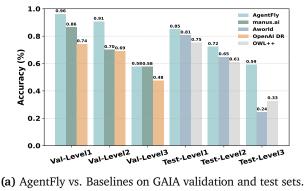
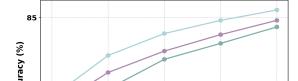
# AgentFly: Fine-tuning LLM Agents without **Fine-tuning LLMs**

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# **Abstract**

In this paper, we introduce a novel learning paradigm for adaptive Large Language Model (LLM) agents that eliminates the need for fine-tuning the underlying LLMs. Existing approaches are often either rigid, relying on static, handcrafted reflection workflows, or computationally intensive, requiring gradient updates of LLM model parameters. In contrast, our method enables low-cost continual adaptation via memory-based online reinforcement learning. We formalise this as a Memory-augmented Markov Decision Process (M-MDP), equipped with a neural case-selection policy to guide action decisions. Past experiences are stored in an episodic memory, either differentiable or non-parametric. The policy is continually updated based on environmental feedback through a memory rewriting mechanism, whereas policy improvement is achieved through efficient memory reading (retrieval). We instantiate our agent model in the deep research setting, namely AgentFly, which attains top-1 on GAIA validation (87.88% Pass@3) and 79.40% on the test set. It reaches 66.6% F1 and 80.4% PM on the DeepResearcher dataset, outperforming the state-of-the-art training-based method, while case-based memory adds 4.7% to 9.6% absolute points on out-of-distribution tasks. Our approach offers a scalable and efficient pathway for developing generalist LLM agents capable of continuous, real-time learning without gradient updates, advancing machine learning towards open-ended skill acquisition and deep research scenarios. The code is available at https://github.com/Agent-on-the-Fly/AgentFly.

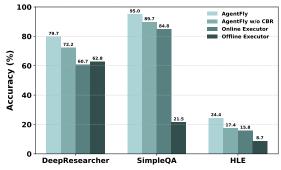




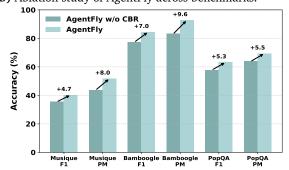


Iteration

(c) Continual learning curves across memory designs.



(b) Ablation study of AgentFly across benchmarks.



(d) AgentFly's accuracy improvement on OOD datasets.

Figure 1: Overview of AgentFly evaluation across baselines, benchmarks, memory designs and generalisation.

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### 1. Introduction

A Large Language Model (LLM) agent refers to a system that leverages one or more LLMs to autonomously perform complex tasks through interaction, reasoning, and decision making, often with access to external tools, memory, or environments (Christianos et al., 2023, Yang et al., 2025). Unlike passive LLMs that respond to prompts in isolation, LLM agents operate proactively and iteratively, guided by explicit goals. They are increasingly deployed as autonomous problem solvers (Choudhary et al., 2021, Wei et al., 2022, Yao et al., 2023) spanning various domains. Notable examples include deep research agents (OpenAI, 2025, Google, 2025, ByteDance, 2025), tool-enhanced execution systems (Li et al., 2025c, Zheng et al., 2025, Qian et al., 2025), and code generation agents (Cui et al., 2021, Guo et al., 2024, Grosnit et al., 2024, Guo et al., 2025), all of which demonstrate strong capabilities in complex scientific and engineering tasks.

Despite recent progress, current LLM agents typically follow two prevailing paradigms, each exhibiting fundamental limitations. The first approach builds specialised frameworks with fixed workflows and hard-coded reasoning, which work well for narrow tasks but lack flexibility. After deployment, such agents are static: they neither incorporate online information nor adapt to novel situations. The second paradigm focuses on updating the LLM itself through parameter tuning of underlying LLMs – via supervised fine-tuning or reinforcement learning – which allows for more flexible behaviour (Christianos et al., 2023, Shi et al., 2025) but comes at a high computational cost. These approaches are inefficient for continuous adaptation and online learning, impractical for agents deployed in open-ended scenarios. This observation raises a central research challenge towards generalist agents:

How can we build LLM agents that learn continuously from a changing environment without the prohibitive cost of fine-tuning the underlying LLMs?

Inspired by human memory mechanisms, we address this challenge by proposing a memory-based learning framework that enables continual adaptation without modifying the underlying LLMs. We observe that humans' performance steadily improves because each experience is (i) encoded as an episodic trace (Pritzel et al., 2017), (ii) distilled into abstract rules during sleep-dependent consolidation (Squire et al., 2015), (iii) selectively reinforced by dopamine-driven credit assignment (Glimcher, 2011), and (iv) retrieved through case- or analogy-based reasoning when similar problems arise (Ashley, 1992). Thus, instead of fine-tuning the base model, LLM agents leverage an external memory to store past trajectories – including successes and failures labels – and draw from similar past experiences to guide decision making. This approach aligns with the principles of case-based reasoning (CBR) (Aamodt and Plaza, 1994, Guo et al., 2024, 2025), a psychologically grounded learning strategy supported by evidence that humans often solve problems by recalling analogous past situations (Anderson, 2013, Ross, 1989). For example, in a deep research scenario, deep research agents that have previously succeeded on a web-based task can leverage their experience to solve never-seen and structurally similar tasks (Wiratunga et al., 2024). Our method offers a novel path to continual learning for deep research agents – efficient, generalizable, and inspired by how humans learn.

To this end, we introduce AgentFly, a non-parametric, learn-on-the-fly framework for CBR (Smyth and McClave, 2001, Hatalis et al., 2025), instantiated as a planner–executor architecture grounded in a memory-based Markov Decision Process (MDP). AgentFly comprises three principal components: (i) a planner, (ii) a tool-enabled executor, and (iii) a growing *Case Bank* that stores past trajectories as episodic memory. Instead of relying solely on the LLM's parametric memory, which is fixed after training, online case-based reasoning in AgentFly is implemented by storing rich episodic traces.

Our experiments are conducted on 4 benchmarks, where GAIA (Mialon et al., 2023) for long-horizon tool use, DeepResearcher (Zheng et al., 2025) for real-time web research, SimpleQA (Wei et al., 2024) for factual precision, and HLE (Phan et al., 2025) for long-tail academic reasoning. We use a planner–executor architecture with GPT-4.1 as the planner and o4-mini as the default executor (o3 for GAIA), instrumented with tools, namely AgentFly. We achieve top-1 on GAIA validation (87.88% Pass@3) and 79.40% on the private test leaderboard, and it reaches 66.6% F1 and 80.4% PM on the DeepResearcher dataset, outperforming the state-of-the-art training-based system, while case-based memory adds 4.7 to 9.6 absolute points on out-of-distribution tasks and yields 95.0% PM on SimpleQA. To our knowledge, we are the first to cast case-based continual learning for LLM agents, achieving the top-level performance on the GAIA benchmark, thereby providing a principled framework for continual adaptation of Deep Research agents.

# 2. Related Work

We first review methods that equip LLMs with continual-learning capabilities. Then, we discuss approaches that augment agents with external tools and multi-agent coordination. Lastly, we introduce agent memory mechanisms, characterising design choices in representation, retrieval, and decay, and their implications for continual learning.

### 2.1. Continual-learning in LLM Agent Systems

Continual-learning strategies for LLM agents can be categorised into two camps. Parametric approaches (Zhu et al., 2025b,a) update the LLM through post-training (e.g., Reinforcement Learning (Wang et al., 2025)) or supervised fine-tuning (e.g., START (Li et al., 2025a)), achieving high task fidelity at the expense of considerable compute, data, and the danger of catastrophic forgetting (Li et al., 2024). It is often assumed that achieving the capability to solve complex reasoning problems requires substantial changes to the model's parameters, and therefore, full fine-tuning is widely applied during RL (Liu et al., 2025). However, when tackling long-horizon, complex tasks (Mialon et al., 2023, Phan et al., 2025), LLM agent systems must spend substantial time rolling out trajectories to gather training data, and they additionally depend on large volumes of human-annotated questions. Differently, non-parametric approaches freeze the LLM and attach an external memory to optimise the prompt construction process. Human intelligence relies heavily on memory systems, especially episodic memory, which supports learning from both successes and failures (Baddeley, 1983). Cognitive science suggests that such memories are segmented and selectively replayed to inform future decisions (Anderson et al., 1997, Khosla et al., 2023, Fountas et al., 2024). This inspired early AI paradigms like Case-Based Reasoning (CBR) (Francis and Ram, 1993). While modern Retrieval-Augmented Generation (RAG) systems (Lewis et al., 2020) share surface similarities with CBR, they typically query static document corpora and lack mechanisms for continual adaptation (Gao et al., 2023).

