TOWARDS UNIFIED ALIGNMENT BETWEEN AGENTS, HUMANS, AND ENVIRONMENT

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ABSTRACT

The rapid progress of foundation models has led to the prosperity of autonomous agents, which leverage the universal capabilities of foundation models to conduct reasoning, decision-making, and environmental interaction. However, the efficacy of agents remains limited when operating in intricate, realistic environments. In this work, we introduce the principles of Unified Alignment for Agents (UA^2) , which advocate for the simultaneous alignment of agents with human intentions, environmental dynamics, and self-constraints such as the limitation of monetary budgets. From the perspective of UA^2 , we review the current agent research and highlight the neglected factors in existing agent benchmarks and method candidates. We also conduct proof-of-concept studies by introducing realistic features to WebShop (Yao et al., 2022a), including user profiles to demonstrate intentions, personalized reranking for complex environmental dynamics, and runtime cost statistics to reflect self-constraints. We then follow the principles of UA^2 to propose an initial design of our agent, and benchmark its performance with several candidate baselines in the retrofitted WebShop. The extensive experimental results further prove the importance of the principles of UA^2 . Our research sheds light on the next steps of agent research with improved problem-solving abilities.

1 INTRODUCTION

Recent days have witnessed the rapid development of autonomous agents, which leverage the proficiency of Large Language Models (LLMs) or Large Multimodal Models (LMMs) (OpenAI, 2023; Touvron et al., 2023; Team et al., 2023; Jiang et al., 2024) to interact with environments for task execution. Several seminal works on foundation model agents have exhibited promising results in both digital and embodied scenarios, including but not limited to web task automation (Deng et al., 2023; Zhou et al., 2023b; Zheng et al., 2024), open-ended world exploration (Wang et al., 2023a; Zhu et al., 2023), interactive coding (Chen et al., 2023c; Qian et al., 2023; Xu et al., 2023), and robotic tasks (Ahn et al., 2022; Mirchandani et al., 2023; Huang et al., 2023b; Ma et al., 2023; Wang et al., 2023b).

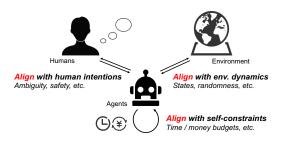


Figure 1: A working system of agents that consists of three roles: humans to be assisted, an environment to interact with, and the agents themselves. The principles of Unified Alignment for Agents (UA^2) suggest that the agents should align with the three roles in a unified manner by recognizing *human intentions*, adapting to *environmental dynamics*, and adhering to *self-constraints*.

Aside from existing literature, the development of foundation model agents in realistic, complex scenarios is still in its infancy. While different agent benchmarks have been proposed (Liu et al., 2023b; Mialon et al., 2023; Ma et al., 2024), the methodologies of agents are still being proposed and evaluated in synthetic, simplified settings, which results in the bottlenecked performance of agents in real-world deployment when attempting to satisfy the expectations of humans with realistic demands (Kinniment et al., 2023). This naturally leads to the question: *What are the principles that the agents should follow to improve their real-world capabilities?*

To answer the question, we first take a systematic view of agents during the operation. We recognize the working system of agents as a composition of three roles: *humans* that propose the goals to be assisted, an *environment* that provides feedback for interaction, and foundation model *agents* themselves to act in the environment to assist the human user. In complex scenarios, the intentions of humans can be ambiguous (Tamkin et al., 2022; Li et al., 2023a) or concerned with safety requirements (Ruan et al., 2023; Yuan et al., 2024). Moreover, the underlying dynamics of the environment can be complicated to identify (LeCun, 2022; Hu & Shu, 2023), and affected by temporality (Fan et al., 2022) or stochasticity (Wu et al., 2023). Last but not least, the agents themselves can also be constrained by a certain amount of budgetary limits (*e.g.*, monetary and time expenses) during operations, an aspect often overlooked in the existing agent research. While each of the aspects is noted by different aforementioned works, none of them emphasize the holistic comprehension of all the roles in the working system.

