

# Enhancing Tool Retrieval with Iterative Feedback from Large Language Models

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## Abstract

Tool learning aims to enhance and expand large language models' (LLMs) capabilities with external tools, which has gained significant attention recently. Current methods have shown that LLMs can effectively handle a certain amount of tools through in-context learning or fine-tuning. However, in real-world scenarios, the number of tools is typically extensive and irregularly updated, emphasizing the necessity for a dedicated tool retrieval component. Tool retrieval is nontrivial due to the following challenges: 1) complex user instructions and tool descriptions; 2) misalignment between tool retrieval and tool usage models. To address the above issues, we propose to enhance tool retrieval with iterative feedback from the large language model. Specifically, we prompt the tool usage model, i.e., the LLM, to provide feedback for the tool retriever model in multi-round, which could progressively improve the tool retriever's understanding of instructions and tools and reduce the gap between the two standalone components. We build a unified and comprehensive benchmark to evaluate tool retrieval models. The extensive experiments indicate that our proposed approach achieves advanced performance in both in-domain evaluation and out-of-domain evaluation.

## 1 Introduction

Large language models (LLMs) have demonstrated remarkable success in language-related tasks and are considered a potential pathway to achieving artificial general intelligence (Zhao et al., 2023). However, despite their powerful capabilities, LLMs are still limited in many aspects, such as knowledge update and mathematical reasoning. A promising way to overcome these limitations is to empower LLMs with external tools, known as tool learning. Tool learning not only enhances LLMs' performance on existing tasks but also allows them to tackle tasks that were previously beyond their reach. Besides,

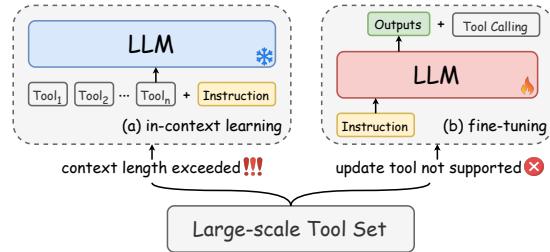


Figure 1: Illustration of two tool-learning approaches in LLMs: (a) in-context learning and (b) fine-tuning. The challenges posed by the extensive and frequently updated tools require the external tool retrieval component.

the ability to use tools is a crucial hallmark on the path to advanced intelligence.

Existing tool learning methods have preliminarily demonstrated that LLMs could effectively utilize specific tools to complete corresponding tasks. They either leverage LLMs' in-context learning ability to facilitate tool usage with tool descriptions (Shen et al., 2023) or fine-tune LLMs to integrate tool learning capabilities into parameters, e.g., Toolformer (Schick et al., 2023). However, as illustrated in Figure 1, existing methods still face significant challenges in real-world scenarios due to the following reasons. 1) The number of tools is usually vast, making it impossible for LLMs to handle them all with the limited input length of in-context learning. 2) Tools would frequently and irregularly update, rendering finetuning-based approaches costly and impractical. Therefore, a tool retrieval component, which aims to select appropriate tools from a large-scale tool set, is essential for LLMs.

Despite the practicality and necessity, tool retrieval has been inadequately studied. Some approaches have adopted traditional document retrieval methods to retrieve tools for LLMs (Li et al., 2023; Patil et al., 2023; Qin et al., 2023b). However, we argue that they overlook the unique challenges of tool retrieval for LLMs: 1) Complex user in-

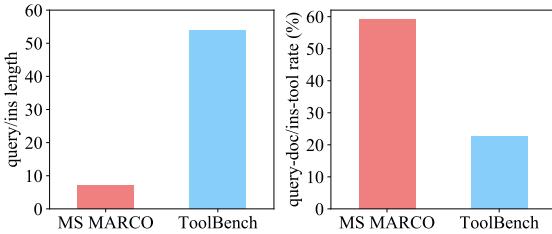


Figure 2: Comparison between the document retrieval and tool retrieval datasets. Tool retrieval presents more challenges due to the complex instructions (in the left figure) and the lower reputation rate (in the right figure).

structures and tool descriptions. As illustrated in Figure 2, compared with document retrieval, user instructions are usually ambiguous and complex, and the reputation rate between instructions and corresponding tool descriptions is much lower. Unfortunately, the retriever model is typically limited in its capacities because of the efficiency requirements, which makes tool retrieval more difficult and challenging. 2) Misalignment between tool retrieval and tool usage models. Previous approaches deploy the tool retriever separately from the downstream tool-usage model, which hinders the LLM from knowing which tools are really useful from the tool-usage perspective. Thus, it will result in a tool recognition gap between the tool retriever and tool usage model, degrading the tool-use performance further.