### 2.2. Tool-augmented LLM

Language agents increasingly incorporate external tools to overcome context limitations and computational bottlenecks. prompt-based methods, including WebGPT (Nakano et al., 2021), embed tool calls directly in the generation trace. However, tackling long-horizon tasks are often required multi-hop tool calls. Therefore, recent works propose multi-agent pipelines, such as AutoGen (Wu et al., 2023), OWL (Camel-AI, 2025) and DeerFlow (ByteDance, 2025) to coordinate specialised agents via dialogue. To address long-horizon decision-

making in dynamic, multi-turn interactions with external tool environments, Agentic Reinforcement Learning (Agentic RL) has emerged as a promising training paradigm. This approach shifts LLM training from static task-solving (e.g., math or code) to dynamic, agent—environment reasoning. Supervised Fine-tuning methods, including Toolformer (Schick et al., 2023), API-Bench (Li et al., 2023), and GRPO-based optimisation (Wang et al., 2025, Qian et al., 2025, Feng et al., 2025) teach models when and how to invoke APIs, but require costly retraining and often assume a fixed, small toolset (e.g., Code and Search). However, without explicit planning, deciding when and which tools to invoke remains a major bottleneck for long-horizon tasks. We model planning as a stateful MDP with explicit memory for past cases. By bringing case-based reasoning into planning, the executor is steered toward strategic tool calls and consistently strong performance.

# 2.3. Agent Memory Mechanism

Recent work has centred on endowing LLM agents with explicit memory structures. A growing body of work (Camel-AI, 2025, Liang et al., 2025, Google, 2025, ByteDance, 2025) has shown that current LLM agents are designed for fixed environments, limiting their ability to evolve. While some efforts, such as ReAct-style agents and reflective prompting pipelines (Shinn et al., 2023, Yao et al., 2023) demonstrate improvement through feedback, they remain constrained by pre-defined heuristics and do not achieve true lifelong learning. DS-Agent (Guo et al., 2024) stabilises planning by mining prior Kaggle solutions and turning them into executable pipelines. Agent-K (Grosnit et al., 2024) adds structured memory and credit assignment to reuse past work, enabling end-to-end automation of Kaggle-style workflows. Furthermore, Agent-KB (Tang et al., 2025) and Alita (Qiu et al., 2025) construct shared knowledge bases and optimised toolsets for agentic problem-solving. However, most systems keep adding cases without selective curation, leading to the classic swamping problem where retrieval costs outweigh utility (Francis and Ram, 1993).

LLM agents are increasingly equipped with long-term memory that grows and adapts over time, allowing them to accumulate knowledge, recall prior context, and adjust behaviour based on experience. Memory-Bank (Zhong et al., 2024) couples retrieval with an Ebbinghaus-style forgetting schedule so older, low-utility items decay while user-relevant facts are reinforced. Building on this idea, SAGE (Liang et al., 2024) unifies reflection with an Ebbinghaus-based memory optimiser to support continual self-refinement. Mem0 (Chhikara et al., 2025) adopts a structured memory mechanism with explicit operations (ADD, UPDATE, DELETE, NOOP). A-MEM (Xu et al., 2025) maintains memory via a typological network. MemInsight (Salama et al., 2025) pushes further on semantics by augmenting raw memories with summaries and tags to aid retrieval. Several lines of work distil operational knowledge from interaction traces: ExpeL (Zhao et al., 2024) collects trajectories and converts them into reusable natural-language insights and rules; AutoGuide (Fu et al., 2024) compresses offline logs into concise, conditional, context-aware guidelines; and Agent Workflow Memory (Wang et al., 2024) induces frequently used subtask sequences as auxiliary skills. Finally, Agent-KB (Tang et al., 2025) and Alita (Qiu et al., 2025) construct shared knowledge bases and optimised toolsets to support agentic problem solving. Differently, we formulate planning as a memory-augmented MDP and learn a neural case-selection policy over an episodic case bank via online soft Q-learning, enabling continual adaptation without fine-tuning the underlying LLM parameters.

# 3. Methodology: Memory-Based MDP with Case-based Reasoning Policy

In this work, we integrate LLM agents with case-based reasoning, a classic problem-solving paradigm that solves new problems by learning from solutions to previously encountered similar problems. As such, LLM

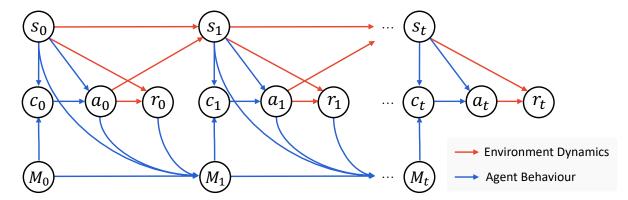


Figure 2: A graphical model of memory-based markov decision process.

agents can achieve continuous improvement without parameter fine-tuning by learning from experiences stored in memory. To begin with, we model the sequential decision-making process of CBR agents as a Memory-Based Markov Decision Process (M-MDP) as below.

**Definition 3.1** (Memory-Based Markov Decision Process). A Memory-Based Markov Decision Process is a tuple  $\langle S, A, \mathcal{P}, \mathcal{R}, \gamma, \mathcal{M} \rangle$ , where S is the state space, A is the action space,  $\mathcal{P}: S \times A \to \Delta(S)$  is the transition dynamics,  $\mathcal{R}: S \times A \to \mathbb{R}$  is the reward function,  $\gamma \in [0,1)$  is the discount factor, and  $\mathcal{M} = (S \times A \times \mathbb{R})^*$  is the memory space.

The graphical model of M-MDP is illustrated in Figure 2. Note that the key difference from standard MDP is that we introduce a memory space as a set of past experiences. In the CBR agent setting, both state space and action space are defined as the set of all finite-length sequences over a predefined vocabulary  $\mathcal{V}$ .

With the M-MDP formulation, the behaviour of the CBR agent can be formally described as follows. At timestep t, we maintain a case bank (i.e., the memory)  $M_t = \{c_i\}_{i=1}^{N_t}$ , with each case  $c_i$  a tuple  $(s_i, a_i, r_i)$ , and  $N_t$  the number of cases in the current case bank. Given the current state  $s_t$ , the CBR agent first retrieves a case  $c_t \sim \mu(\cdot \mid s_t, M_t)$ , and then reuses and adapts it via the LLM, i.e.,  $a_t \sim p_{\text{LLM}}(\cdot \mid s_t, c_t)$ . Here,  $\mu$  denotes the case retrieval policy, whose implementation details will be presented later. Taking the action  $a_t$ , the CBR agent receives the reward  $r_t = \mathcal{R}(s_t, a_t)$  and observes the next state  $s_{t+1} \sim \mathcal{P}(\cdot \mid s_t, a_t)$ . The CBR agent also retains the new case in the case bank, i.e.,  $M_{t+1} = M_t \cup \{(s_t, a_t, r_t)\}$ . In this way, we can define the overall policy of the CBR agent as below.

**Definition 3.2** (Case-Based Reasoning Agent). A Case-Based Reasoning Agent is an agent that makes decisions based on both the current state and a finite memory of past experiences. Formally, let  $s \in S$  denote the current state;  $M \in \mathcal{M}$  denote the current case bank, consisting of past cases c;  $a \in A$  denote the action;  $\mu(c \mid s, M)$  denote a case retrieval policy, assigning a probability distribution over M given the current state s;  $p_{LLM}(a \mid s, c)$  denote the action likelihood of a large language model (LLM) conditioned on the current state s and a retrieved case  $c \in M$ . Then, the overall policy  $\pi$  of a CBR agent is defined as:

$$\pi(a|s,M) = \sum_{c \in M} \mu(c|s,M) p_{LLM}(a|s,c). \tag{1}$$

Overall, the trajectory  $\tau$  of the CBR agent can be described as:  $\tau = \{M_0, s_0, c_0, a_0, r_0, M_1, s_1, c_1, a_1, r_1, \cdots\}$ . The

probability of sampling the trajectory  $\tau$  can be modelled as:

$$p(\tau) = \prod_{t=0}^{T-1} \underbrace{\mu(c_t \mid s_t, M_t)}_{\text{(1) Retrieve}} \underbrace{p_{\text{LLM}}(a_t \mid s_t, c_t)}_{\text{(2) Reuse\&Revise}} \underbrace{\mathbb{I}[r_t = \mathcal{R}(s_t, a_t)]}_{\text{(3) Evaluation}} \underbrace{\mathbb{I}[M_{t+1} = M_t \cup (s_t, a_t, r_t)]}_{\text{(4) Retain}} \underbrace{\mathcal{P}(s_{t+1} \mid s_t, a_t)}_{\text{(5) Transition}}, \quad (2)$$

where  $\mathbb{I}(\cdot)$  is the indicator function, assigning probability 1 if the condition holds and 0 otherwise, modelling the deterministic reward function and memory update, and T denotes the maximum trajectory length. Note that the reward function and memory update can also be probabilistic in some specific cases, which we leave as future work. Among them, (1) Retrieve, (2) Reuse and Revise, and (4) Retain describe the agent behaviour; (3) Evaluation and (5) Transition model the environment dynamics.