In this work, we propose the principles of Unified Alignment for Agents (UA^2) by drawing connections with the alignment research in the sense of both LLMs and reinforcement learning literature (Sutton & Barto, 2018; Ouyang et al., 2022; Bai et al., 2022; Ji et al., 2023; Burns et al., 2023). The goal of UA² is to enhance the awareness of the foundation model agents to their working system, aligning with *human intentions, environmental dynamics*, and *self-constraints* in a unified manner. From the perspective of UA², we review the existing research on agents and point out the neglected factors in the design of existing benchmarks and candidate methodologies of agents.

To further demonstrate the essence of UA^2 , we conduct proof-of-concept studies by constructing an upgraded version of WebShop (Yao et al., 2022a). In the retrofitted WebShop, we add the design of the *human intentions* of shoppers for agents to track and infer, the *environmental dynamics* with personalized re-ranking algorithms that evolve with agent actions, and the *self-constraints* by implementing a counter of monetary and temporal costs. On top of the retrofitted environment, we initiate an agent method guided by the principles of UA^2 , and benchmark its performance as well as several other candidate agent baselines. The results reveal the suboptimality of the agent baselines that violate the principles of UA^2 . The results further support our advocacy that the agents should achieve a unified alignment with humans, the environment, and the agents themselves. Our research sheds light on the future steps of autonomous agents, including synergizing agents with alignment techniques, constructing agent benchmarks and methods that follow the principles of UA^2 , and envisioning self-evolving agents through lifelong interaction and continual alignment.

2 PRINCIPLES OF UNIFIED ALIGNMENT FOR AGENTS

2.1 ROLES IN A WORKING SYSTEM OF AGENTS

A working system of agents consists of three roles (Figure 1): agents, humans, and the environment.

Agents are the core component of the entire system. Agents are responsible for understanding human intentions and generating appropriate responses or actions to interact with the environment. Proficient agents should provide accurate, informative, and engaging interactions during task execution.

Humans are the main role to be assisted in the system. The tasks assigned by humans can be viewed as the initial inputs to the working system, which reflects the underlying goals and human intentions.

Environment refers to the situation where the agents operate. It encompasses the external factors and conditions that can influence the agents' behavior, performance, and interactions. The feedback from the environment affects the reasoning of the agents, as well as their following actions.

Realistic working systems of agents are composed of diverse, ambiguous human intentions, changing environments with complex dynamics, as well as self-constraints over the agents themselves. This leads to the necessity of agents to operate towards the unified alignment with all the roles.

2.2 UNIFIED ALIGNMENT WITH ALL THE ROLES

While three distinct roles exist in a working system of agents, we argue that the agents should align with all the roles in a unified manner. To promote the orchestration of agents, humans, and the environment, the agents should work in the direction of eliminating the gap between agents and

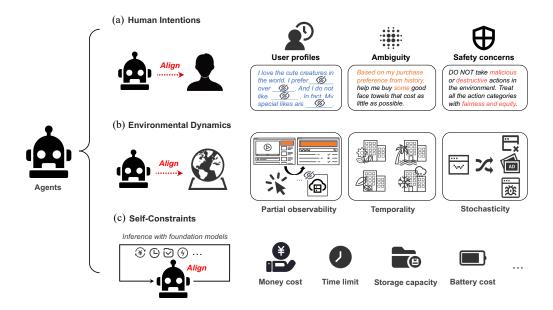


Figure 2: Illustrations of the principles of unified alignment with (a) *human intentions*, (b) *environmental dynamics*, and (c) *self-constraints*. The principles of unified alignment for agents emerge from all the roles in an agent working system: agents, humans, and environment.

humans, agents and the environment, as well as adapting to the constraints imposed on the agents themselves. Based on this, we propose the principles of Unified Alignment for Agents (UA^2) :

