval tasks with ToolE dataset.

2 Related Work

Tool Retrievals for Tool-Use. ReAct [\(Yao et al.,](#page-10-5) [2023\)](#page-10-5) pioneers the interaction and reasoning with diverse tools using in-context reasoning traces, particularly in decision-making and multi-step reasoning environments. [Schick et al.](#page-10-2) [\(2023\)](#page-10-2) proposes a self-supervised training method with API demonstrations. [Patil et al.](#page-9-4) [\(2023\)](#page-9-4) and [Hsieh et al.](#page-9-5) [\(2023\)](#page-9-5) demonstrate that augmenting LLMs with tool document significantly improves their ability to generate correct API calls by mitigating hallucinations, compared to prompting with demonstrations alone.

[Yuan et al.](#page-10-6) [\(2024\)](#page-10-6) also shows unifying tool instruction leads to better tool usage. However, tool document retrieval for LLM tool learning is currently under-explored, as most work simply uses LLM agents to retrieve a limited number of tools. [Patil](#page-9-4) [et al.](#page-9-4) [\(2023\)](#page-9-4) first demonstrate that LLMs generate more reliable outputs with the integration of a retrieval system using BM25 [\(Robertson et al.,](#page-10-7) [2009\)](#page-10-7) and GPT-index [\(Liu,](#page-9-10) [2022\)](#page-9-10), but still introduce more hallucination and errors compared to the ground truth retriever. Some works [\(Qin et al.,](#page-10-3) [2023;](#page-10-3) [Kong](#page-9-11) [et al.,](#page-9-11) [2023;](#page-9-11) [Gao et al.,](#page-8-2) [2024\)](#page-8-2) train a Sentence-Bert transformer model using the fully labeled query-API document pairs as a tool retriever. The key distinction between our approach and existing tool retrieval systems lies in our emphasis on zero-shot usage, eliminating the need for any labeled data.

Generative Document Expansion. Appending relevant terms, such as queries, to documents effectively enriches document representation for sparse retrievals. [Nogueira et al.](#page-9-12) [\(2019\)](#page-9-12) demonstrated this by using a language model to generate search queries for improved retrieval in search engines. [Lewis et al.](#page-9-13) [\(2021\)](#page-9-13) introduced Probably Asked Questions (PAQ) by generating the question given a passage and an answer, and a retriever trained using PAQ demonstrated the strength in accuracy, speed, and space efficiency for selective QA. [Ma](#page-9-14) [et al.](#page-9-14) [\(2023a\)](#page-9-14) trains a dense retriever after applying document expansion. Our approach also leverages document expansion with generative language models, but with a focus on tool selection rather than search engine or question-answering tasks. We further emphasize the ability to extract the user intents from queries to better match the varying complexities of downstream tasks.

Generative Query Expansion. Augmenting user queries with hypothetical information is a popular approach in both dense and sparse retrieval methods. Query2doc [\(Wang et al.,](#page-10-8) [2023\)](#page-10-8) expands queries with pseudo-generated documents through few-shot prompting. [Jagerman et al.](#page-9-15) [\(2023\)](#page-9-15) further extends this idea by studying different prompting methods. [Liu et al.](#page-9-16) [\(2022\)](#page-9-16) improves query expansion by balancing diversity and relevance through a combination of effective filtering and documents fusion. [Shen et al.](#page-10-9) [\(2024\)](#page-10-9) augments queries with potential answers by prompting LLMs with a composition of the query and its in-domain candidates. [Mackie et al.](#page-9-17) [\(2023\)](#page-9-17) enriches the original query with useful terms from diverse generation

Figure 2: An overview of Re-Invoke for tool retrieval tasks. (Top) A query generator generates diverse synthetic queries from the tool documents and each synthetic query is concatenated with the tool document to create multiple copies of the expanded tool document. (Bottom) An intent extractor synthesizes multiple underlying intents from the user queries in order to retrieve the relevant tools.

subtasks. [Chuang et al.](#page-8-3) [\(2023\)](#page-8-3) proposes a query expansion and reranking approach to train a reranker after query expansion. Alternatively, [Gao](#page-8-4) [et al.](#page-8-4) [\(2023\)](#page-8-4) proposes a zero-shot dense retrieval system by first instructing LLMs to generate a hypothetical document given the query for semantic retrievals. Those approaches primarily focus on generative pseudo-relevance feedback by enriching user queries within the retrieval system. They are fundamentally different from our approach, which focuses on query understanding rather than query expansion.

Query Rewriting. LLM-aided query rewriting is commonly used in conversational search engine to precisely understand user's contextual search intent through in-context learning [\(Yu et al.,](#page-10-10) [2020;](#page-10-10) [Ye et al.,](#page-10-11) [2023;](#page-10-11) [Mao et al.,](#page-9-18) [2023;](#page-9-18) [Anand et al.,](#page-8-5) [2023\)](#page-8-5). Some works even train the query rewriter in a rewrite-retrieve-read pipeline, allowing interaction with the search engine [\(Feng et al.,](#page-8-6) [2023;](#page-8-6) [Ma](#page-9-19) [et al.,](#page-9-19) [2023b\)](#page-9-19). While LLMs are primarily used to summarize user context in conversations in these works, Re-Invoke focuses on extracting underlying intents for tool uses, rather than solely for information retrieval.