**Soft Q-Learning for CBR Agent.** To optimise the CBR policy  $\pi$  in Eq. (1), we aim to learn the case retrieval policy  $\mu$  with the LLM component  $p_{\rm LLM}$  fixed. In this context, the "action" of  $\mu$  is to select a case c = (s, a, r) from the case bank M. To optimise it while encouraging diversity in retrieved cases, we apply the maximum entropy RL framework (Haarnoja et al., 2018) and derive the following optimisation objective:

$$J(\pi) = \mathbb{E}_{\tau \sim p} \left[ \sum_{t=0}^{T-1} \left[ \mathcal{R}(s_t, a_t) + \alpha \mathcal{H} \left( \mu \left( \cdot | s_t, M_t \right) \right) \right] \right], \tag{3}$$

where  $\mathcal{H}$  denotes the entropy, and  $\alpha$  denotes the hyper-parameter of the entropy weight in the final reward. Under this framework, the value function can be defined as:

$$V^{\pi}(s_t, M_t) = \sum_{c \in M_t} \mu(c|s_t, M_t) [Q^{\pi}(s_t, M_t, c) - \alpha \log \mu(c|s_t, M_t)]. \tag{4}$$

Also, the Q value function for taking an "action" (i.e., selecting a case), given a state, can be defined as:

$$Q^{\pi}(s_t, M_t, c_t) = \mathbb{E}_{a \sim p_{\text{IJM}}(\cdot | s_t, c_t), s_{t+1} \sim \mathcal{P}(\cdot | s_t, a_t)} \left[ \mathcal{R}(s_t, a_t) + \gamma V^{\pi}(s_{t+1}, M_{t+1}) \right], \tag{5}$$

where  $M_{t+1}$  denotes the updated memory after  $(s_t, a_t, r_t)$  is added. Let  $d^{\pi}(s, M) = \sum_{t=0}^{\infty} \gamma^{t-1} \mathbb{P}(s_t = s, M_t = M)$  denote the discounted visitation frequency of (s, M) under  $\pi$ . The expected value function objective is then defined as:

$$J(\pi) = \mathbb{E}_{(s,M)\sim d^{\pi}} \left[ V^{\pi}(s,M) \right] = \mathbb{E}_{(s,M)\sim d^{\pi}} \left[ \sum_{c\in M} \mu(c|s,M) \left[ Q^{\pi}(s,M,c) - \alpha \log \mu(c|s,M) \right] \right]. \tag{6}$$

Then, we can derive the closed-form solution of the optimal retrieval policy as a softmax over the optimal Q value:

$$\mu^*(c|s,M) = \frac{\exp(Q^*(s,M,c)/\alpha)}{\sum_{c' \in M} \exp(Q^*(s,M,c')/\alpha)}.$$
 (7)

The detailed derivation can be found in Appendix A. In this way, we can derive the optimal retrieval policy by learning the Q-function Q, which can be achieved by the temporal difference (TD) learning in soft Q-learning (Haarnoja et al., 2017) as:

$$Q(s_t, M_t, c_t) \leftarrow Q(s_t, M_t, c_t) + \eta \left[ r_t + \gamma \alpha \log \sum_{c' \in M_{t+1}} \exp\left(Q(s_{t+1}, M_{t+1}, c_{t+1})\right) - Q(s_t, M_t, c_t) \right], \quad (8)$$

where  $\eta$  denotes the learning rate. Next, we provide a simpler way to learn the Q-function by learning a similarity kernel over states.

# Algorithm 1 Fine-tuning CBR agent with soft Q-learning and state similarity

**Require:** Kernel network parameters  $\theta$ , LLM policy  $p_{\text{LLM}}$ , entropy weight  $\alpha$ , discount factor  $\gamma$ , learning rate  $\eta$ , target-network update period K, averaging weight  $\beta$ , initial case bank  $M_0 = \emptyset$ , initial episodic memory  $\mathcal{D} = \emptyset$  and initial replay buffer  $\mathcal{B} = \emptyset$ 

```
1: Initialize target retrieval network \bar{\theta} \leftarrow \theta
 2: for timestep t = 0, 1, 2, ... do
          Retrieve: Sample case c_t \sim \mu_{\theta}(\cdot \mid s_t, M_t)
                                                                                    ▶ Memory Reading, following Eq. (7) and Eq. (9)
 3:
          Reuse & Revise: Sample action a_t \sim p_{\text{LLM}}(\cdot \mid s_t, c_t)
 4:
          Execute a_t and observe reward r_t and next state s_{t+1}
 5:
          Retain: M_{t+1} = M_t \cup \{(s_t, a_t, r_t)\}
 6:
          Store transition (s_t, c_t, r_t, s_{t+1}, M_{t+1}) in \mathcal{B}
 7:
          Append Episodic Memory \mathcal{D} \leftarrow \mathcal{D} \cup \{(s_t, c_t, Q_t)\}
 8:
                                                                                                                                  ▶ Memory Writing
          Sample mini-batch \{(s_i, c_i, r_i, s_i', M_i')\} \sim \mathcal{B}
 9:
          \theta \leftarrow \theta - \eta \ \nabla_{\theta} \mathcal{L}_i
                                                                                                                               \triangleright Following Eq. (10)
10:
          if t \mod K = 0 then

    □ Update target network

11:
                \bar{\theta} \leftarrow \beta \bar{\theta} + (1 - \beta)\theta
12:
          end if
13:
14: end for
```

Enhance Q-Learning Based on State Similarity. As in Eq. (8), we can learn the Q function from scratch via TD learning. However, directly learning the Q function is challenging due to complex state and case descriptions in the form of natural language. To this end, we propose to approximate the Q value via kernel-based estimation, following episodic control (EC) algorithms (Pritzel et al., 2017). Specifically, we maintain an episodic memory  $\mathcal{D} = \{(s, c, Q)\}$ , including the state, the retrieved case, and the Q value of each interaction. Then, we approximate the Q function via a kernel network  $k_{\theta}(\cdot, \cdot)$ , parametrised by  $\theta$ :

$$Q_{\text{EC}}(s, M, c; \theta) = \sum_{\substack{(s', c', Q') \in \mathcal{D}_c}} \frac{k_{\theta}(s, s') Q'}{\sum_{(\hat{s}, \hat{c}, \hat{Q}) \in \mathcal{D}_c} k_{\theta}(s, \hat{s})}, \tag{9}$$

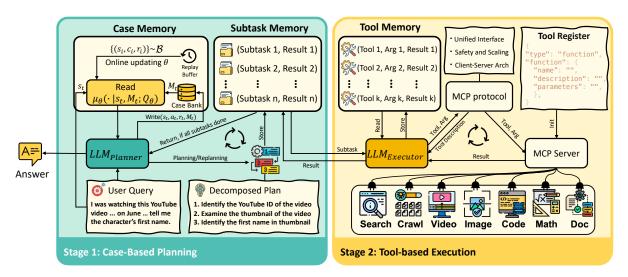
where  $\mathcal{D}_c = \{(s_i, c_i, Q_i) \in \mathcal{D} : c_i = c\}$  denotes the past interactions stored in the episodic memory  $\mathcal{D}$  with the same retrieved case c. By substituting Eq. (9) in Eq. (8), we can learn the Q function by optimising the kernel parameter  $\theta$  via TD learning, i.e.,

$$\mathcal{L}(\theta) = \mathbb{E}_{(s,c,r,s',M,M')} \left[ \left( Q_{\text{EC}}(s,M,c;\theta) - \left[ r + \gamma \alpha \log \sum_{c' \in M'} \exp(Q_{\text{EC}}(s',M',c';\bar{\theta})) \right] \right)^2 \right], \tag{10}$$

where  $\bar{\theta}$  denotes the target kernel network, s' denotes the next state and  $M' = M \cup \{c\}$  denotes the updated case bank. More specifically, we provide the gradient of the TD learning loss with respective of  $\theta$  as:

$$\nabla_{\theta} \mathcal{L}(\theta) = 2 \mathbb{E}_{(s,c,r,s',M,M')} \left[ (f_{\theta}(s,c) - y) \sum_{i \in \mathcal{D}_c} w_i(s,c;\theta) \left( Q_i - f_{\theta}(s,c) \right) \nabla_{\theta} \log k_{\theta}(s,s_i) \right], \tag{11}$$

where 
$$w_i = \frac{k_{\theta}(s,s_i)}{\sum_{s_i \in \mathcal{D}_c} k_{\theta}(s,s_j)}$$
,  $f_{\theta}(s,c) = \sum_{(s_i,Q_i) \in \mathcal{D}_c} w_i Q_i$ , and  $y = r + \gamma \alpha \log \sum_{c' \in M'} \exp(f_{\bar{\theta}}(s',c'))$ .



**Figure 3:** The architecture of AgentFly with parametric memory. AgentFly is instantiated as a planner–executor framework alternating between Case-Based Planning (Stage 1) and Tool-Based Execution (Stage 2). The planner is an LLM-based CBR agent enhanced by a Case Memory module that supports both Write, which records new cases and online refines the Q-function, and Read, which retrieves cases via the learned retrieval policy for adaptive case selection. The executor is an LLM-based MCP client that invokes external tools hosted on the MCP servers through the MCP protocol.