To address the above issues, we propose to enhance tool retrieval with iterative feedback. Our motivation is to utilize the LLM to enhance the comprehension ability of the tool retriever and bridge the gap between the two independent models. At each iteration, we conduct a feedback generation process by asking the LLM to provide feedback step-by-step, conditioned on the user instruction and retrieved tools from the retriever. The LLM will first comprehend the instruction and tool functionalities thoroughly, and then assess the effectiveness of those retrieved tools. According to the assessment, the LLM will refine the user instruction to improve the tool retrieval process. The refined instruction will substitute previous user instruction and be used to retrieve a new list of tools from the tool set. In the next iteration, the new candidate tool list will be fed into the LLM for a new round of LLMs’ feedback. During this iterative process, the tool retriever is expected to provide more appropriate tools for the tool-usage model. In this manner, the comprehension capability and tool preference of LLMs could be pro-

gressively incorporated into the retriever, and thus the tool retriever’s performance could be continuously enhanced. We build a comprehensive tool retrieval benchmark, named TR-bench. The benchmark takes into account real-world practices with updated tools, and therefore encompasses both in-domain and out-of-domain settings. The experimental results show our approach achieves the best performance among the current methods with both in-domain and out-of-domain settings.

The key contributions are summarized:

- We identify the importance of tool retrieval in tool learning and present the distinct challenges of tool retrieval.
- We propose to enhance tool retrieval with iterative feedback from the LLM. By leveraging iterative feedback, the tool retriever model gets continual improvements, ultimately reducing the misalignment between them.
- We build a comprehensive tool retrieval benchmark with in-domain and out-of-domain settings, which will also aid future tool retrieval research. The extensive experiments illustrate our approach has demonstrated superior performance.

## 2 Related Work

### 2.1 Tool Learning in LLMs

Tool learning aims to equip LLMs with external tools to enhance and expand their capabilities (Schick et al., 2023; Tang et al., 2023; Yao et al., 2023; Qin et al., 2023a; Shen et al., 2023). Generally, existing tool learning methods could be categorized into in-context learning and fine-tuning approaches. The former approach encourages LLMs to use tools with descriptions, documentation, or demonstrations, while the latter one trains the parameters of LLMs using specially created tool-use datasets. However, no matter whether the in-context learning or fine-tuning approach encounters severe challenges in real-world scenarios, where the candidate tools are extensive and frequently updated. Therefore, it is crucial to equip LLMs with a tool retrieval component to select appropriate tools from a large-scale tool set. Recent works have proposed a stopgap measure through traditional document retrieval methods (Li et al., 2023; Patil et al., 2023; Qin et al., 2023b). In this work, we aim to develop a specialized method for retrieving tools.

## 159 2.2 Document Retrieval

160 Early popular document retrieval methods rely on  
 161 sparse retrieval that calculates the relevance of doc-  
 162 uments to a query based on the frequency of query  
 163 terms in each document, e.g., BM25 (Robertson  
 164 and Zaragoza, 2009). With the development of  
 165 language models (Devlin et al., 2019), the dense  
 166 retrieval (Zhao et al., 2024; Mitra and Craswell,  
 167 2017) paradigm has gained considerable attention  
 168 in the research community. By encoding queries  
 169 and documents into high-dimensional vector rep-  
 170 resentations and computing their relevance scores  
 171 through inner product calculations, the paradigm  
 172 can capture semantic relationships between queries  
 173 and documents, thereby enhancing retrieval per-  
 174 formance (Karpukhin et al., 2020). However, tool  
 175 retrieval presents unique challenges, rendering tra-  
 176 ditional document retrieval methods suboptimal.  
 177 We address these challenges by harnessing LLMs’  
 178 feedback to iteratively refine the tool retrieval pro-  
 179 cess.

## 180 3 Preliminaries

### 181 3.1 Task Definition

182 Given a user’s instruction, tool retrieval aims to  
 183 select a small number of tools, which could aid the  
 184 LLM in answering the instruction, from a large-  
 185 scale tool set. Formally, we define the user instruc-  
 186 tion as  $q$  and the tool set as  $D = \{d_1, d_2, \dots, d_N\}$ ,  
 187 where  $d_i$  represents the description of each tool and  
 188  $N$  is the total number of tools. The retriever model  
 189  $R$  needs to measure the relevance  $R(q, d_i)$  between  
 190 the instruction  $q$  and each tool description  $d_i$ , and  
 191 return  $K$  tools, denoted as  $D = \{d_1, d_2, \dots, d_K\}$ .

### 192 3.2 Dense Retriever

193 Dense retriever usually leverages the encoder-  
 194 based LLM to encode the user instruction  $q$  and a  
 195 tool description  $d$  into dense embeddings  $E(q)$  and  
 196  $E(d)$ , respectively. Then, it could measure the rele-  
 197 vance between  $q$  and  $d$  by calculating the similarity  
 198 score between these two embeddings, denoted as  
 199  $R(q, d) = \text{sim}(E(q), E(d))$ .