3 Method: Re-Invoke

We formulate the tool retrieval task as retrieving the most relevant tools that a downstream agent can execute to fulfill user queries, given a list of tool documents describing the intended tool usage.

Re-Invoke, our proposed fully unsupervised retrieval method designed for tool retrieval tasks, is

illustrated in Fig. [2.](#page-2-0) It consists of two core components: (1) *Query generator*: for each tool document, LLMs generate diverse synthetic queries answerable by the corresponding tool. These queries enrich the tool document and are then indexed by encoding them into the embedding space when the tool documents are ingested offline. (2) *Query intent extractor*: during online inference, LLMs extract the core tool-related intent(s) from user queries, filtering out irrelevant background context. Each user intent is then encoded into the same embedding space as the tool documents for similarity matching. Pseudo-code of Re-Invoke is described in Algorithm [1.](#page-3-0)

3.1 Query Generator

Tool documents, provided by developers to explain tool usage, are often vague or incomplete, which can lead to incorrect tool retrievals. Additionally, the existing text embedding model designed for information retrieval tasks may not accurately model the semantic relationship between tool usage and user queries [\(Patil et al.,](#page-9-4) [2023;](#page-9-4) [Qin et al.,](#page-10-3) [2023\)](#page-10-3). In practice, tool developers often include usage examples in the tool documents to help users better understanding how to use the tools.

Following this intuition, we instruct LLMs to predict user queries by reading the provided tool document. The generated queries then serve as examples of intended tool usages. We encourage LLMs to produce creative and complex queries that the tool can address. This process is compatible with any LLMs, including enterprise models such

Figure 3: An illustration of the multi-view similarity ranking algorithm during retrieval. Multiple intents can be extracted from the user query and we first compute the similarity scores between the expanded tool documents and each intent in the embedding space. We rank and retrieve the top tools from each intent as the final retrieved tools.

as GPT-4 [\(OpenAI,](#page-9-20) [2023b\)](#page-9-20), Gemini API [\(Google,](#page-9-21) [2024\)](#page-9-21), and open-source models like LLaMa [\(Tou](#page-10-12)[vron et al.,](#page-10-12) [2023\)](#page-10-12). The prompt template is detailed in Appendix [A.](#page-11-0)

To introduce variation and cover the potential query space, we increase the sampling temperature and sample the model response multiple times. Examples of the query generator outputs can be found in Appendix [B.](#page-14-0) Finally, each synthesized query is concatenated with the original tool document to create augmented tool documents, facilitating better tool retrievals (see Fig. [2\)](#page-2-0).

3.2 Intent Extractor

Tool augmented LLM agents often function as chatbots, interacting with users who express their intents in diverse and potentially verbose ways. Users

may unconsciously provide extraneous background information before stating their actual tasks, which can confuse downstream tool retrieval when trying to identify the underlying intents [\(Qian et al.,](#page-10-13) [2024\)](#page-10-13). Additionally, users might express multiple intents in a single conversational query, which current retrieval system may struggle to capture due to the query complexity. To address these, we leverage LLM's reasoning and query understanding capabilities through in-context learning to extract tool-related intents, thereby improving retrieval accuracy. This approach also allows for the effective extraction of multiple intents if the user query contains different requests. We then encode these intents replacing the original user queries into the embedding space during tool retrieval. This technique enables the retrieval system to recommend all the relevant tools for each individual intent (see Fig. [2\)](#page-2-0). The prompt template for extracting user intent using LLMs is available in Appendix [A.](#page-11-0)

3.3 Multi-view Similarity Ranking

As each intent extracted from the user queries could retrieve different relevant tools, we introduce a multi-view similarity ranking method to consider all tool-related intents expressed in the user query. We aggregate similarity scores between each intent and the expanded tool document. By incorporating multiple perspectives within the embedding space, it provides a robust measure of relevance between expanded tool documents and user queries.

We first aggregate the embedding values from multiple copies of the expanded tool document with synthetic queries to represent each tool document in the embedding space. Instead of grouping the entire tools retrieved by all the intents described in the user query before ranking, we rank the tools individually within each intent and retrieve the top

tool from each intent until the specified number of candidates have been retrieved. To achieve this, we design an ordering function to consider both the rank of the retrieved tool within each intent and the similarity score value between the tool and the intent. The proposed formulation allows us to capture the relevance of each intent to different aspects of the tool document, as represented by the generated queries.

The multi-view similarity ranking algorithm is explained using an example in Fig. [3.](#page-3-1) The final retrieved 2 tools from the query include the top tool book_flight retrieved from the intent "book a flight from New York City to San Francisco this weekend" and the top tool find_restaurant retrieved from the intent "find highly rated restaurants in downtown San Francisco". The detailed implementation is described in Appendix [C.](#page-15-0)