# 4. Implementation: Deep Research Agent

We implement stateful prompt engineering via M-MDP methodology (§ 3) in Deep Research scenarios (Huang et al., 2025), where agents must solve complex, long-horizon tasks by iteratively interacting with their environment, invoking external tools, retrieving information from external sources, and processing heterogeneous data for dynamic reasoning. As illustrated in Figure 3, AgentFly alternates between two core stages: Case-Based Planning and Tool-Based Execution.

#### 4.1. Framework

To address the challenges of long-horizon reasoning, AgentFly follows the plan-and-act paradigm (Erdogan et al., 2025), where the planner and executor operate in an alternating loop to iteratively advance task completion. For effective coordination, AgentFly integrates three memory modules:Case Memory (vectorised storage of prior cases for high-level planning), Subtask Memory (text-based storage of active subtasks and their results), and Tool Memory (text-based logs of tool interactions for each subtask).

In the planning stage, Planner, instantiated as an LLM-driven CBR agent, receives the task instruction and queries the case memory for relevant case triplets  $(s_i, a_i, r_i)_{i=1}^K$ , where  $s_i$  is the task,  $a_i$  is the plan,  $r_i$  indicates success, and K is the retrieval count. This process is supported by a Case Memory module, which retrieves relevant experiences from a case bank through either a similarity-based retriever or online-updating Q-function, thus enabling the planner to leverage both parametric and non-parametric memory as priors. The retrieved cases are concatenated with the current task instruction to form the prompt, guiding the LLM to generate a plan for each subtask. Once the initial task is decomposed, a Subtask Memory module orchestrates the interaction between the planner and executor, recording generated subtasks and their execution outcomes. After each iteration, the planner uses the accumulated execution history to assess task

completion. If the task is unfinished, the planner replans based on updated context; otherwise, the final result is returned, and the case memory is updated with new experiences only upon task completion.

The execution stage is managed by an Executor, powered by a general-purpose LLM, which is responsible for executing each subtask as an autonomous episode (Sumers et al., 2023) using the MCP protocol. Unlike prior agents (Zheng et al., 2025, Weng et al., 2025), AgentFly's executor supports rich reasoning and flexible tool composition. For each subtask, the executor consults tool memory, determines the appropriate tool invocation, and updates results.which operates as a Model Context Protocol (MCP)<sup>1</sup> client. The executor reads pending subtasks from the subtask memory, accesses relevant history from a Tool Memory (scoped per subtask), and determines whether to invoke an external tool or return a result. MCP serves as a standardized, model-agnostic interface, enabling flexible coordination with diverse external tools and data sources. By unifying access under a single protocol layer, AgentFly can seamlessly integrate dynamic reasoning and compositional tool use across multiple domains.

# 4.2. Case Memory Management

The case memory is an online-growing case bank  $M_t$  operated with Write and Read operations, available in non-parametric and parametric variants. In the non-parametric setting, Write simply appends  $(s_t, a_t, r_t)$ , and Read retrieves cases by similarity for computational efficiency. In the parametric setting, Write further online updates a Q-function to shape the retrieval distribution, while Read is driven by the learned Q-function, thereby realising adaptive case selection. More details are provided in Appendix B.

**Memory Storage.** Following the CBR agent in Definition 3.2, the Write operation appends each historical case  $(s_t, a_t, r_t)$  to the case bank  $M_t$ , after each time step t:

Write
$$(s_t, a_t, r_t, M_t) = M_{t+1} = M_t \cup \{(s_t, a_t, r_t)\}.$$
 (12)

In this process, the state  $s_t$  is encoded using a frozen text encoder, while the action  $a_t$  and reward  $r_t$  are preserved in their original forms, as only the state representation requires vectorisation for subsequent retrieval operations. This Write operation is continuously performed throughout the agent's execution, allowing the case bank to grow into a comprehensive and transferable repository of experiences incrementally. By accumulating both successes and failures, the memory not only enables retrospective analysis for informed avoidance of past mistakes but also provides successful trajectories that prospectively guide future planning.

Non-Parametric Memory Retrieval. A cornerstone of AgentFly is its dynamically evolving Case Bank, which underpins its continual learning capability. At each planning step, this non-parametric memory module receives the task instruction and then retrieves relevant cases, comprising a mixture of successful and failed cases. This CBR method mirrors human analogical learning, where previously encountered outcomes shape decision-making (Aamodt and Plaza, 1994). Specifically, we retrieve the K nearest past cases from the case bank by computing the semantic similarity between the current state and past states. This design follows the mainstream CBR paradigm, which assumes that similar problems should have similar solutions (Wiratunga et al., 2024, Guo et al., 2025), thereby allowing the agent to prioritise cases whose historical contexts are most aligned with the current task. Formally, the Read operator of the non-parametric memory is defined as:

$$\operatorname{Read}_{\operatorname{NP}}(s_t, M_t) = \operatorname{TopK}_{(s_i, a_i, r_i) \in M_t} \operatorname{sim} (\operatorname{enc}(s_t), \operatorname{enc}(s_i)), \tag{13}$$

<sup>1</sup>https://github.com/modelcontextprotocol

where  $s_t$  and  $M_t$  denote the query and case bank at time step t, respectively. Here, enc(·) represents the pretrained textual encoder and sim(·) denotes the cosine similarity function.

Parametric Memory Retrieval. To empower the agent to selectively leverage high-utility cases to augment planning from past experiences, we design a differential memory mechanism in AgentFly via a parametric Q-function. When writing new cases to the case bank, the parametric method, in contrast to the non-parametric approach that merely appends the tuple as in Eq. (12), concurrently updates the Q-function online. Meanwhile, with CBR applied only for planning in AgentFly, the CBR planner can be simplified to a single-step setting instead of a multi-step M-MDP. This single-step setting collapses the TD target in Eq. (10) to the immediate reward, thereby simplifying the learning objective. Without bootstrapping, the updating reduces to a supervised learning paradigm, which avoids non-stationary targets. Therefore, we can train a parametric Q-function  $Q(s,c;\theta)$  end-to-end, dispensing with the kernel-based estimation in Eq. (9). Accordingly, the single-step Q-learning loss can be formulated as:

$$\mathcal{L}(\theta) = \mathbb{E}_{(s,c,r)} \left[ \left( Q(s,c;\theta) - r \right)^2 \right], \tag{14}$$

where the tuple  $\{(s,c,r)\}$  is stored in the replay buffer  $\mathcal{B}$  and Q is implemented as a neural network. Noting that the reward signal in deep research tasks is binary  $(r \in \{0,1\})$ , we replace the Mean Squared Error (MSE) objective with a cross-entropy (CE) loss, since MSE loss suffers from vanishing gradients near 0/1, whereas CE loss provides more numerically stable signals. Thus, we reformulate the training objective as a binary classification loss:

$$\mathcal{L}(\theta) = \mathbb{E}_{(s,c,r)} \left[ -r \log Q(s,c;\theta) - (1-r) \log \left( 1 - Q(s,c;\theta) \right) \right], \tag{15}$$

where Q can be seen as a normalised value representing the probability  $p(r = 1 | s, c; \theta)$ , i.e., the likelihood that the retrieved case c is a good reference for the current state s given the case bank s. Unlike the non-parametric approach that only preserves new cases, the parametric memory also refines the Q-function during Write, enabling each update to both record a new case and update the overall Q-value landscape.

During retrieval, the learned Q-function is used to compute the retrieval policy distribution via Eq. (7), from which cases can be sampled. To reduce the randomness of case selection and enhance the interpretability of the agent's decision process, the Read operation of the parametric memory applies a TopK operator to select the K cases with the highest Q-values, which are used as planning references:

$$\operatorname{Read}_{P}(s_{t}, M_{t}) = \operatorname{TopK}_{c_{i} \in M_{t}} Q(s_{t}, c_{i}; \theta). \tag{16}$$

By continually updating the Q-function with new samples, the parametric memory module learns to capture the latent patterns between states and cases, thereby producing a closer approximation to the underlying distribution of the case retrieval policy  $\mu^*$ .

# 4.3. Tool Usage

Besides the inherent requirement for long task execution sequences and multi-turn interactions, deep research tasks also place stringent demands on the atomic actions, which require the agent to be able to acquire external information and subsequently process, integrate, and analyse it. Thus, we design a suite of tools for AgentFly accessible via the MCP protocol, comprising modules for information retrieval such as search engines and web crawlers, as well as components for processing and analysing multimodal information, including video and image data, and files in various formats.

**External Information Acquisition.** To support open-ended tasks requiring access to up-to-date external knowledge (e.g., GAIA, BrowseComp), we design a search toolkit that integrates both retrieval and content acquisition capabilities. Specifically, we employ searxng <sup>2</sup>, a self-hosted metasearch engine that aggregates results from multiple sources such as Google <sup>3</sup>, Bing <sup>4</sup>, Duckduckgo <sup>5</sup>, and Brave <sup>6</sup>. Retrieved candidates are then re-ranked based on semantic similarity to the query context, ensuring relevance and precision. To supplement this, we incorporate Crawl4AI <sup>7</sup> to fetch and parse the full web content of selected results when deeper understanding is required by the executor. In other words, the search tool functions as a coarse filter based on keyword matching in the user query, while the crawler serves as a fine-grained mechanism to extract detailed information from the retrieved sources when necessary.