200 Dense retriever is trained via the contrast learn-  
 201 ing objective, which is designed to minimize the  
 202 distance between the instruction embedding and  
 203 embeddings of positive tools (the instruction’s  
 204 ground-truth tools) while maximizing the distance  
 205 between the instruction embedding and embed-  
 206 dings of negative tools. The objective can be for-

207 mulated as follows,

$$\mathcal{L} = -\frac{1}{B} \sum_{i=1}^B \log \frac{e^{R(q_i, d_i^+)}}{e^{R(q_i, d_i^+)} + \sum_j e^{R(q_i, d_{ij}^-)}}, \quad (1)$$

209 where  $B$  denotes the batch size,  $d_i^+$  denotes the  
 210 positive tool, and  $d_{ij}^-$  represents the  $j$ -th negative  
 211 tool to the instruction  $q_i$ .

212 However, due to the efficiency requirements,  
 213 dense retrieval utilizes a dual-encoder architecture,  
 214 which has limited ability to understand instructions.  
 215 In this study, our goal is to improve the tool re-  
 216 trieval process with the feedback from the tool-  
 217 usage model, i.e., the LLM.

## 218 4 Methodology

### 219 4.1 Overview

220 Recent studies have found that LLMs show a great  
 221 capability in acting as a critic (Zheng et al., 2023)  
 222 and could provide comprehensive feedback to im-  
 223 prove performance across a range of tasks (Madaan  
 224 et al., 2023; Asai et al., 2023). Inspired by those  
 225 observations, we propose an innovative framework  
 226 that leverages the LLM’s feedback to improve the  
 227 tool retrieval process iteratively.

228 As illustrated in Figure 3, at each iteration, the  
 229 LLM will provide feedback on the current-turn re-  
 230 trieval results. Specifically, the LLM will first com-  
 231 prehend the user instruction and tool functionalities  
 232 thoroughly. Then, it will assess the effectiveness  
 233 of those retrieved tools for handling the instruction.  
 234 Based on the assessment, the LLM could provide  
 235 a refinement to the retrieval model, refining the  
 236 user instruction if necessary. To ensure that the  
 237 retriever model is aware of the iteration round, we  
 238 conduct an iteration-aware feedback training pro-  
 239 cess to adapt the retriever model with continuously  
 240 refined user instructions.

### 241 4.2 Feedback Generation

242 Assuming at the iteration step  $t$ , given the refined  
 243 instruction  $q^t$ , we could utilize retriever model  $R$  to  
 244 retrieve a list of top- $K$  tools  $\{d_1^t, \dots, d_K^t\}$ . We then  
 245 conduct a three-step feedback generation process  
 246 by feeding those retrieved tools and associated tool  
 247 descriptions into the LLM as follows.

248 **Comprehension.** Firstly, the LLM is prompted  
 249 to give comprehension on both the given instruction  
 250 and retrieved tools. The prompt provided to LLM  
 251 includes two parts: (1) summarize the abstract user  
 252 goals by ignoring detailed entity information in the

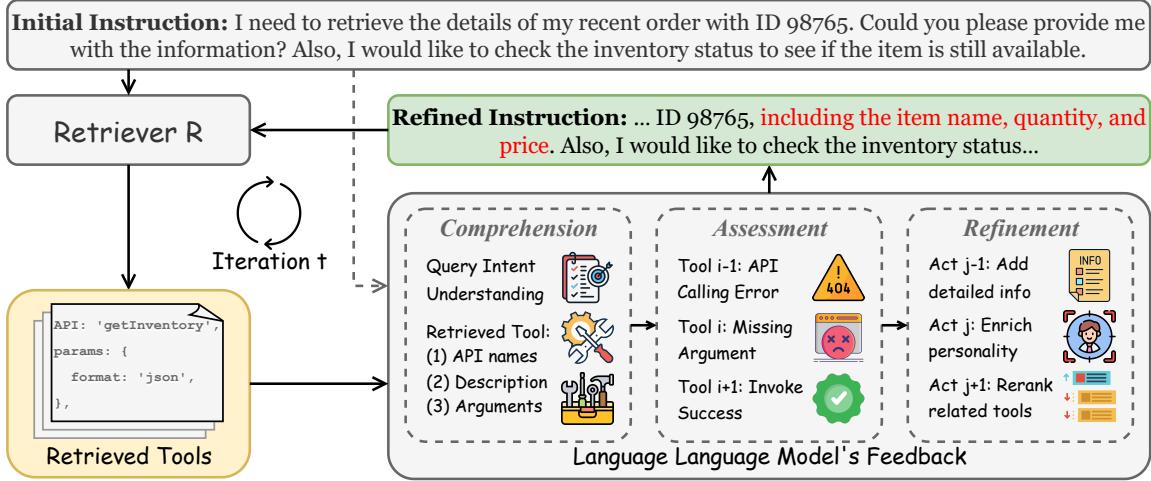


Figure 3: Illustration of our proposed iterative tool retrieval method. At each iteration, the LLM follows a three-step feedback generation process, which includes comprehension, assessment, and refinement, to improve the instruction.

given instruction; (2) understand the functionalities of retrieved tools, focusing on the category, name, description, input and output parameters of given tools. This step can be formulated as,

$$F_C = LLM(P_C, q^t, \{d_1^t, \dots, d_K^t\}), \quad (2)$$

where  $F_C$  denotes LLM’s comprehension output and  $P_C$  denotes the prompt provided to LLM.