4 Experimental Settings

4.1 Benchmark Datasets

A variety of benchmark datasets containing tools across different domains have been proposed to assess tool-augmented LLMs. These include APIBench [\(Patil et al.,](#page-9-4) [2023\)](#page-9-4), API-Bank [\(Li et al.,](#page-9-22) [2023\)](#page-9-22), ToolBench [\(Xu et al.,](#page-10-4) [2023\)](#page-10-4), ToolAlpaca [\(Tang et al.,](#page-10-14) [2023\)](#page-10-14), ToolBench [\(Qin et al.,](#page-10-3) [2023\)](#page-10-3), ToolE [\(Huang et al.,](#page-9-23) [2023\)](#page-9-23) and ToolQA [\(Zhuang](#page-10-15) [et al.,](#page-10-15) [2023\)](#page-10-15). To evaluate Re-Invoke's tool retrieval performance, we select ToolBench [\(Qin et al.,](#page-10-3) [2023\)](#page-10-3) and ToolE [\(Huang et al.,](#page-9-23) [2023\)](#page-9-23) datasets, as both datasets provide ground truth query and tool document pairs that reflect real-world scenarios. We use the same ToolBench dataset to evaluate the end to end performance when integrating the LLM agent with the proposed Re-Invoke retriever. Detailed data statistics on the benchmark datasets can be found in Appendix [D.](#page-16-0)

Following the approach in [Qin et al.](#page-10-3) [\(2023\)](#page-10-3), we use nDCG@k metric^{[1](#page-4-0)} to evaluate retrieval performance on the benchmark datasets. We report nDCG@5 in the following sections and the detailed retrieval metrics including recall $@k^2$ $@k^2$ can be found in Appendix [E.](#page-17-0) For end-to-end performance evaluation, we use pass rate following the same evaluation protocol proposed in [Qin et al.](#page-10-3) [\(2023\)](#page-10-3).

4.2 Unsupervised Retrieval Baselines

As the proposed method is training free, we establish the following baselines to benchmark Re-Invoke's unsupervised tool retrieval performance: (a) Sparse retrieval using BM25: We directly calculate relevance between the user query and the tool documents using BM25. We use the default normalization parameter $k = 1.5$ for term fre-

(b) Dense retrieval using text embedding: We encode both query and entire tool documents using Google Vertex AI's textembedding-gecko@003 model^{[3](#page-4-2)} and compute the cosine similarity on the embedding values.

quency and offset parameter $b = 0.75$ for docu-

ment length normalization.

(c) HyDE as a dense retrieval method: Following [Gao et al.](#page-8-4) [\(2023\)](#page-8-4), we use LLMs to generate a hypothetical tool document for each user query. We then calculate document-document similarity using embeddings to retrieve the real tool document. In our experiment, we use Google Vertex AI's text-bison@001 model^{[4](#page-4-3)} to generate the hypothetical tool document. The instruction template can be found in Fig. [6](#page-13-0) in Appendix [A.](#page-11-0) Both hypothetical and real tool documents are encoded using the Vertex AI text embedding API.

AnyTool [\(Du et al.,](#page-8-7) [2024\)](#page-8-7) proposes hierarchical agents by leveraging LLM as a tool retriever for large-scale API calls, but the "hierarchy of the tools" structure may not be available in general tool use cases. It also results in significantly higher latency and cost when the number of tools scale up. Therefore, this method is excluded in our baselines.

4.3 Re-Invoke

We use Google Vertex AI's text-bison@001 model (with 0.7 temperature) in the query generator to generate 10 diverse synthetic queries per tool document. Other parameters remain default. We explored various concatenation methods (prepending, appending, repetition) and found they yield similar retrieval metrics. Therefore, we append each generated query to the original tool document in the format: "Documentation: <tool document> Query: <predicted query>" to create different copies of the expanded tool document. For evaluation, we vary the number of synthetic queries (see ablation study in Sec. [6.1\)](#page-6-0).

¹ [https://scikit-learn.org/stable/modules/](https://scikit-learn.org/stable/modules/generated/sklearn.metrics.ndcg_score.html) [generated/sklearn.metrics.ndcg_score.html](https://scikit-learn.org/stable/modules/generated/sklearn.metrics.ndcg_score.html)

² [https://www.tensorflow.org/ranking/api_docs/](https://www.tensorflow.org/ranking/api_docs/python/tfr/keras/metrics/RecallMetric) [python/tfr/keras/metrics/RecallMetric](https://www.tensorflow.org/ranking/api_docs/python/tfr/keras/metrics/RecallMetric)

³ [https://cloud.google.com/vertex-ai/docs/](https://cloud.google.com/vertex-ai/docs/generative-ai/embeddings/get-text-embeddings) [generative-ai/embeddings/get-text-embeddings](https://cloud.google.com/vertex-ai/docs/generative-ai/embeddings/get-text-embeddings)

⁴ [https://cloud.google.com/vertex-ai/docs/](https://cloud.google.com/vertex-ai/docs/generative-ai/model-reference/text) [generative-ai/model-reference/text](https://cloud.google.com/vertex-ai/docs/generative-ai/model-reference/text)

Table 1: nDCG@5 metrics on ToolBench I1, I2, I3 and ToolE single-tool, multi-tool datasets using both sparse and retrieval methods. In the sparse retrieval method, we apply BM25 retrieval and HyDE retrieval based on BM25 as two baselines. text-bison@001 is used to generate hypothesis documents in the HyDE method. We integrate Re-Invoke with BM25 embedding using text-bison@001, gpt-3.5-turbo and Mistral-7B-Instruct-v0.3 as three different backbone LLMs. In the dense retrieval method, we apply Vertex AI text embedding retrieval and HyDE retrieval based on Vertex AI text embedding as two baselines. text-bison@001 is used to generate hypothesis documents in the HyDE method. We also integrate Re-Invoke with the Vertex AI text embedding using text-bison@001, gpt-3.5-turbo and Mistral-7B-Instruct-v0.3 as three different backbone LLMs. The highest nDCG@5 metric is marked in bold.