Multimodal Heterogeneous Information Processing. To support downstream reasoning over heterogeneous data sources, we implemented a versatile and fine-grained document processing toolkit that automatically extracts information from a broad spectrum of file types and modalities. For example, images are captioned using a vision-language model (VLM); audio is transcribed via automated speech recognition; PowerPoint files are parsed slide-by-slide with embedded image descriptions; spreadsheets are converted to a readable row-wise layout; archives are unpacked; plain text and code files are read directly; JSON and XML are parsed into structured objects; Word documents are translated into Markdown; and videos receive natural-language summaries from VLMs. For PDFs or unsupported formats, a fallback extraction via Chunkr AI <sup>8</sup> or plain-text parsing is used. This toolkit offers a unified interface for accessing and interpreting content across diverse file types and modalities, streamlining the handling of heterogeneous data in real-world scenarios.

Reasoning. The reasoning and analysis toolkit integrates code execution and mathematical computation to support robust, automated analysis within the AgentFly framework. The Code tool provides a sandboxed environment for writing, running, and managing code within a unified workspace. Users can create files, execute shell or Python commands, and inspect outputs – all within a persistent task directory. Python scripts are validated against a security whitelist to ensure safe execution, supporting commonly used libraries such as numpy, pandas, and torch. The workspace maintains state across steps, enabling iterative development. This agent is crucial for solving data analysis, automation, or dynamic code generation tasks. Complementing this, the Math tool handles fundamental arithmetic operations.

# 5. Experiments

In this paper, we investigate the Deep Research agent, which necessitates tool use and supports multiple rounds of interaction with external, real-world environments. To comprehensively evaluate the agent's capabilities, we select four datasets, each representing a distinct aspect of the research challenge: (i) long-horizon tool use and planning (GAIA) (Mialon et al., 2023), (ii) real-time web-based research (DeepResearcher) (Zheng et al., 2025), (iii) concise factual accuracy (SimpleQA) (Wei et al., 2024), and (iv) exploration at the frontier of human knowledge (HLE) (Phan et al., 2025).

```
2
https://github.com/searxng/searxng-docker
3
https://www.google.com/
4
https://www.bing.com/
5
https://duckduckgo.com/
6
https://brave.com/
7
https://github.com/unclecode/crawl4ai
8
https://chunkr.ai/
```

Method	N	Q	T	Q	Hotp	otQA	2W	/iki	Mus	ique	Bamb	oogle	Pop	QA	A	vg
	F1	PM	F1	PM	F1	PM										
Prompt Based																
CoT	19.8	32.0	45.6	48.2	24.4	27.9	26.4	27.3	8.5	7.4	22.1	21.6	17.0	15.0	23.6	26.1
CoT + RAG	42.0	59.6	68.9	75.8	37.1	43.8	24.4	24.8	10.0	10.0	25.4	27.2	46.9	48.8	37.7	43.2
Search-o1 (Web) (Li et al., 2025c)	32.4	55.1	58.9	69.5	33.0	42.4	30.9	37.7	14.7	19.7	46.6	53.6	38.3	43.4	35.2	45.0
Training Based																
Search-r1-base (Jin et al., 2025)	45.4	60.0	71.9	76.2	55.9	63.0	44.6	47.9	26.7	27.5	56.5	57.6	43.2	47.0	48.3	53.8
Search-r1-instruct (Jin et al., 2025)	33.1	49.6	44.7	49.2	45.7	52.5	43.4	48.8	26.5	28.3	45.0	47.2	43.0	44.5	39.6	45.6
R1-Searcher (Song et al., 2025)	35.4	52.3	73.1	79.1	44.8	53.1	59.4	65.8	22.8	25.6	64.8	65.6	42.7	43.4	47.1	53.7
DeepResearcher (Zheng et al., 2025)	39.6	61.9	78.4	85.0	52.8	64.3	59.7	66.6	27.1	29.3	71.0	72.8	48.5	52.7	51.8	60.5
Ours																
AgentFly (GPT-4.1 + o4-mini)	42.0	74.6	85.5	93.9	66.5	81.6	81.4	94.1	40.6	53.3	86.2	92.8	64.0	72.5	66.6	80.4

**Table 1:** Performance comparison of prompt-based, training-based, and our approach on seven open-domain QA datasets. We report the F1 score and PM scores. The last two columns give the weighted average (*Avg*) across all benchmarks, where Bamboogle contributes 125 examples and every other dataset 512 examples. The results of prompt-based and training-based methods using Qwen2.5 (7B) are referred to *DeepResearcher* (Zheng et al., 2025).

#### 5.1. Datasets

To evaluate the general-purpose reasoning capabilities of AgentFly, we adopt the GAIA benchmark (Mialon et al., 2023), which comprises 450 non-trivial questions with unambiguous answers – 300 in the test set and 150 in the validation set. Each question requires varying levels of tool use and autonomous planning, and the dataset is stratified into three difficulty levels: Level 1: Requires approximately 5 steps using a single tool; Level 2: Requires 5–10 steps involving multiple tools; Level 3: Involves up to 50 steps with no restrictions on the number or type of tools. Each level includes a public validation split and a private test split with hidden ground-truth answers and metadata.

We further evaluate AgentFly on broader benchmarks compiled in DeepResearcher (Zheng et al., 2025), which draws from seven open-domain QA datasets: Natural Questions (NQ) (Kwiatkowski et al., 2019), TriviaQA (TQ) (Joshi et al., 2017), HotpotQA (Yang et al., 2018), 2Wiki (Ho et al., 2020), MusiQue (Trivedi et al., 2022), Bamboogle (Press et al., 2022), and PopQA (Mallen et al., 2022). Each dataset contributes 512 examples, except Bamboogle, which provides 125 high-quality samples curated to minimise contamination and emphasise web-based synthesis.

Additionally, we include two challenging benchmarks: 1) SimpleQA (Wei et al., 2024), consisting of 4,330 fact-seeking questions, focuses on factual accuracy. 2) Humanity's Last Exam (HLE) (Phan et al., 2025), with 2,500 questions across diverse academic subjects, assesses the limits of broad-domain reasoning.

### 5.2. Evaluation Metrics

As each GAIA query has a single reference answer, we follow the GAIA leaderboard and use the Exact Match (EM) metric, which marks a prediction as correct only if it exactly matches the ground-truth answer after standard normalisation (lowercasing, punctuation and article removal, whitespace normalisation). The EM score reflects the percentage of perfectly matched answers.

However, EM cannot accurately reflect the capabilities of an LLM agent, as it overlooks the diversity of expression. We use the macro-F1 score to evaluate the DeepResearcher, SimpleQA, and HLE datasets.

Agent name	Model family	Average score (%)	Level 1 (%)	Level 2 (%)	Level 3 (%)
	Valiadation Datase	t			
AgentFly (Pass@3)	GPT4.1, o3	87.88	96.23	90.70	61.54
Alita	Claude 4 Sonnet, GPT-40	87.27	88.68	89.53	76.92
Skywork Super Agents v1.1	skywork-agent, Claude 3.7 Sonnet, Whisper	82.42	92.45	83.72	57.69
Langfun Agent	Gemini 2.5 Pro	79.39	88.68	80.23	57.69
AWorld	GPT-4o, DeepSeek-V3, Claude 4, Gemini 2.5 Pro	77.58	88.68	77.91	53.85
Manus	-	73.30	86.50	70.10	57.70
OWL-Workforce	Claude 3.7 Sonnet	69.09	84.91	67.44	42.31
OpenAI DeepResearch	03	67.40	74.30	69.10	47.60
OWL-Roleplaying	GPT-4o and o3-mini	58.18	81.13	54.65	23.08
Open Deep Research	o1	55.15	67.92	53.49	34.62
	Test Dataset				
Su Zero Ultra	_	80.40	93.55	77.36	65.31
h2oGPTe Agent v1.6.33	Claude 3.7 Sonnet, Gemini 2.5 Pro	79.73	89.25	79.87	61.22
AgentFly	GPT4.1, o3	79.40	90.32	75.47	71.43
h2oGPTe Agent v1.6.32	Claude 3.7 Sonnet, Gemini 2.5 Pro	79.07	90.32	77.99	61.22
Aworld	GPT-40, DeepSeek-V3, Claude 4 sonnet, Gemini 2.5 Pro	77.08	93.55	76.73	46.94

**Table 2:** Top results on the GAIA Leaderboard as of June 26, 2025, AgentFly achieves the Top-1 performance on the validation set and the test set in open-source agent frameworks.

Meanwhile, Partial Match (PM) indicates the partial semantic match scores between LLMs' generated answers and gold answers. We utilise GPT-40-mini as the answer evaluator to give the scores and the prompt the same as DeepResearcher (Zheng et al., 2025).