**Assessment.** The LLM will assess the effectiveness of retrieved tools for handling the instruction based on its comprehension of the user’s intent and tool functionalities. The assessment is conducted from two perspectives: 1) identify which of the user’s goals could and could not be solved by the retrieved tools with corresponding reasons; and 2) analyze whether the ranked order of retrieved tools corresponds with their significance in addressing the user’s intent with specific reasons. The step can be formulated as,

$$F_A = LLM(P_A, q^t, \{d_1^t, \dots, d_K^t\}, F_C), \quad (3)$$

where  $F_A$  denotes the LLM’s assessment output.

**Refinement.** Lastly, the LLM will refine user instruction based on its assessment. Specifically, we ask the LLM to determine whether the refinement is necessary based on the two following questions: 1) Whether all the user’s goals have been solved by currently retrieved tools, 2) and whether all existing appropriate tools are given the highest ranking priorities by the retriever. If one of the answers is not “yes”, we prompt the LLM to provide a potential refinement for retrieval improvement. Otherwise, the LLM will directly return a special token “N/A” without conducting any refinement.

The feedback from the LLM is finalized made on the current user instruction  $q^t$ . Specifically, we prompt the LLM to generate refined instruction with enriched information in two dimensions: 1) more detailed and personalized content about those user’s intent which have not been solved by current tools, helping the retriever explore other relevant tools; (2) more scenario-specific tool-usage information about existing appropriate tools, helping the retriever give higher ranking priority to those tools. This step can be formulated as,

$$F_R = LLM(P_R, q^{t-1}, \{d_1^{t-1}, \dots, d_K^{t-1}\}, F_A), \quad (4)$$

where  $P_R$  is the corresponding prompt and  $F_R$  denotes LLM’s refinement output, i.e., the new refined instruction  $q^{t+1}$ .

### 4.3 Iteration-Aware Feedback Training

We concatenate a special token “Iteration  $t$ ” in front of the instruction, where  $t$  is the instruction’s iteration step (e.g., “Iteration  $t - 1$ ” for  $q^{t-1}$  and “Iteration  $t$ ” for  $q^t$ ). The final training loss is formulated as the sum of losses in each iteration as follows,

$$\mathcal{L}_{feedback} = \sum_{t=1}^T \alpha^t \mathcal{L}(q^t), \quad (5)$$

where  $\alpha^t$  is a balancing factor. In this way, the LLM’s comprehensive knowledge of the user requirements could be injected into the retriever through those refined instructions. Besides, with the aid of iteration-aware tokens and joint-training manner, the retriever could maintain a balance be-

313      between newly learned knowledge and previously  
 314      acquired knowledge.

315      We also employ the hard negative sampling in  
 316      training. Concretely, for each given instruction,  
 317      we randomly sample an incorrect tool from the re-  
 318      trieval top- $K$  tool list. The high similarity scores  
 319      of those tools indicate that they are prone to be mis-  
 320      taken as correct tools by the retriever. In feedback  
 321      training, we utilize those tool-instruction pairs as  
 322      hard negative samples.

323      Then, the loss function for each iteration could  
 324      be calculated as,

$$325 \quad \mathcal{L} = -\frac{1}{B} \sum_{i=1}^B \log \frac{e^{R(q_i, d_i^+)}}{e^{R(q_i, d_i^+)} + \sum_{j \neq i} e^{R(q_i, d_{ij}^-)} + \sum e^{M(q_i, d_{ij}^H)}}, \quad (6)$$

326      where  $d_{ij}^H$  denotes the hard negative sample. By  
 327      distinguishing the subtle differences in the tool de-  
 328      scriptions, the retriever could achieve a deeper un-  
 329      derstanding of the tool functionalities and their re-  
 330      lation with user instructions.

#### 331      4.4 Inference

332      At the time of inference, the feedback generation  
 333      process keeps working while the feedback training  
 334      process ceased. The retriever will update the candi-  
 335      date tool list based on the refined user instruction  
 336      from LLM’s feedback iteratively, until output the  
 337      final retrieved tools.