- 1. Alignment with *human intentions*. The agents need to correctly recognize the intentions of the human users. While the goal is usually specified with a textual sentence, the ambiguity of language expression can affect the understanding and decision-making of agents.
- 2. Alignment with *environmental dynamics*. The agents need to interact with the environment to achieve the goal required by human users. To succeed, the agents should raise their awareness of the operation laws of the environment. This is also advocated in (LeCun, 2022; Hu & Shu, 2023) that proposes to incorporate a world model into an agent system.
- 3. Alignment with *self-constraints*. The underscored factor of current agent research comes from the constraints imposed on the agents themselves, including time/money budget limits. For foundation model agents, the underlying models (*e.g.*, proprietary LLMs/LMMs) are costly for inference, which hurdles the performance in realistic scenarios.

2.3 Challenges from the Principles of UA^2

Figure 2 illustrates the principles of UA^2 . In this section, we pose the challenges raised from UA^2 .

Challenges in the alignment with *human intentions.* When the interaction between humans and the agent is a single-turn process, it is equivalent to LLM alignment (Ouyang et al., 2022) in the form of a prompt-response pair. However, in realistic settings, human intentions are often not perfectly covered in a single prompt, but rather reflected by preferences not directly visible from instructions (*e.g.*, personal preferences and safety concerns). Challenges arise for the agents to infer authentic human intentions with multiple turns of interactions by either eliciting human preferences (Li et al., 2023a), or learning to self-correct from environmental feedback (Huang et al., 2023a), or both.

Challenges in the alignment with *environmental dynamics*. The interactive environments for agents in realistic scenarios can be highly complicated, which requires the agent to recognize the hidden state from the history of observations. Considering the dynamics function $\mathbf{s}_{n+1} \sim \pi(\mathbf{s}_n, \mathbf{a}_n)$ where \mathbf{s}_n and \mathbf{a}_n stand for the *n*-th step state and action, respectively, its complexity includes:

Partial observability. This is reflected by the complexity of the function that transforms the historical observations {o_{<n}} into the authentic state of the current step s_n.

Туре	Benchmarks	Human Intentions	Environmental Dynamics	Self-Constraints
	Androidenv (Toyama et al., 2021)	None	Partial Obs.	None
	WebShop (Yao et al., 2022a)	None	Full Obs. [†]	None
Digital	Mind2Web (Deng et al., 2023)	None	Partial Obs.	None
	ToolBench (Qin et al., 2023)	None	Full Obs. & Temp. & Stoch.	None
	WebArena (Zhou et al., 2023b)	Fixed and Given	Partial Obs.	None
	VirtualHome (Puig et al., 2018)	None	Partial Obs.	None
	BabyAI (Chevalier-Boisvert et al., 2019)	None	Partial Obs.	None
	ALFWorld (Shridhar et al., 2020)	None	Partial Obs.	None
	MineDojo (Fan et al., 2022)	None	Partial Obs. & Stoch.	None
Embodied	ScienceWorld (Wang et al., 2022a)	None	Partial Obs.	None
Embouleu	Interactive Gibson (Xia et al., 2020)	None	Partial Obs.	#Actions
	AGENT (Shu et al., 2021)	None	Partial Obs.	#Actions
	RFUniverse (Fu et al., 2022)	Fixed and Given	Partial Obs.	#Actions
	BEHAVIOR-1K (Li et al., 2023b)	None	Full Obs.	#Actions
	HAZARD (Zhou et al., 2024)	None	Partial Obs. & Temp.	#Actions
	SmartPlay (Wu et al., 2023)	None	Partial Obs. & Stoch.	None
Mixed	AgentBench (Liu et al., 2023b)	None	Partial Obs.	None
	AgentBoard (Ma et al., 2024)	None	Partial Obs. & Temp. & Stoch.	None

Table 1: Existing agent benchmarks from the perspective of alignment with *human intentions, environmental dynamics*, and *self-constraints*. "Temp." stands for temporality, and "Stoch." stands for stochasticity. "#Actions" means that the step count in the environment will be reported as a metric. † WebShop is fully observable as long as the URL is covered in each observation.