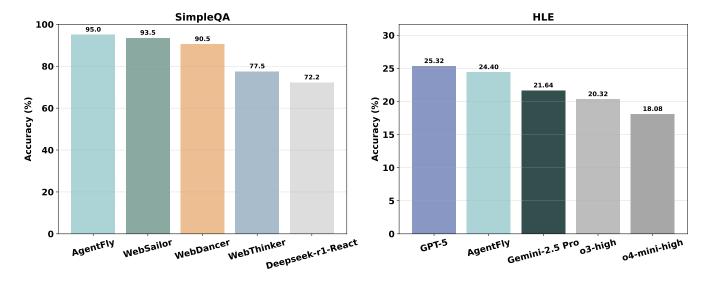
#### 5.3. Model Configurations

The Planner is powered by GPT-4.1, the Executor by o3 for GAIA and o4-mini for other datasets, the image processing by GPT-40, the video agent by Gemini 2.5 Pro and the audio agent by Assembly AI. For the non-parametric CBR, we encode sentences with SimCSE and rank candidate cases using cosine similarity. For the parametric CBR, we initialise sentence representations with SimCSE and implement the Q-function as a two-layer MLP to assign the Q value. Meanwhile, the CBR planner's state at each step often contains information inherited from previous states. To avoid redundant storage, only the state, action, and reward from the final step of each trajectory are written to memory, ensuring that the case bank remains both compact and informative.

The Offline Executor setting refers to one static executor, removing the planner, case memory, and all external tools, so it reflects only raw parametric knowledge from LLMs. The Online Executor starts from that stripped-down baseline but reconnects the same executor to live search and other MCP tools, reflecting the value of real-time retrieval and tool execution. AgentFly (w/o CBR) keeps episodic memory disabled, allowing us to measure the extra gain delivered specifically by case-based reasoning.

### 5.4. Experimental Results

**Deep Researcher.** We include this dataset to test real-time web research, evidence retrieval, cross-page synthesis, and multi-hop reasoning. As shown in Table 1, AgentFly augmented with MCP tools (e.g., search engine, browser) reaches an average 66.6% F1 across the seven DeepResearcher benchmarks, nearly doubling the 37.7% F1 of the CoT + RAG baseline. This demonstrates that real-time, online retrieval tools can rival or



**Figure 4:** Performance on SimpleQA and HLE. The SimpleQA results are from WebSailor (Li et al., 2025b), and the HLE results are from the official website.

even exceed carefully curated static databases.

GAIA (Validation & Test). To assess robustness in long-horizon planning, tool orchestration, and execution, we employ the GAIA benchmark. AgentFly attains the top-1 ranking on the validation set and 4th place on the test set, outperforming most existing agent frameworks (Table 2). Notably, it surpasses widely used open-source frameworks, including Manus (Liang et al., 2025), Aworld (Alibaba, 2025), and OWL (Camel-AI, 2025), on both validation and test sets.

For the GAIA validation evaluation, we initialise memory from scratch and iteratively store both successful and failed trajectories in the case bank over three iterations. Using GPT-4.1 as the planner and o3 as the executor, AgentFly achieves 87.88% accuracy on the validation set. For the GAIA test set, performance is based solely on the case bank accumulated during validation, yielding an accuracy of 79.40%. Although AgentFly demonstrates strong overall performance, challenges remain for Level 3 tasks that require extended reasoning horizons and advanced tool coordination.

Humanity's Last Exam (HLE). To evaluate the frontier of human knowledge and the complex reasoning ability in long-tail, specialised domains, we include the HLE <sup>9</sup>. Using our planner executor architecture, with planner GPT-4.1 and executor o4-mini with tools, AgentFly attains 24.4% PM, ranking second overall and within 0.92 points of GPT-5 at 25.32%, while outperforming Gemini-2.5-Pro at 21.64%, o3-high at 20.32%, and o4-mini-high at 18.08%. These results demonstrate that continual learning through CBR effectively transforms episodic experiences into reusable knowledge, offering a complementary pathway to generalisation even in long-tail domains where conventional tool usage and retrieval methods struggle.

**SimpleQA.** To evaluate AgentFly's reliability and robustness against hallucination in single-hop factual question answering, we employ the SimpleQA benchmark. As illustrated in Figure 4, AgentFly, implemented with a planner–executor framework (GPT-4.1 as the planner and o4-mini as the executor) augmented with tool use, achieves the highest accuracy among all baselines. Specifically, it reaches an accuracy of

<sup>9</sup>https://scale.com/leaderboard/humanitys\_last\_exam

Dataset	K=	=0	K=	=1	K=	=2	K=	=4	K=	=8	K=	:16	K=	:32
	F1	PM												
NQ (Kwiatkowski et al., 2019)	39.5	67.8	41.1	74.4	41.3	72.7	41.9	73.0	41.7	73.8	42.1	73.2	42.2	75.4
TQ (Joshi et al., 2017)	81.1	89.1	86.1	93.8	86.2	93.9	86.3	94.1	85.8	94.1	85.9	94.3	85.5	93.9
HotpotQA (Yang et al., 2018)	62.0	76.0	65.4	80.7	65.7	81.3	67.4	84.2	66.6	82.0	65.5	82.0	66.4	83.2
2Wiki (Ho et al., 2020)	78.3	90.0	81.3	94.9	80.9	94.1	81.0	94.7	82.0	94.5	81.1	93.6	81.0	94.1
Musique (Trivedi et al., 2022)	35.6	43.8	39.8	50.2	40.1	52.1	41.6	51.0	41.0	52.1	39.6	51.4	40.3	50.4
Bamboogle (Press et al., 2022)	77.5	83.2	85.9	91.2	84.1	91.2	84.7	90.4	84.9	91.2	85.2	92.0	83.0	87.2
PopQA (Mallen et al., 2022)	57.9	63.9	62.6	70.1	63.4	71.3	63.6	70.9	62.7	69.2	64.1	70.9	63.2	69.4
Average	59.9	72.2	63.6	77.9	63.7	78.1	64.5	78.5	64.1	78.2	63.9	78.1	63.9	78.1

**Table 3:** The performance of AgentFly on the DeepResearcher dataset across different numbers of cases. We use gpt-4.1 as the planner and o4-mini as the executor.

Method	Iter 1	Iter 2	Iter 3	Iter 4	Iter 5					
	Baseline									
AgentFly w/o CBR	78.65	80.93	82.62	83.53	84.47					
Case-based Continual Learning										
AgentFly w/ Non-Parametric CBR AgentFly w/ Parametric CBR	79.84 <b>80.46</b>	81.87 <b>82.84</b>	83.09 <b>84.10</b>	84.03 <b>84.85</b>	84.85 <b>85.44</b>					

**Table 4:** Performance improvement of AgentFly over five learning iterations on the DeepResearcher dataset, demonstrating the benefit of accumulating cases in the Case Bank.

95.0%, outperforming WebSailor (93.5%), WebDancer (90.5%), WebThinker (77.5%), and DeepSeek-r1-React (72.2%). These results demonstrate that AgentFly provides strong factual reliability and substantially mitigates hallucination on straightforward single-hop queries, establishing a new state-of-the-art over prior web-agent baselines.

#### 5.5. Ablation Studies

We analyse AgentFly's hyper-parameter selection, component-wise Analysis, learning curves for both parametric and non-parametric case-based reasoning, out-of-distribution performance, and token costs.

# 5.5.1. Hyper-parameter Selection

Increasing the number of retrieved cases in CBR raises computational cost and can introduce noise from irrelevant examples. To evaluate this, we vary K in 0, 2, 4, 8, 16, 32 on the DeepResearcher dataset. As shown in Table 3, performance improves up to K = 4 – yielding the highest F1 (64.5) and PM (78.5) – but plateaus or slightly declines for larger K. This suggests that CBR benefits from a small, high-quality memory, unlike few-shot prompting, where more examples often help (Agarwal et al., 2024). Careful case selection and memory curation are thus crucial for continual learning.