338      Concretely, assume that we have obtained a re-  
 339      triever  $R$  after the feedback training. For each  
 340      initial test instruction  $q_{test}^0$ , we add a special to-  
 341      ken “Iteration 0” in front of the instruction. Then  
 342      we use the trained retriever  $R$  to retrieve an ini-  
 343      tial tool list  $D_{test}^0$ , containing  $K$  candidate tools  
 344       $\{d_1, d_2, \dots, d_K\}$ . The retrieved  $D_{test}^0$  and  $q_{test}^0$  will  
 345      be fed to the LLM for feedback generation, includ-  
 346      ing instruction refinement, as discussed in Section  
 347      4.2. After obtaining the refined instruction  $q_{test}^1$ ,  
 348      we add a token “Iteration 1” to it and then input  
 349      it to  $R$  for the next-round tool retrieval. Then, we  
 350      can get an updated tool list  $D_{test}^1$  for a new round  
 351      of feedback generation. As such, we could obtain  
 352      a final tool list  $D_{test}^T$  after  $T$  iterations.

## 353      5 Experiments

### 354      5.1 Setup

355      **Datasets and evaluation.** To assess the tool  
 356      retrieval performance of models, we conduct a tool re-  
 357      trieval benchmark, referred to as **TR-bench**, based  
 358      on three datasets, including ToolBench (Qin et al.,

		scenarios	# instructions	# tool set
Training Set	ToolBench-I1	86,643	-	
	ToolBench-I2	84,270	-	
	ToolBench-I3	25,044	-	
	ToolBench-All	195,937	-	
In-domain Evaluation	ToolBench-I1	796	10,439	
	ToolBench-I2	573	13,142	
	ToolBench-I3	218	1,605	
	ToolBench-All	1,587	13,954	
Out-of-domain Evaluation	Teval	553	50	
	UltraTools	1,000	498	

359      Table 1: Statistics of the TR-bench, which is conducted  
 360      from ToolBench (Qin et al., 2023b), T-Eval (Chen et al.,  
 361      2023), and UltraTools (Huang et al., 2024).

362      2023b), T-Eval (Chen et al., 2023), and Ultra-  
 363      Tools (Huang et al., 2024). To address real-world  
 364      requirements, we conduct evaluations in both *in-  
 365      domain* and *out-of-domain* settings. Specifically,  
 366      the training set is from ToolBench, while the test  
 367      set of ToolBench is employed for in-domain evalua-  
 368      tion, and the test sets from T-Eval and UltraTools  
 369      are used for out-of-domain evaluation. The statis-  
 370      tics of TR-bench are summarized in Table 1.

371      Following previous work (Qin et al., 2023b), we  
 372      adopt the Normalized Discounted Cumulative Gain  
 373      (NDCG) (Järvelin and Kekäläinen, 2002), an ideal  
 374      ranking metric for tool retrieval since it could eval-  
 375      uate the relevance and quality of retrieved tool can-  
 376      didates according to their ranked orders. We report  
 377      NDCG@ $m$  ( $m = 1, 3, 5, 10$ ), where  $m$  refers to  
 378      top- $m$  ranked search results for evaluation.

379      **Baselines.** We compare our method against rep-  
 380      resentative retrieval methods. 1) BM25 (Robertson  
 381      and Zaragoza, 2009): the classical sparse retrieval  
 382      method; 2) Ada Embedding: the closed-sourced  
 383      OpenAI’s text-embedding-ada-002 model<sup>1</sup>; 3)  
 384      ToolRetriever (Qin et al., 2023b): a dense retrieval  
 385      approach specifically finetuned on tool retrieval  
 386      datasets.

387      **Implementation details.** We employ Sentence-  
 388      BERT (Reimers and Gurevych, 2019) to train our  
 389      retriever model based on BERT-base (Devlin et al.,  
 390      2019). We set the learning rate to  $2e-5$  with 500  
 391      warm-up steps. The batch size in training is set  
 392      to 64. We utilize ChatGPT (gpt-3.5-turbo-0125)<sup>2</sup>  
 393      as the LLM for giving feedback. The number of  
 394      tool candidates  $K$ , the balancing factor  $\alpha$ , and the

<sup>1</sup><https://platform.openai.com/docs/guides/embeddings/embedding-models>.

<sup>2</sup><https://openai.com/index/introducing-chatgpt-and-whisper-apis/>.