- Time-variant property. This is reflected by the temporal effect in the dynamics function, where the evolution of time t leads to the variation of $\mathbf{s}_{n+1} \sim \pi(\mathbf{s}_n, \mathbf{a}_n, t)$.
- Stochasticity. The $\pi(\mathbf{s}_n, \mathbf{a}_n)$ can be interlaced with (nearly) independent random events.

In this way, constructing a precise world model for an agent system requires delicate techniques beyond ad-hoc exploration, coarse-grained memory, or ungrounded planning.

Challenges in the alignment with *self-constraints*. The self-constraints of agents are the oftenoverlooked desiderata in the design of existing agent methodologies. Taking the budgetary limits into account, the agent system should re-use the accumulated experiences during the lifelong learning process (Majumder et al., 2023), and balance the resources invested in the different learning modules. Furthermore, in scenarios where the self-constraints change with different episodes, additional challenges emerge for the agents to adapt to the constraints autonomously.

3 LITERATURE REVIEW FROM THE LENS OF UA²

3.1 BENCHMARKS

In this section, we begin with a comprehensive review of current benchmarks in agent research, from the perspective of UA^2 . Representative benchmarks in both digital (Toyama et al., 2021; Yao et al., 2022a) and embodied (Puig et al., 2018; Chevalier-Boisvert et al., 2019) environments are summarized in Table 1. By rendering realistic simulations (Puig et al., 2023; Szot et al., 2021) and carefully configured tasks (Li et al., 2023b), current benchmarks offer diverse environments for both language-based and embodied agents (Xi et al., 2023) to operate and interact within (Maes, 1995). Instead of focusing on environmental authenticity (Fu et al., 2022) or general task complexity, we assess the benchmarks prioritizing the alignment principles of UA^2 . In practice, we consider the following three aspects:

- 1. *Human intentions*: Whether the authentic goals need to be inferred during task execution, or the intentions of humans are precisely conveyed in the descriptions.
- 2. *Environmental dynamics*: Whether the state transitions of the environment are intrinsically endowed with partial observability, temporality, or stochasticity.
- 3. *Self-constraints*: Whether the status of budgetary resources is reflected, including time consumption, the maximum number of actions or reasoning steps, etc.

In terms of human intentions, most benchmarks (Qin et al., 2023; Liu et al., 2023b) provide explicit task instructions for more effective evaluation, rather than considering human intentions as hidden

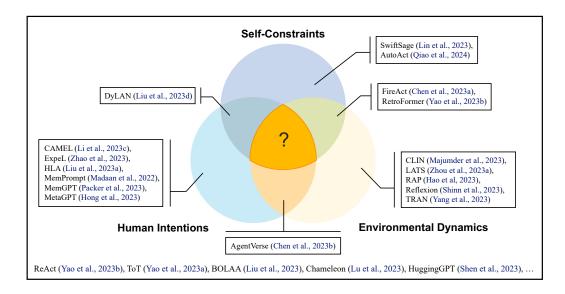


Figure 3: The dissection of alignment endeavors for different representative agent techniques. Generally speaking, the methods that actively coordinate with humans excel at aligning with *human intentions*. The methods that are grounded with external feedback from the environment align well *environmental dynamics*. The methods that adopt adaptive strategies or fine-tuning demonstrate better alignment with *self-constraints*. While the advanced techniques mostly align with one role or two in the working system of agents, much room lies in the quest for UA^2 .

attributes for agents to discover. By incorporating human interactions, several embodied simulators (Puig et al., 2023; Xia et al., 2019) facilitate tasks with vague goal descriptions (Paul et al., 2022; Liu et al., 2023c), necessitating agents to engage with humans to gather sufficient information for task completion. In contrast, digital benchmarks hardly account for this aspect. The most relevant digital environment in this aspect is WebArena (Zhou et al., 2023b), which deliberately defines consistent human intentions across episodes. However, the intentions are also explicitly stated in the instructions, which bypasses the intention elicitation process of agents with humans.