#### 5.5.2. Component-wise Analysis

From Table 5, we observe a consistent pattern across HLE, SimpleQA, and DeepResearcher. Moving from an offline executor to live tools generally reduces hallucination and increases both F1 and PM, though the

Model	Humanities/SC	Math	Chemistry	Other	Physics	Engineering	Biology/Medicine	CS/AI	Avg
Offline Executor	5.2/9.6	7.1/5.8	2.3/7.9	2.9/11.4	7.6/4.6	12.8/14.0	5.2/17.7	6.5/11.9	6.4/8.7
Online Executor	10.8/24.9	13.1/16.0	6.9/9.3	14.0/16.3	7.8/10.2	7.5/5.3	5.7/17.2	13.3/15.4	11.2/15.8
AgentFly w/o CBR	25.5/29.2	24.9/16.3	17.4/21.1	24.8/24.1	18.4/10.8	15.8/8.8	10.0/18.7	25.4/12.4	22.2/17.4
AgentFly	28.4/33.0	30.9/24.2	18.7/22.7	28.5/32.4	22.9/19.1	15.9/12.1	14.0/26.1	28.5/18.5	26.7/24.4

#### (a) HLE

Model	Art	Geography	Science & Tech	Politics	Sports	Other	TV Shows	Music	History	Video Games	Avg
Offline Executor	16.5/19.6	25.7/31.1	20.1/24.7	25.8/24.8	18.8/19.0	15.8/14.9	12.6/13.3	15.7/17.6	25.9/26.6	15.5/13.3	19.7/21.5
Online Executor	49.7/82.9	45.1/82.5	59.4/87.7	51.6/86.9	46.6/90.1	48.7/86.4	39.5/84.3	43.1/88.5	49.7/83.8	34.7/78.6	48.5/84.8
AgentFly w/o CBR	83.8/92.2	71.8/84.9	87.1/94.1	83.7/90.8	77.4/86.4	81.2/90.7	70.0/81.6	80.7/89.1	79.1/86.1	81.2/88.9	81.0/89.7
AgentFly	86.9/96.4	76.6/91.7	89.3/96.9	87.1/95.6	82.2/93.5	84.2/95.4	77.3/90.8	83.3/95.0	85.7/94.8	86.3/95.6	84.7/95.0

#### (b) SimpleQA

Method	NQ	TQ	HotpotQA	2Wiki	Musique	Bamboogle	PopQA	Avg
Offline Executor	39.7/70.1	75.8/89.1	50.7/67.2	44.8/56.0	26.9/35.7	76.0/84.0	48.0/53.5	48.8/62.8
Online Executor	23.3/55.3	41.9/80.7	34.4/67.8	33.6/66.2	23.0/39.7	45.8/77.6	24.9/50.2	30.8/60.7
AgentFly w/o CBR	39.5/67.8	81.8/89.1	62.0/76.0	78.3/90.0	35.6/43.8	77.5/83.2	57.9/63.9	59.9/72.2
AgentFly	42.0/74.6	85.5/93.9	66.5/81.6	81.4/94.1	40.6/53.3	86.2/92.8	64.0/72.5	66.6/80.4

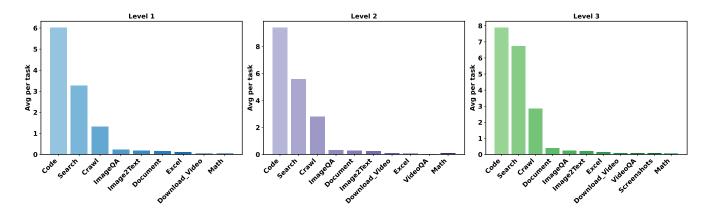
#### (c) DeepResearcher

**Table 5:** Ablation results across three benchmarks. Each cell shows F1/PM. We use gpt-4.1 as the planner and o4-mini as the executor.

magnitude depends on task type (SimpleQA:  $+28.8 \, \text{F1} / +63.3 \, \text{PM}$ , HLE: +4.8 / +7.1), and may even hurt on open-domain data (DeepResearcher: -18.0 / -2.1). Introducing planning (AgentFly w/o CBR) yields robust gains on each benchmark (HLE: +11.0 / +1.6, SimpleQA: +32.5 / +4.9, DeepResearcher: +29.1 / +11.5), indicating that explicit decomposition and tool orchestration systematically improve execution. Finally, case-based reasoning provides consistent, additive improvements (HLE: +4.5 / +7.0, SimpleQA: +3.7 / +5.3, DeepResearcher: +6.7 / +8.2). For HLE, however, without sufficient domain knowledge encoded in the backbone model, neither tool usage nor planning alone can reliably produce correct answers on long-tail, expert-level tasks. For DeepResearcher, we also identify data contamination (Shumailov et al., 2024) across the seven evaluated benchmarks, evidenced by a noticeable drop in both F1 and PM when moving from the offline executor to the online executor without planning (DeepResearcher:  $-18.0 \, \text{F1} / -2.1 \, \text{PM}$ ). This aligns with broader findings in the field (Sun et al., 2022, Yu et al., 2022, Zhou et al., 2025): simply using external knowledge can sometimes negatively affect the model, while the internal knowledge within the model plays an important role in QA tasks and can even outperform RAG.

# 5.5.3. Continual Learning Ability Boosted by Parametric and Non-Parametric CBR

Figure 1c and Table 4 present the continual learning curves across different memory designs for the AgentFly framework, comparing the performance of three configurations: AgentFly with non-parametric CBR or parametric CBR and AgentFly without CBR. The results demonstrate that the full AgentFly architecture consistently outperforms the ablated versions across all iterations, achieving higher accuracy at each step. Notably, removing CBR leads to a noticeable decline in performance, highlighting the effectiveness and complementary benefits of both parametric CBR and non-parametric CBR components in enhancing the



**Figure 5:** The average number of each task type per level, highlighting the dominance of code, search, and crawl tasks as difficulty level increases.

continual learning capability of AgentFly. More importantly, we observe a learning curve of the accuracy on the DeepResearcher dataset with increased iterations, suggesting that memory-based approaches can effectively enhance LLM agents without requiring parameter updates.

Although we attempted to locate any performance drops along the learning curve, in practice, such inflexion points are elusive. With only about 3k training data, the Case Bank saturates quickly. Each additional iteration, therefore, contains progressively fewer previously unseen (and thus potentially failing) cases. In our simulated, open-ended, but ultimately finite environment, we observe rapid convergence with only marginal gains after a few iterations. Consequently, adding many more iterations yields diminishing returns and contributes little to our understanding of memory-based continual learning.

# 5.5.4. Generalisation across Tasks

To assess out-of-distribution (OOD) generalisation, we follow the evaluation protocol of Zheng et al. (2025). Specifically, MusiQue (Trivedi et al., 2022), Bamboogle (Press et al., 2022), and PopQA (Mallen et al., 2022) are selected as OOD datasets due to their distinct question styles and information distributions, while NQ (Kwiatkowski et al., 2019), TQ (Joshi et al., 2017), HotpotQA (Yang et al., 2018), and 2Wiki (Ho et al., 2020) are used for training. We first collect and store trajectories from the training datasets in the case bank. During inference, AgentFly retrieves the four most relevant cases from the case bank for each target query. As shown in Figure 1d, AgentFly achieves substantial improvements on all OOD benchmarks, with absolute gains ranging from 4.7% to 9.6%. These results highlight the effectiveness of case-based reasoning in enhancing generalisation to unseen tasks.

# 6. Discussion and Analysis

Building on the results in § 5 that establish the effectiveness of AgentFly, we further analyse its efficiency and operational behaviour. Specifically, we (i) analyse the average number of tool calls per task across three difficulty levels to assess how the MCP framework adapts as task complexity increases, (ii) characterise tool-call statistics, and (iii) evaluate the impact of using reasoning-oriented versus general-purpose models.

Planner	Executor	Level 1	Level 2	Level 3	Average
gpt-4.1	о3	77.36%	69.77%	61.54%	70.91%
o3	o3	73.58%	63.95%	38.46%	63.03%
Qwen3-32B-Fast	o4-mini	62.26%	56.98%	26.92%	53.94%
Qwen3-32B-Slow	o4-mini	56.60%	36.05%	23.08%	40.61%

**Table 6:** The impact of fast and slow think mode on GAIA valiadation dataset (pass@1).

# 6.1. The Number of Tokens per Task

As shown in Figure 5, code, search, and crawl tasks dominate across all levels, with their usage increasing notably as difficulty rises. Importantly, while overall tool usage grows with task complexity, the most challenging problems increasingly rely on the model's internal reasoning to interpret and aggregate evidence from prior tool outputs, rather than simply calling more tools via MCP. This highlights the importance of effective integration between planning, memory, and evidence aggregation for solving open-ended, long-horizon deep research tasks.

#### 6.2. Statistics of MCP Tools

As shown in Figure 6, we randomly sample 10 tasks from the GAIA validation, respectively, to calculate the tokens and costs per task. Average response tokens rise sharply with task difficulty: Level 1 queries required 26k input tokens and 4.7k output tokens, Level 2 grew to 48k/6.9k, and Level 3 peaked at 121k/9.8k. This highlights that the primary computational burden in complex scenarios stems from integrating and analysing multi-step tool outputs, rather than from generating long responses.

We observe that the output tokens remain stable across task levels, as the final answers typically require only short responses. This demonstrates that our system effectively controls generation length and avoids unnecessary verbosity during inference. However, due to the

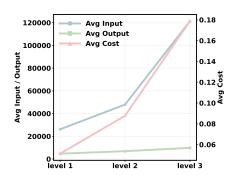


Figure 6: Token costs on the GAIA.

complexity and unpredictability of real-world environments, the input context grows significantly with task difficulty. As tasks become more complex, more detailed observations, plans, tool outputs, and intermediate reasoning steps must be incorporated into the input prompts, resulting in a substantial increase in the number of input tokens.

# 6.3. The Impact of Fast and Slow Think Mode

Table 6 compares the impact of fast- and slow-thinking planners on overall system performance (pass@1) across different task difficulties. The results show that pairing the fast, non-deliberative GPT-4.1 planner with the o3 executor yields the highest average accuracy (70.9%), outperforming the more deliberative o3 planner (63.03%) even when both use the same executor. Similarly, when using the o4-mini executor, GPT-4.1 achieves a substantial 16.4% improvement over o3. The Qwen3-32B models further confirm this trend, with the fast planner consistently outperforming its slow counterpart.