We use the same Google Vertex AI's LLM model in the intent extractor to synthesize the intents from the user queries. We then extract dense embedding vectors from both augmented tool documents and extracted intents using Google Vertex AI's textembedding-gecko@003 model. We also apply Re-Invoke using BM25 embedding vectors as a sparse retrieval method.

In our Re-Invoke design, we average the embedding values from multiple copies of the expanded tool document as a representation of the tool document. We then compute the embedding similarity score between each extracted intent and the expanded tool documents, and rank the tool documents with the ordering function described in Sec. [3.3.](#page-3-2) We compare our designed aggregation function with others in Sec. [6.1.](#page-6-0)

5 Experimental Results

5.1 Baseline Retrieval Performance

As shown in Table [1,](#page-5-0) semantic retrieval using Vertex AI text embedding significantly outperforms the sparse retrieval BM25 across all five benchmark datasets. This aligns with the findings in [Patil et al.](#page-9-4) [\(2023\)](#page-9-4) and [Qin et al.](#page-10-3) [\(2023\)](#page-10-3). Even without specific pre-training on tool retrieval tasks, the existing enterprise text embedding API can effectively represent the semantic relationship between user queries and relevant tool documents.

Compared to its dense retrieval counterpart,

HyDE retrieval using Vertex AI text embedding performs less favorably. This suggests that the HyDE approach introduces a concept drift between the actual and hypothetical tool documents. The metric degradation can likely be attributed to information loss within the hypothetical documents.

5.2 Retrieval Performance of Re-Invoke

Re-Invoke consistently outperforms both sparse and dense retrieval baselines across all benchmark datasets, as shown in Table [1](#page-5-0) (See Table [6](#page-17-1) in Appendix for complete results). When combined with BM25 sparse embeddings, nDCG@5 is significantly increased. Similarly, Re-Invoke with Vertex AI text embedding yields significant performance gains. This improvement stems from the proposed LLM-powered tool document enrichment and user intent extraction.

The application of Re-Invoke significantly improves both sparse and dense retrieval performance although we observe that applying Re-Invoke on top of the sparse retrieval method still underperforms the dense retrieval counterparts. To further analyze the impact of Re-Invoke on improving retrievals, we examine specific user queries and compare the retrieved tools between the baseline and Re-Invoke (see Appendix [F\)](#page-18-0).

We also replicate our experiment using Ope $nAI's$ gpt-3.[5](#page-5-1)-turbo model⁵ and Mistral AI's

⁵ [https://platform.openai.com/docs/models/](https://platform.openai.com/docs/models/gpt-3-5-turbo) [gpt-3-5-turbo](https://platform.openai.com/docs/models/gpt-3-5-turbo)

Tool Retriever	$\mathbf{11}(\%)$			12(%)		$13\left(\% \right)$	Average $(\%)$
	Instruction	Tool	Category	Instruction	Category	Instruction	
None	39.70	44.72	47.50	64.50	55.33	61.00	52.13
ToolLLM's	47.50	42.00	53.00	62.50	56.78	54.00	52.63
Re-Invoke (ours)	48.00	49.75	53.03	65.33	58.29	62.00	56.07

Table 2: End-to-end performance on the ToolBench datasets. We follow [Qin et al.](#page-10-3) [\(2023\)](#page-10-3) to use pass rate as the evaluation metric. We integrate ToolLLaMA with DFSDT as the agent, using a set of reference tools without a retriever, ToolLLM's retriever, and Re-Invoke retriever. The highest performance metric is marked in bold.

Mistral-7B-Instruct-v0.3 model [\(Jiang et al.,](#page-9-24) [2023\)](#page-9-24) as the backbone LLMs. The same backbone LLM is used in both the query generator and intent extractor. Applying the same settings including prompt and decoding parameters as those described in text-bison@001, Re-Invoke achieves a similar trend across all benchmark datasets (see Table [1\)](#page-5-0). This demonstrates Re-Invoke's compatibility with various foundation models to improve the baseline retrieval methods.

5.3 End-to-End Performance Evaluation

We employ the proposed Re-Invoke as the tool retriever and the ToolLLaMA with Depth-First Search-Based Decision Tree (DFSDT) approach as the agent. Comprehensive implementation details can be found in ToolLLM [\(Qin et al.,](#page-10-3) [2023\)](#page-10-3). We adopt the pass rate metric proposed in ToolLLM [\(Qin et al.,](#page-10-3) [2023\)](#page-10-3) for evaluation metrics. Pass rate calculates the percentage of instructions successfully completed within limited budgets. We evaluate on six subsets of the ToolBench benchmark dataset: *I1-Instruction*, *I1-Category*, *I1-Tool*, *I2- Instruction*, *I2-Category* and *I3-Instruction*, using OpenAI's gpt-3.5-turbo model as an evaluator.