The benchmarks for agents are designed to mirror the complexities of the real-world dynamics (Puig et al., 2023). Most benchmarks assume the environment is partially observable where agents are required to accomplish tasks through exploration and interaction (Xia et al., 2020). Some benchmarks also include stochastic factors (Wu et al., 2023; Zhou et al., 2024) or evolve with time (Qin et al., 2023). Nevertheless, the synthesis of fine-grained realistic dynamics remains underdeveloped in benchmark design, resulting in the lack of evaluations of agent methodologies therein.

As for *self-constraints*, embodied benchmarks (Xia et al., 2020; Li et al., 2023b) use the number of actions as a metric to reflect the operational cost in real-world deployments, such as the path length in navigation tasks (Anderson et al., 2018). In this context, AGENT (Shu et al., 2021) further explicitly evaluates the trade-offs between cost and reward. However, existing digital benchmarks overlook cost and time constraints in the assessments, which should be equally important.

In essence, existing agent benchmarks are still inadequate from the lens of UA^2 . In general, the development of digital benchmarks lags behind that of embodied benchmarks. This underscores the need for more realistic environments to enhance the development of agent techniques.

3.2 Methods

In this section, we review the representative agent methods. For each method, we investigate whether it actively seeks alignment with *human intentions, environmental dynamics*, or *self-constraints*.

To align with *human intentions*, the agent methods should coordinate with humans through reasoning or experience summarization. HLA (Liu et al., 2023a) and MemPrompt (Madaan et al., 2022) interact with humans for multiple rounds to solicit authentic human intentions. Multi-agent frameworks like CAMEL (Li et al., 2023c), AgentVerse (Chen et al., 2023b), and DyLAN (Liu et al., 2023d) leverage a group of agents for role-playing and inter-discussion to improve the understanding of human instructions. ExpeL (Zhao et al., 2023) and MemGPT (Packer et al., 2023) also align with human intentions through the analysis of human goals in an iterative manner.

To align with *environmental dynamics*, the agents should ground themselves with external information from the environment. Reflexion (Shinn et al., 2023), LATS (Zhou et al., 2023a), and Agent-Verse (Chen et al., 2023b) use external reward feedback as conditions to rectify their actions and improve the alignment with the environment. RetroFormer (Yao et al., 2023b), TRAN (Yang et al., 2023), CLIN (Majumder et al., 2023), and FireAct (Chen et al., 2023a) integrate the (abstracted) trajectories accumulated through the interaction with the environment into the prompts or data for fine-tuning. This results in an in-context or parametrized world model, which narrows the gap of alignment with the environment. RAP (Hao et al., 2023) can also be categorized as aligning with the environment through simulation of the underlying foundation models.

To align with *self-constraints*, the agents should adopt an adaptive strategy in the process of task execution and/or group construction. The representative works in this vein include SwiftSage (Lin et al., 2023), Retroformer (Yao et al., 2023b), and DyLAN (Liu et al., 2023d). Finetuning a small-sized foundation model is also beneficial to the obedience of self-constraints (Chen et al., 2023a; Qiao et al., 2024), which eliminates the need to call the costly APIs of proprietary models.

In addition to the aforementioned frameworks, there are also basic techniques for agents, such as ReAct (Yao et al., 2022b) and Tree-of-Thoughts (Yao et al., 2023a), that serve as the foundational elements in most of the advanced agents. An overview of the analysis is illustrated in Figure 3.