Methods	SINGLE-TOOL (I1)			CATEGORY (I2)			COLLECTION (I3)			ALL		
	N@1	N@3	N@5	N@1	N@3	N@5	N@1	N@3	N@5	N@1	N@3	N@5
BM25	18.37	17.97	19.65	11.97	9.85	10.95	25.23	18.95	20.37	15.84	13.98	15.63
Ada Embedding	57.52	54.90	58.83	36.82	28.83	30.68	54.59	42.55	46.83	46.59	41.06	43.95
ToolRetriever	84.20	89.59	89.65	68.24	77.43	77.90	81.65	87.24	87.13	75.73	83.19	83.06
<b>Ours</b>	<b>90.70</b>	<b>90.95</b>	<b>92.47</b>	<b>89.01</b>	<b>85.46</b>	<b>87.10</b>	<b>91.74</b>	<b>87.94</b>	<b>90.20</b>	<b>88.53</b>	<b>87.00</b>	<b>88.83</b>
% improve	7.72%	1.52%	3.15%	30.44%	10.37%	11.81%	12.36%	0.80%	3.52%	16.90%	4.58%	6.95%

Table 2: In-domain evaluation on TR-bench in terms of NDCG@m under scenarios including single-tool (*I1*), intra-category multi-tool (*I2*), intra-collection multi-tool (*I3*), and the whole data (*All*). % improve represents the relative improvement achieved by our method over the previously best tool retrieval method.

Methods	T-EVAL				ULTRATOOLS			
	N@1	N@3	N@5	N@10	N@1	N@3	N@5	N@10
BM25	52.12	43.19	45.23	52.91	15.10	14.13	16.03	18.34
Ada Embedding	80.11	69.11	71.95	79.62	31.46	33.75	39.91	46.40
ToolRetriever	82.10	72.03	74.15	<b>80.76</b>	48.20	<b>47.73</b>	53.01	58.93
<b>Ours</b>	<b>84.45</b>	<b>73.31</b>	<b>74.45</b>	80.25	<b>49.30</b>	47.50	<b>54.30</b>	<b>59.92</b>
% improve	2.86%	1.78%	0.40%	-0.06%	2.28%	-0.48%	2.43%	1.68%

Table 3: Out-of-domain evaluation on TR-bench in terms of NDCG@m under two scenarios, T-Eval (Chen et al., 2023) and UltraTools (Huang et al., 2024). % improve represents the relative improvement achieved by our method over the previously best tool retrieval method.

iteration round  $T$  are set to 10, 1, and 3, respectively. We have trained the model several times to confirm that the improvement is not a result of random chance and present the mid one. Our experiments were conducted on four NVIDIA A6000 GPUs with 48 GB of memory

## 5.2 Main Results

**In-domain evaluation.** The results of the in-domain evaluation are reported in Table 2. It is observed that non-finetuned retrieval methods, i.e., BM25 and Ada Embedding, perform much worse than other finetuned methods. This is reasonable since non-finetuned methods have not been specifically adopted for tool retrieval. While Tool Retriever outperforms non-finetuned methods, the performance is still not satisfying. In comparison, our proposed method consistently outperforms all finetuned and non-finetuned baselines. Significantly, our method maintains strong performance in the intra-category multi-tool (*I2*) scenario, even as other methods' performance declines, demonstrating the robustness of our proposed method across different scenarios. The above results prove the effectiveness of our method in enhancing tool retrieval accuracy, particularly in challenging scenarios with multi-tools.

**Out-of-domain evaluation.** Since the tools are usually frequently updated in real-world, we further test all methods in the out-of-domain setting,

Methods	N@1	N@3	N@5	N@10
Ours	89.01	85.46	87.10	88.41
w/o warm-up	85.51	81.36	84.47	86.92
w/o hard-negative	86.04	80.41	84.00	85.98
w/o joint & hard-neg	83.77	77.67	81.21	83.69

Table 4: Ablation study of our method under the intra-category multi-tool (*I2*) scenario.

where the training data from ToolBench and the test data from T-Eval and UltraTools are used. The experimental results are shown in Table 3. We could observe that our method significantly outperforms other baselines across both scenarios. This demonstrates that our method not only excels in in-domain benchmarks but also maintains robust performance across varied scenarios, revealing its generalization ability of tool retrieval.

## 5.3 Ablation Study

We conduct ablation studies to investigate the efficacy of different components in our methods. First, we remove the warm-up training by directly conducting our method on an retriever based on Sentence-BERT. Then, we analyze the contribution of hard negative sampling in our method by removing the hard-to-distinguish samples from the training. In addition, we assess the efficacy of joint training in our method, by substituting it with a loss  $\mathcal{L}_{feedback} = \mathcal{L}(q^t)$ , with respect to

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Iteration	N@1	N@3	N@5	N@10	Efficiency
1	85.69	80.48	83.94	86.27	6.12s
2	87.78	83.48	86.31	88.26	8.59s
3	89.01	85.46	87.10	88.41	10.30s

Table 5: Analysis on iteration round under the intra-category multi-tool instructions (I2) scenario. The efficiency is measured by the time consumption to complete one user instruction.