We compare the agent performance with different tool retriever settings: using a set of reference tools without retrievers, ToolLLM's API retriever [\(Qin et al.,](#page-10-3) [2023\)](#page-10-3) trained using the labeled querytool pairs, and our Re-Invoke retriever without any training data. The reference set of tools are provided in the ToolBench dataset, but they might not be the ground-truth tools as same task could be solved with a different set of tools. All pass-rate evaluation results are reproduced. Table [2](#page-6-1) demonstrates that our unsupervised Re-Invoke retriever outperforms both baselines with the set of reference tools and a trained tool retriever across all the benchmark datasets. This aligns with the finding in ToolLLM [\(Qin et al.,](#page-10-3) [2023\)](#page-10-3) that a tool retriever can expand the search space to find more appropriate

tools for a given task. Therefore, using tools retrieved by Re-Invoke can improve the agent performance by suggesting more relevant tools given the task even compared to using the reference toolset. These evaluation results provide evidence that our Re-Invoke retriever can effectively retrieve relevant tools from a vast pool (16,000+ APIs) and it leads to more reliable downstream agent behaviors on the tool use. Importantly, Re-Invoke is completely unsupervised, eliminating the needs for training.

6 Discussions

6.1 Ablation Studies

Re-Invoke component evaluation. In this study, we evaluate the tool retrieval performance on each individual Re-Invoke components: query generator and intent extractor using Vertex AI text embedding API. The results in Table [3\(](#page-7-0)A) provide the evidence that both designed components contribute positively to final retrieval metrics in Re-Invoke. Specifically, we observe consistent retrieval performance improvement across all the benchmark datasets when integrating the query generator with the baseline retrieval method. Similar improvement is also demonstrated when applying intent extractor with the baseline. When integrating both query generator and intent extractor, Re-Invoke achieves the highest retrieval metrics. Note that no improvement is observed on ToolBench I1 dataset when applying intent extractor mainly because ToolBench I1 dataset consists of APIs under the same tool, and each individual intent retrieves overlapped set of APIs. We discuss the scenarios when each component performs better in Sec. [6.3.](#page-7-1)

Query generator evaluation. We investigate the retrieval performance with different document augmentation settings using the query generator alone including (1) whether to append the document with the synthetic query, (2) number of synthetic queries and (3) aggregation function. Table [3\(](#page-7-0)B,C,D)

Method		ToolBench		ToolE			
	11	I2	I3	single-tool	multi-tool		
(A) INCLUDING CRITICAL COMPONENTS IN RE-INVOKE							
Baseline + Query generator (Sec. 3.1) + Intent extractor (Sec. 3.2) + Query generator & Intent extractor (Re-Invoke)	0.5962 0.6286 0.5910 0.6110	0.3880 0.4135 0.5157 0.5379	0.4633 0.4906 0.5843 0.5955	0.6522 0.7813 0.6756 0.7821	0.5296 0.6906 0.6258 0.7231		
(B) USING GENERATED QUERIES ONLY IN QUERY GENERATOR							
Synthetic query only Appending the synthetic query to the document	0.4924 0.6286	0.3050 0.4135	0.4121 0.4906	0.7535 0.7813	0.6814 0.6906		
(C) VARYING THE NUMBER OF SYNTHETIC QUERIES IN QUERY GENERATOR							
1 synthetic query 5 synthetic queries 10 synthetic queries	0.5962 0.6242 0.6286	0.3741 0.4091 0.4135	0.4543 0.4882 0.4906	0.7388 0.7777 0.7813	0.6503 0.6724 0.6906		
(D) VARYING THE AGGREGATION FUNCTION IN QUERY GENERATOR (MAX VS MEAN)							
Maximum similarity score Mean similarity score	0.6104 0.6286	0.3867 0.4135	0.4760 0.4906	0.7716 0.7813	0.6333 0.6906		

Table 3: nDCG@5 metrics of ablation studies on ToolBench I1, I2, I3 datasets and ToolE single-tool, multi-tool datasets. We evaluate the impact of each critical component in Re-Invoke: the query generator and the intent extractor. Within query generator component, we further compare nDCG@5 metrics across different number of synthetic queries, different aggregation functions to aggregate the relevance scores, and appending the synthetic queries to the tool documents or not. The highest retrieval metric is marked in bold.

	ToolBench	ToolE			
Metric	T1 12		13	single- $\&$ multi-tool	
recall $@5$ recall $@10$	0.7787 0.8402	0.7665 0.8311	0.9043 0.9464	0.9131 0.9462	

Table 4: Round-trip consistency recall metrics on synthetic queries in the query generator.

clearly validate that our design choices in the query generator: appending the synthetic query to the tool document with 10 synthetic queries and aggregating the similarity scores on the augmented tool documents with mean function, outperforms the alternatives. We observe that replacing the tool document with the synthetic queries could lead to potential information loss during the retrieval stage and augmenting the tool document is preferred. Mean similarity score is more robust when considering diverse synthetic queries in the query generator. Increasing the number of diverse synthetic queries improves the retrieval performance and demonstrates the effectiveness in enriching the tool documents with diverse synthetic queries.

6.2 Round-Trip Consistency Evaluation

We define the synthetic query quality using the round-trip consistency criteria [\(Alberti et al.,](#page-8-8) [2019\)](#page-8-8), *i.e.*, the synthetic queries should retrieve the same tool documents used to generate them. Specifically, we compute recall $@k$ as a round-trip consistency metric to quantify if the tool document used to generate the synthetic query are among the top- k documents after retrieval using the synthetic query (see Table [4\)](#page-7-2). The relatively high recall $@10$ metric across all the benchmark datasets suggests query generator's effectiveness to distinguish highly similar tool documents during retrieval. The round-trip consistency recall metric is lower on ToolBench I1 and I2 datasets, mainly caused by the larger toolset size compared to ToolBench I3 and ToolE datasets.