Despite the emergence of diverse agent methodologies, plenty of room still exists for the unified alignment of agents with *human intentions, environmental dynamics*, and *self-constraints* simultaneously. Challenges lie in the construction of the agent framework (Sumers et al., 2023), which requires an elaborate design to strike a good balance of alignment with all three roles. Counterexamples in this sense are Reflexion (Shinn et al., 2023) and LATS (Zhou et al., 2023a), which leverage multiple rounds of sampling to achieve better alignment with the environment, but the self-constraints are significantly violated at the same time due to the high cost. Moreover, the capability of the underlying foundation model dominates the potential of the sophisticated alignment endeavors of an agent. Therefore, it is essential to promote the synergy between the development of foundation models (such as alignment techniques) and the research of agents.

4 PROOF-OF-CONCEPT STUDIES

In this section, we conduct proof-of-concept studies to validate the importance of UA^2 in the design of both benchmarks and methods for agents. Section 4.1 covers several realistic features we introduced into WebShop (Yao et al., 2022a), which are selected according to the principles of UA^2 . In Section 4.2, we introduce our agent method design following the principles of UA^2 . Section 4.3 covers the experiments of several agent candidate baselines and our method in the retrofitted environment, and Section 4.4 reports the results as well as our discussions and findings.

4.1 Environment Construction

We conduct the case studies by first upgrading the WebShop environment. WebShop is a simulated online shopping environment with 1.18M real-world shopping items gathered from Amazon, and 12,087 textual shopping instructions collected from human annotators. While serving as a high-quality testbed for the instruction-following and planning abilities of foundation model agents, we further improve the complexity of WebShop by introducing the realistic factors around the three roles in the agent working system: *human intentions, environmental dynamics*, and *self-constraints*.

Human intentions. In reality, different human users own unique, potentially invisible preferences about the properties and categories of shopping items. Given this, we configure 10 different users for testing, each possessing a basic preference (in text) that corresponds with a certain hidden attribute of items. We equip each user with a group of 50 consecutive artificially constructed instructions with user profiles, ambiguous descriptions, and preferences to be inferred by tracking the purchase

history. The rules of reward computation for each instruction follow those of the original WebShop. For details of the task construction and the instructions with user profiles, see Appendix A.1.

Environmental dynamics. To narrow the gap with realistic online shopping scenarios, we implement fine-grained personalized reranking algorithms on top of the original search engine in Web-Shop. The algorithms include collaborative filtering (Sarwar et al., 2001) and a Determinantal Point Process (DPP) based method (Chen et al., 2018). With personalized reranking schemes, the website is constantly evolving with user actions, which better reflects the complexity of realistic environmental dynamics. The details of the implementation are listed in Appendix A.2.

Self-constraints. To measure the expenses of the agents themselves during the operating process, we implement the runtime environment to count for the temporal and monetary expenditures for the agent working system. The monetary cost consists of the API calls of the proprietary foundation models, and the time consumption indicates the normalized endurance of interaction between the agents and the interactive environment (detailed in Appendix A.3).

4.2 AGENT DESIGN WITH THE PRINCIPLES OF UA^2

Following the principles of UA^2 , we initiate our agent by introducing the structured memory module on top of ReAct (Yao et al., 2022b). Shown in Figure 4, the introduced module is formed by two components: *low-level* action insights and *high-level* intra-task experience.

Low-level action insights are a list of key actions exploited from different runs in the environment under the same task instruction. The key actions are extracted from the high-reward trajectories with an analyzer, with which the contributions of actions are computed in task-solving. The analyzer adopts a batched inference (Cheng et al., 2023) to tag all actions at the same time. The structured memory is then maintained with the key actions paired with their corresponding human instructions.

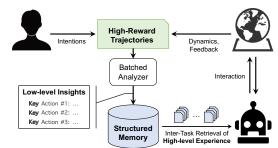


Figure 4: Overview of our agent design that follows the principles of UA^2 . By continually analyzing and retrieving structured memory from similar tasks of the same user, the agent extrapolates experience across different tasks.