Methods	N@1	N@3	N@5
ToolRetriever (BERT-based)	68.24	77.43	77.90
Ours (BERT-based)	89.01	85.46	87.10
ToolRetriever (RoBERTa-based)	76.61	69.81	74.99
Ours (RoBERTa-based)	85.40	78.72	81.50

Table 6: Analysis on different base models under the intra-category multi-tool instructions (I2) scenario.

only the refined instructions  $q^t$  at current iteration  $t$ . Table 4 reports the ablation test performance (i.e., NDCG@m ( $m = 1, 3, 5, 10$ )) under the intra-category multi-tool instructions (I2) scenario on ToolBench.

From the results, we can observe that our method achieves comparably high NDCG scores even without warm-up training, indicating that it does not heavily rely on prior tool-use knowledge. When hard negative sampling is removed, the performance degradation illustrates that hard negative sampling could enable the model to discriminate between similar tool functionalities. Besides, the model’s performance further declines when joint training is removed, demonstrating that the model could balance new and previous knowledge in this joint-training manner.

#### 5.4 In-depth Analysis

**Analysis on iteration round.** The iteration round is an important factor in our method. We conduct experiments to investigate changes in effectiveness and efficiency with different iteration round  $T$ . The results are presented in Table 5, and the efficiency is measured by the cost of time to complete one user instruction on average.

By analyzing the results in Table 5, we gain two findings. 1) We could observe a continuous improvement as the iteration round increases. This shows that the tool retriever progressively enhances its performance with the aid of LLMs’ feedback. 2) In terms of time efficiency, we find that adding one additional round of refinement takes an average of 6.12s/instruction, primarily resulting from the

Embedding Size	N@1	N@3	N@5	N@10
300	87.61	83.49	85.20	86.50
512	87.61	82.85	84.67	85.81
768	89.01	85.46	87.10	88.41
1024	88.66	83.91	85.94	87.04
2048	88.74	83.95	85.98	87.43

Table 7: Analysis on embedding sizes under the intra-category multi-tool instructions (I2) scenario.

time waiting for LLM’s feedback when calling the OpenAI API. As the number of iterations increases, we can see that the extra inference time required for each instruction decreases. This is due to the fact that there will be fewer instructions requiring refinement as retrieval performance improves.

**Analysis on base models.** We further analyze the impact of different base models on the performance. Specifically, we replace the base model BERT in our method with another classic language model, RoBERTa (Liu et al., 2019). The results are shown in Table 6. As we can see, our method still achieves significant improvement over the baseline with the same RoBERTa model. Another observation is that RoBERTa is more effective in serving as a base model for the retrieval application, which benefits from its effective training strategies. The improvements demonstrate the robustness of our method with different base models.

**Analysis on embedding sizes.** Since the retriever model  $R$  encodes the textual instruction and tool description into dense vectors, we explore the impact of the embedding size on retrieval performance. as shown in Table 7. From the table, we can find that larger embedding sizes result in greater performance improvements compared to smaller embedding sizes. This is probably due to the fact that embeddings with larger sizes could accommodate more knowledge. However, when the embedding size increases from 768 to 2048, there is a slight decrease in performance. This suggests that a specific embedding size is sufficient, and larger embedding sizes may pose challenges to training. It is worth noting that larger embedding sizes necessitate higher training costs and increased inference memory. Therefore, we recommend an optimal embedding size of 768.

#### 5.5 Case Study

As shown in Figure 4, we conduct case study by using an example of instruction refinement to take a closer look at the effect of our method.