6.3 Re-Invoke Performance Analysis

We analyze the Re-Invoke performance under different scenarios from the results in Table [3\(](#page-7-0)A). For relatively short tool documents with minimal human-readable descriptions, tool document expansion alone can significantly boost retrieval performance through generative relevance feedback. The documents in the ToolE datasets only include the tool name and descriptions and we can see that *query generator* alone achieves larger performance gains. However, if a tool document lacks API and parameter descriptions, LLMs may struggle to accurately infer usage, relying solely on names. This can lead to generated queries that do not reflect realworld tool usage scenarios. In contrast, for complex user queries with extensive background context or requiring multiple tools simultaneously, *intent extractor* becomes crucial for improving tool retrieval performance. This component ensures individual tool-related contexts are extracted effectively. Tool-Bench I2 and I3 datasets both contain the queries that need to be handled by calling the APIs from multiple tools and categories on RapidAPI hub, *intent extractor* component alone achieves more significant retrieval performance gains.

6.4 Latency and Computational Cost Analysis

The query generator in Re-Invoke creates the synthetic queries offline when the tool documents are ingested, resulting no additional latency during serving. The number of LLM calls during tool document indexing is proportional to the number of synthetic queries per document and the total number of documents. On the other hand, intent extractor employs an LLM to extract the user intents from the user query during online inference, which incurs an extra LLM call with associated latency and computational cost.

To mitigate the latency and cost increase, techniques such as knowledge distillation from larger to smaller LLMs, or quantization, offer promising avenues for reducing both latency and computational overhead.

7 Conclusion

In this work, we present Re-Invoke, a fully unsupervised tool retrieval approach designed to scale LLM tool learning to large toolsets. We leverage LLMs to enhance tool document context with diverse synthetic queries, extract essential tool-related intents into executable requests through intent extraction. Re-Invoke offers a fresh perspective on scalable tool retrieval, prioritizing context enhancement and intent understanding without any training data.

8 Limitations

Synthetic query diversity and quality. Re-Invoke achieves query diversity through simple LLM response sampling with a zero-shot prompt. To further enhance the quality and reduce concept drift between synthetic and real-world queries, more sophisticated query generation methods could be explored. This might include techniques such

as controlled prompting, iterative refinement, or utilizing external knowledge bases.

Intent extractor. Re-Invoke relies on in-context learning and LLM's internal knowledge to extract tool related intents. Future work could include using the downstream agent's execution results as a feedback to refine intent extraction.

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Appendix

A Prompt Templates

In this section, we list all the prompt templates used in our experiments. Fig. [4](#page-11-1) is the prompt to generate a synthetic query from the tool document. Fig. [5](#page-12-0) shows the prompt to extract the user intents. Fig. [6](#page-13-0) describes the prompt to generate hypothetical tool document given a user query used in the HyDE retrieval baseline.

Suppose you are an assistant and you have access to the following API to answer user's queries. You are provided with a tool and its available API function including the description and parameters. Your task is to generate a possible user query that can be handled by the API. You must include the input parameters required in the API call. Please be creative and generate random but specific information for the required parameters. Now you are given the API documentation below: <tool document> Please generate a user query that you will need to call this tool. Note the generated query should be complex enough to describe the scenarios that you will need to call the provided API to address them.

The relevant query is:

Figure 4: Prompt template to generate the synthetic queries from the tool document.

Instructions Suppose you are a query analyzer and your task is to extract the underlying user intents from the input query. You should preserve all the underlying user request and the extracted user intents should be easily understood without extra context information. You should carefully read the given user query to understand its different intents. Then identify what are the specific intents. Each individual intent should be separated by a newline. Here are some examples of how you should solve the task. **Example** Query: I'm planning to travel to Paris next weekend to visit my family, could you help me book a round trip flight ticket? I want to fly in economy class. Intent: book a round-trip flight ticket in economy class to Paris next weekend Query: I'm a potential buyer looking for a condominium in the city of Miami. I am specifically interested in properties that have a minimum of two bathrooms. It should have walkable distance to the grocery stores. Intent: buy a real estate in Miami with a minimum of two bathrooms and walkable distance to the grocery stores Query: I want to learn Spanish by talking to the native speakers at any time. Additionally, can you recommend some interesting books, preferably fictions, so that I can learn by reading? Also include the websites that I can buy them. Intent: learn Spanish by talking to the native speakers recommend fictions to learn Spanish by reading suggest the websites to buy Sanish fictions **Begin!** Query: <user query> Intent:

Figure 5: Prompt template to extract the underlying intents from user queries.

```
Suppose you are an assistant and you have access to the API documentation to answer user's queries.
Please generate an API documentation in the JSON format that can be called to handle this query.
The API documentation should be general enough to handle the cases beyond the provided queries.
Please provide detailed descriptions on the parameters.
**Examples**
Query: I'm planning to travel to Paris next weekend to visit my family, could you help me book a
round trip flight ticket? I want to fly in economy class.
The API documentation is:
{
    "api_name": "flights",
    "api_description": "Search the flight ticket on a specific travel date."
    "required_parameters": [
        {
            "name": "departure_date",
            "type" DATETIME,
            "description": "The departure date for the flight."
        },
        {
            "name": "from",
            "type" STRING,
            "description": "The city where the flight departs."
        },
        {
            "name": "to",
            "type" STRING,
            "description": "The city where the flight arrives."
        },
        {
            "name": "fare_class",
            "type": STRING,
            "description": "The fare class for the flight, economy, business or first."
        }
    ],
    "optional_parameters": [
        {
            "name": "return_date",
            "type": DATETIME,
            "description": "The return date for the flight."
        }
    ]
}
**Begin!**
Query: <user query>
The API documentation is:
```
Figure 6: One-shot prompt template to generate hypothetical tool document given a user query.

B Example Synthetic Queries

We show 10 different generated user queries from the documentation newsSearch API in the ToolBench dataset in Fig. [7.](#page-14-1)

{"category_name": "Data", "tool_name": "Web Search", "api_name": "newsSearch", "api_description": "Get news articles relevant for a given query.", "required_parameters": [{"name": "pageSize", "type": "NUMBER", "description": "The number of items per page. The maximum value is 50.", "default": "10"}, {"name": "autoCorrect", "type": "BOOLEAN", "description": "Automatically correct spelling.", "default": true}, {"name": "q", "type": "STRING", "description": "The user's search query string.", "default": "taylor swift"}, {"name": "pageNumber", "type": "NUMBER", "description": "The page to view.", "default": "1"}], "optional_parameters": [{"name"": "toPublishedDate", "type": "STRING", "description": "The published date and time for the newest article allowed. For example: *2015-05-16T05:50:06.* See [https://www.c-sharpcorner.com/blogs/date-and-time-format-in-c-sharp -programming1](url)for more possible DateTime formats.", "default": "null"}, {"name": "safeSearch", "type": "BOOLEAN", "description": "A filter used to filter results for adult content.", "default": false}, {"name": "fromPublishedDate", "type": "STRING", "description": "The published date and time for the oldest article allowed. For example: *2015-05-16T05:50:06.* See [https://www.c-sharpcorner.com/blogs/date-and-time-format-in-c-sharp-programming1](url)for more possible DateTime formats. "", "default": "null"}, {"name": "withThumbnail"", "type": "BOOLEAN", "description": "Show results with image thumbnails.", "default": false}], "method": "GET"}

Show me news articles about the latest coronavirus outbreak in the United States. I would like to see the articles from the past week, and I would like them to be safe for work.

I would like to see a list of news articles about the latest developments in the field of artificial intelligence. Please show me the results from the past year and make sure that they are safe for work.

I'd like to get a list of news articles about the latest developments in the field of artificial intelligence. Please show me articles from the past 24 hours, and include images with the results.

I would like to get a list of news articles about the latest developments in artificial intelligence. Please show me the results in chronological order, with the most recent articles first. I would also like to see images of the articles.

I want to get the news articles about the latest news about the new album by Taylor Swift. I want the results to be from the past month and I want them to be safe for work.

I want to know the latest news about the war in Ukraine. Please show me the results from the past 24 hours, and make sure that they are safe for work.

I want to find news articles about the latest developments in the field of artificial intelligence. Please show me articles from the past year that are safe for work and have image thumbnails.

I would like to find news articles about the latest developments in AI. Please show me the results from the past month and make sure to include images in the results.

I would like to know about the latest news articles on the topic of artificial intelligence. Please show me the results in chronological order, with the newest articles first. I would also like to see thumbnails of the articles.

I would like to find news articles about the latest developments in artificial intelligence. Please show me the results from the past week and make sure they are safe for work.

Figure 7: The document on the example newsSearch tool and 10 different synthetic queries that are relevant to the provided tool.

C Multi-view Similarity Ranking Algorithm Implementations

In this section, we describe the multi-view similarity ranking algorithm (Sec. [3.3\)](#page-3-2) implementations. As each tool document is concatenated with a synthetic query to create m copies, we iterate each augmented tool document and compute the average embedding on each copy of the same tool document. We iterate each user intent from a user query and each tool document to compute the embedding similarity score between the individual intent and tool document. Within each intent, we also compute the reversed ranking order of the tools using the similarity score. To allow each intent to be considered during retrieval, we use a tuple to represent the ranking score to include both the reversed ranking order and similarity score value: we compare the reversed ranking order followed by the similarity score value if the reversed ranking order is the same. We then group all the intents and retrieve the top k documents based on the ranking score. The pseudo-code is available in Algorithm [2,](#page-15-1) with a detailed working example in Fig. [8.](#page-15-2)

Algorithm 2: Pseudo-code of Re-Invoke's ranking method

Data: n extracted intents $q_1, q_2, ..., q_n$ from query Q, List of tool documents D with each document d concatenated with m synthetic queries and each concatenated document is denoted as $d_1, d_2, ..., d_m$, Text embedding model f_{enc}