Analysis of system traces reveals several key reasons for the fast planner's superiority. The planner relying on the o3 model often either answers directly – skipping plan generation altogether – or produces overly verbose plans, which can mislead the executor with incomplete instructions. Additionally, in complex multi-step reasoning fields, the slow planner tends to compress solutions into a single, convoluted chain of thought, while the fast planner effectively decomposes problems into manageable sub-tasks.

Overall, these findings highlight that in modular LLM systems, concise and structured planning leads to more effective downstream execution. Overly deliberative planning not only introduces unnecessary context and redundancy but also induces role confusion, thereby undermining the very specialisation that the two-stage architecture is designed to exploit.

# 7. Conclusion

We introduce AgentFly, a memory-based learning paradigm that enables LLM agents to adapt online search without updating model weights. AgentFly formalises deep research agents as a memory-based Markov Decision Process (MDP) and implements it within a planner–executor framework, leveraging an episodic case bank to record and retrieve trajectories for continual policy improvement. Empirically, we achieve strong performance across GAIA, DeepResearcher, and SimpleQA. Ablation studies reveal that both parametric and non-parametric CBR are critical to the significant performance gains, and that a small, curated memory yields optimal results. These findings motivate future work on deep research tasks using memory-based MDP.

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# A. Derivation of the Optimal Policy in Soft-Q Learning

The soft value function over the state *s* is defined as:

$$V^{\pi}(s, M) = \sum_{c \in M} \mu(c|s, M) [Q^{\pi}(s, M, c) - \alpha \log \mu(c|s, M)]$$
 (17)

The Q function over the state, case pair is defined as:

$$Q^{\pi}(s, M, c) = \mathbb{E}_{a \sim p_{\text{LLM}}(\cdot | s, c), s' \sim \mathcal{P}(\cdot | s, a)} \left[ r(s, a) + \gamma V^{\pi}(s', M') \right], \tag{18}$$

Define the visitation frequency over the state, case bank for the policy  $\pi$  as:  $d^{\pi}(s, M) = \sum_{t=0}^{\infty} \gamma^{t-1} \mathbb{P}(s_t = s, M_t = M)$ . Then, our goal is to derive the optimal retrieval policy by expected value function:

$$J_{\text{MaxEnt}}(\pi) = \mathbb{E}_{(s,M)\sim d^{\pi}} \left[ V^{\pi}(s,M) \right],$$

$$= \mathbb{E}_{(s,M)\sim d^{\pi}} \left[ \sum_{c\in M} \mu(c|s,M) \left[ Q^{\pi}(s,M,c) - \alpha \log \mu(c|s,M) \right] \right]$$
(19)

For simplicity, let  $\mu_c = \mu(c|s, M)$  and  $Q_c = Q^{\pi}(s, M, c)$ , and introduce the Lagrange multiplier  $\lambda$  to constrain that  $\sum_c \mu_c = 1$ . Then, for any state, case bank pair, we have the optimisation objective:

$$\mathcal{J}(\{\mu_c\}, \lambda) = \sum_c \mu_c Q_c - \alpha \sum_c \mu_c \log \mu_c - \lambda (\sum_c \mu_c - 1), \tag{20}$$

whose derivative concerning  $\mu_c$  is:

$$\frac{\partial \mathcal{J}(\{\mu_c\}, \lambda)}{\partial \mu_c} = Q_c - \alpha (1 + \log \mu_c) - \lambda, \tag{21}$$

Let  $\frac{\partial \mathcal{J}(\{\mu_c\},\lambda)}{\partial \mu_c} = 0$ , then we have:

$$\mu_c = \exp(\frac{Q_c}{\alpha} - (\frac{\lambda}{\alpha} + 1))$$

$$= K \exp(\frac{Q_c}{\alpha}),$$
(22)

where  $K = \exp(-\frac{\lambda}{\alpha} - 1)$ . Thus, by performing the normalisation and shaping the optimal Q, we have:

$$\mu_c^* = \frac{\exp(Q_c^*/\alpha)}{\sum_{c'} \exp(Q_{c'}^*/\alpha)}.$$
 (23)

Note that when  $\alpha \to 0$ , the soft Q learning deteriorates to standard Q-learning. The softmax form of the policy is also used in previous LLM-based agents with LLM prior (Yan et al. (2025)).

# B. Analysis of Memory Mechanisms

Method	Kernel	Neural Q	Q-Function	Read	Write	Gradient
Tabular Q-learning	w/o	w/o	Q-Table	Exact Match	Eq. (8)	-
Deep Q-learning	w/o	w/	Neural Network	Eq. ( <mark>7</mark> )	Eq. (24)	Eq. (25)
Neural Episodic Control	w/	w/o	Eq. (9)	Eq. ( <mark>7</mark> )	Eq. (10)	Eq. (11)
Non-Parametric Memory in Sec. 4	w/o	w/o	w/o	Eq. (13)	Eq. (12)	-
Parametric Memory in Sec. 4	w/o	w/	Neural Network	Eq. (16)	Eq. (15)	Eq. (26)

**Table 7:** Detail comparison of memory mechanisms.

Here, we consider several representative memory mechanisms, emphasising their Read and Write operations as summarised in Table 7. Specifically, we discuss tabular and parametric Q-value representations, as well as EC-based methods.

In the tabular setting, the memory maintains an explicit table  $Q: \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ , where Read is a direct lookup of table Q(s, M, a) and Write corresponds to updating the entry for the state–action pair after observing a transition, following the standard TD learning in Eq. (8). To extend beyond discrete spaces, deep Q-learning learns the Q function by a neural network  $Q(s, M, a; \theta)$ , with Read operation sampling cases from the retrieval policy  $\mu$  following Eq. (7) and Write operation updates the parameters  $\theta$  via minimising the TD error:

$$\mathcal{L}(\theta) = \mathbb{E}_{(s,c,r,s',M,M')} \left[ \left( Q(s,M,c;\theta) - \left[ r + \gamma \alpha \log \sum_{c' \in M'} \exp \left( Q\left( s',M',c';\bar{\theta} \right) \right) \right] \right)^2 \right], \tag{24}$$

where  $\bar{\theta}$  is the target Q network. The gradient of the TD learning loss with respect to  $\theta$  is given by:

$$\nabla_{\theta} \mathcal{L}(\theta) = 2\mathbb{E}_{(s,c,r,s',M,M')} \left[ (Q(s,M,c;\theta) - y) \nabla_{\theta} Q(s,M,c;\theta) \right], \tag{25}$$

where  $y = r + \gamma \alpha \log \sum_{c' \in M'} \exp(Q(s', M', c'; \bar{\theta}))$ . This parametric formulation enables generalisation across states and action spaces through the shared parameters  $\theta$ , in contrast to tabular methods, which only memorise individual entries. However, this benefit comes at the cost of optimisation instability and large data demand, since approximation errors may propagate globally through the parameter space. This limitation motivates the EC-based methods in Section 3, where value estimation is regularised through a learnable kernel (see Eq. (9)). Within this memory design, the Read operation samples cases from the retrieval policy distribution defined in Eq. (7) while the Write operation additionally store (s, c, Q) into an episodic memory and updates the kernel parameters  $\theta$  by Eq. (10) with gradient in Eq. (11) optimising the weighting function. This approach only parameterises the kernel to regularise the historical Q-values of matched states, thereby ensuring generalisation across the state space while retaining data-efficient adaptation and improved stability compared with deep Q-learning.

In section 4, the CBR agent is implemented as a planner, applying both non-parametric and parametric memory mechanisms. For the non-parametric variant, the Write operation appends each observed case  $(s_t, a_t, r_t)$  into the case bank as in Eq.(12), while the Read operation retrieves the most relevant experiences by performing cosine-similarity matching between the current query embedding and stored states, followed by a TopK selection as in Eq. (13). This similarity-based retrieval, without further parameterisation,

is a common design in CBR and provides an effective means of reusing past experiences. Alongside the non-parametric approach, the single-step nature of the deep research setting permits fitting a parametric Q-function directly, as the reduced state space substantially lowers data requirements. In the single-step case, the temporal-difference bootstrap vanishes, so the learning objective reduces to Eq.(14). Furthermore, since the reward signal in the deep research scenario is binary, we replace the MSE objective with a CE loss. This choice avoids the vanishing-gradient problem near the boundaries 0 and 1, while providing more numerically stable training signals. Consequently, the final updating objective is reformulated as a binary classification loss in Eq.(15), and the resulting gradient is as follows:

$$\nabla_{\theta} \mathcal{L}(\theta) = \mathbb{E}_{(s,c,r)} \left[ \frac{Q(s,c;\theta) - r}{Q(s,c;\theta)(1 - Q(s,c;\theta))} \nabla_{\theta} Q(s,c;\theta) \right]. \tag{26}$$

To further stabilise case selection, we also apply a TopK operator in the parametric Read operator Eq. (16) rather than sampling from the retrieval policy  $\mu$ .