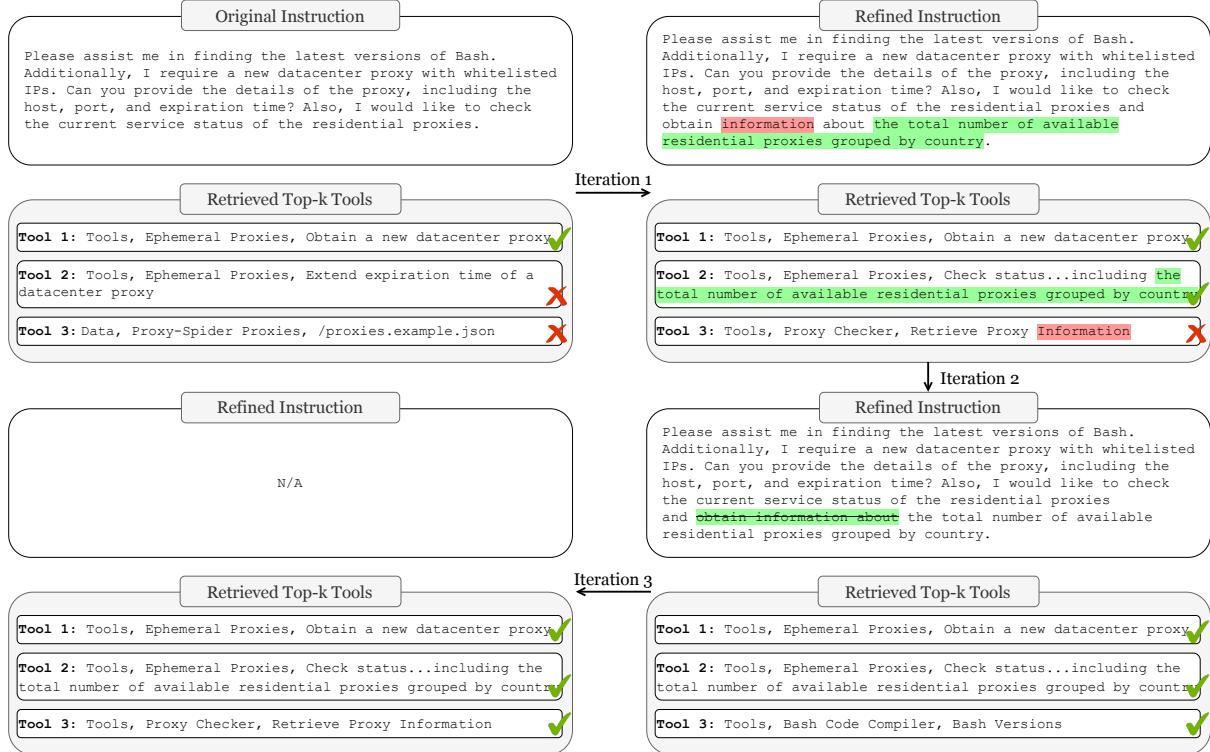


Figure 4: Case study on the effect of user instruction refinement through 3 iterations. The original instruction is revised step-by-step, leading to improved retrieval results.

In the 1<sup>st</sup> iteration, we can observe that the refined instruction has included more detailed information (i.e., “total number”) about the user’s requirements than the original instruction, enabling the retriever to identify more appropriate tools (e.g., Check residential proxies service status). This reveals that the comprehension capabilities of LLMs could be instilled into the retrieval process through feedback. In the 2<sup>nd</sup> iteration, our method further refines the instruction by omitting irrelevant content (i.e., “information”) which may mislead the retriever into retrieving incorrect tools (e.g., Retrieve Proxy Information). Another benefit of the refinement is that some correct tools (e.g., Bash Code Compiler) will move up in positions of the top- $K$  rankings, improving the overall retrieval performance. In the 3<sup>rd</sup> iteration, our method showcases great decision-aware capabilities, where the iterative process could be terminated if no further refinement is deemed necessary.

## 6 Conclusion and Future Work

In this study, we concentrate on the crucial tool retrieval in the tool learning of LLMs. We have identified the bottleneck in the tool retrieval-usage pipeline as the limited tool retrieval model. We

propose the unique challenges of the tool retrieval compared with document retrieval. To improve the current tool retrieval process, we propose leveraging the LLM’s feedback to assess the retrieval results and provide detailed suggestions for refining user instructions. In order to integrate the retriever model into this iterative process, we implement iteration-aware feedback training. This will improve the tool retriever’s capabilities and close the gap between tool retrieval and usage models. We conduct the TR-benchmark to comprehensively evaluate the models’ ability in real-world tool retrieval scenarios. Our method demonstrates the best performance in both in-domain and out-of-domain settings.

In the future, we aim to improve this work from the following aspects. 1) Limited by the training speed, we have applied the offline feedback generation, where feedback is generated before training the tool retriever. We will also assess whether online feedback generation yields further improvements in the future. 2) Furthermore, as the tool retriever serves the subsequent tool usage model in tool learning, we intend to conduct further evaluations of the tool retriever models based on the subsequent tool usage results.

## 566 Limitations

567 1) Undoubtedly, our iterative refinement will re-  
568 duce the inference speed of the tool retrieval. We  
569 have evaluated the efficiency as the number of iter-  
570 ative rounds increases. Fortunately, we observed  
571 that just one additional round of refinement could  
572 yield significant improvements. Furthermore, the  
573 performance enhancement of the tool retrieval is  
574 crucial for the subsequent tool usage model. 2)  
575 Similar to document retrieval, the used datasets in  
576 our work also contain “false negative” samples. For  
577 instance, some tools may be capable of handling  
578 the user’s instruction but are not labeled as pos-  
579 itive. This can disrupt the training and evaluation of  
580 tool retrieval and is a common limitation in many  
581 retrieval scenarios.

## 582 Ethics Statement

583 The datasets used in our experiment are publicly  
584 released and labeled through interaction with hu-  
585 mans in English. In this process, user privacy is  
586 protected, and no personal information is contained  
587 in the dataset. The scientific artifacts that we used  
588 are available for research with permissive licenses.  
589 And the use of these artifacts in this paper is consis-  
590 tent with their intended use. Therefore, we believe  
591 that our research work meets the ethics of the con-  
592 ference.

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