Result: a retrieval score to rank the documents given a user query

1 **Function** rank($q_{1...n}$, $d_{1...m}$, f_{enc}): 2 for $d \in D$ do $\begin{array}{|c|c|c|}\hline \rule{0pt}{12pt}\quad & E_d \leftarrow \frac{1}{m}\sum_{i=1}^m (f_{\text{enc}}(d_i)); \\\hline \end{array}$ ⁴ end 5 **for** $i = 1, ..., n$ do 6 **for** $d \in D$ do $\begin{array}{|c|c|c|c|c|}\hline \hspace{0.2cm} & \hspace{0.2cm} & \hat s(q_i, d) \leftarrow f_{\sf enc}(q_i) \cdot E_d; \hline \end{array}$ $\begin{array}{|c|c|c|c|}\hline \textbf{8}}& & \textbf{rank}(q_i,d) \leftarrow \hat{s}(q_i,d).\textbf{rank}(\textbf{reversed}=\textbf{True},\textbf{axis}=1); \hline \end{array}$ $\begin{array}{|c|c|c|c|}\hline \text{\textit{9}} & \text{\textit{r}}(q_i,d) \leftarrow (\text{rank}(q_i,d),\hat{s}(q_i,d)); \ \hline \end{array}$ 10 end 11 end 12 $r(Q, D) \leftarrow \max_{i=1,2,\dots,n} r(q_i, D);$ 13 return $r(Q, D)$

Figure 8: An example of the multi-view similarity ranking algorithm. From the intent-tool similarity score, we define the ranking score as a tuple of the reversed ranking order (*i.e.*, lowest similarity score will have a reversed ranking order of 1) for each tool within the same intent and similarity score. We then find the maximum ranking score across multiple intents for each tool document to compute the retrieval score. The retrieval score will be used to retrieve and rank the top tools given the user query.

D Data statistics

The statistics for the benchmark datasets of ToolBench I1, I2, I3 and ToolE single-tool and multi-tool are shown in Table [5.](#page-16-1)

Table 5: Data statistics on ToolBench and ToolE benchmark datasets including number of queries, number of tool documents and number of labeled pairs.

E Retrieval performance evaluation

The complete retrieval metrics including nDCG@1, nDCG@5, recall@1 and recall@5 on all the benchmark datasets of ToolBench I1, I2, I3 and ToolE single-tool and multi-tool are shown in Table [6.](#page-17-1)

Table 6: Retrieval metrics (nDCG@1, nDCG@5, recall@1 and recall@5) on ToolBench I1, I2, I3 and ToolE single-tool and multi-tool datasets with different approaches including baselines and Re-Invoke using BM25 and Vertex AI text embedding. We observe the similar tool retrieval performance trend with different retrieval metrics. The highest metric is marked in bold.

F Case Study on Retrieved Tools

In this section, we showcase that tool retrieval can benefit from Re-Invoke using the ToolE dataset as demonstration examples. A few user queries are cherrypicked from the ToolE single-tool and multi-tool datasets that the baseline Vertex AI retriever retrieved the wrong tools while the Re-Invoke recommended the relevant tools. We investigate query generator and intent extractor components separately.

Table [7](#page-19-0) shows the example queries that the correct tools are retrieved with the query generator component. It can be clearly seen that Re-Invoke's query generator component can better distinguish among similar tools to determine which tool is more relevant to user's request. For example, when the user is asking for the weather forecast for a location, the Vertex AI baseline retriever retrieves the very specific airqualityforeast tool while Re-Invoke retrieves the correct WeatherTool tool, which is more tailed to answer user's queries.

Table [8](#page-20-0) lists the correct tools retrieved with the intent extractor component. Similarly, Re-Invoke's intent extractor effectively understands the user intents to recommend the most relevant tools to user's specific request. For example, when the user is asking for recommendations on online courses on machine learning and needs the access to relevant PDFs or URLs, Re-Invoke's intent extractor identifies two intents "recommend a course on machine learning" and "have access to relevant PDFs or URLs for further reading" and successfully retrieves the correct tools CourseTool and PDF&URLTool from each intent. However, the baseline retrieval method retrieves CourseTool and search tools instead.

We have also observed that Re-Invoke can still lead to wrong retrievals, especially when the tools are very similar, e.g., HousePurchasingTool and HouseRentingToo, FinanceTool and CompanyInfoTool. Please see the examples in Table [9.](#page-21-0) When the user is explicitly looking to buy a condominium in the query, Re-Invoke retrieves the wrong HouseRentingTool. We believe those errors can be reduced by designing a more sophisticated approach to generate more explicit synthetic queries that can be used to distinguish among confusing tool documents.

Table 7: A list of cherry-picked example queries from the ToolE single-tool dataset, including top 1 tool retrieved by the baseline and Re-Invoke's query generator using the Vertex text embedding API. Re-Invoke's query generator retrieves the correct tools (in **green**) while the baseline retrieves the wrong tools (in red).

Table 8: A list of cherry-picked example queries from the ToolE multi-tool dataset, including 2 tools retrieved by the baseline and Re-Invoke's intent extractor component using the Vertex text embedding API. Re-Invoke's intent extractor identifies the intents (in green and blue) and retrieves the correct tools (in green and blue) while the baseline retrieves the wrong tools (in $\frac{\text{red}}{\text{red}}$). 4725

Table 9: A list of cherrypicked example queries from the ToolE single-tool dataset, including top 1 tool retrieved by the baseline and Re-Invoke using the Vertex text embedding API. Baseline retrieves the correct tool (in green), while Re-Invoke retrieves the wrong tool (in red).