High-level intra-task experience is formed by

the retrieval of the *low-level* action insights accumulated in the structured memory. According to the similarity of the current human instruction with the previous ones stored in the memory, the key actions are gathered to form an initial plan for the current task. The re-use of high-level experience throughout the stream of tasks promotes efficient intra-task generalization.

We design the agent to differ from previous works, which rely on LLM summarization of unstructured insights (Majumder et al., 2023; Zhao et al., 2023) or multiple-round LLM reflections within a single task (Shinn et al., 2023). Our method aligns with *human intentions, environmental dynamics,* as well as *self-constraints*: (i) The maintenance of the structured memory contributes to the lifelong profiling of a human user. (ii) The storage and retrieval of key actions analyzed from different trajectories improves the awareness of the agent to the environment. (iii) The reuse of structured records saves the agents from planning from scratch for each task, which aligns with *self-constraints* by cost minimization. Appendix B covers the formal descriptions and implementation details.

4.3 EXPERIMENTS

Baselines. We compare the performance of our method with several widely-used agent techniques on the retrofitted WebShop in Section 4.1, including (1) ReAct (Yao et al., 2022b), which harmonizes internal reasoning and external actions, (2) ReAct-SC (ReAct with Self-Consistency), which equips ReAct with sampling and marginalization (Wang et al., 2022b), (3) Reflexion (Shinn et al., 2023), which conducts self-correction by reflecting on past actions and observations, and (4) LATS (Zhou et al., 2023a), which leverages a combination of techniques including ReAct, self-reflection, and Monte Carlo Tree Search (MCTS). Note that we leave the implementation of techniques categorized

Table 2: The performance of averaged reward, success rate (SR) (%), alignment gap (%) with human
intentions (G_{HI}) and environment dynamics (G_{ED}), time (s) and money (\$) cost of all methods
tested in our retrofitted WebShop environment. The best result for each metric is in bold . The better
performance under each metric is indicated by the darker green shades. *LATS is tested on 1/10
subset of the entire task instructions due to the significant cost.

Method	Reward ↑	$\mathrm{SR}(\%)\uparrow$	$G_{\mathrm{HI}}\left(\%\right)\downarrow$	$G_{\mathrm{ED}}\left(\%\right)\downarrow$	Time (s) \downarrow	Money (\$) \downarrow
ReAct	50.3	8.0	11.7	14.9	1.716	0.013
ReAct-SC	49.9	7.4	14.4	14.6	1.720	0.039
Reflexion	44.4	13.8	22.5	25.7	5.539	0.045
LATS*	52.4	10.0	18.5	14.3	125.935	5.508
Ours	51.9	9.6	6.7	14.8	1.779	0.014

as aligning with human intentions in Section 3.2 as future work, since great effort should be taken by involving humans in the interaction loop and adapting to our settings.

Evaluation Metrics. Following the settings of Yao et al. (2022a), we measure the performance of task completion with the average reward and success rate incurred per task. To quantitatively investigate the alignment of different methods under the principles of UA^2 , we introduce three extra metrics. We report the averaged monetary and time cost to reflect the alignment of each method with *self-constraints*. For *human intentions* and *environmental dynamics*, we build ablated versions of the retrofitted WebShop that exclude the introduced feature, respectively. We then test each agent technique on the pair of fully-retrofitted / ablated environments, and finally investigate the difference between the pair of the evaluated rewards. More specifically:

To evaluate the alignment with *human intentions*, we construct an ablated version of the environment in Section 4.1, where the hidden attributes corresponding with user profiles or preferences are excluded from the reward computation. In this ablated environment, the performance of each method should be better than that in the fully-retrofitted environment. We define the alignment gap with human intentions $G_{\rm HI}$ as the relative difference between the two performances:

$$\mathbf{G}_{\mathrm{HI}} = (R_{\mathrm{full}} - R_{\mathrm{HI}})/R_{\mathrm{full}} \times 100\%,\tag{1}$$

where R_{full} and R_{HI} stand for the reward of an agent in the fully-retrofitted environment and the environment excluding the computation of human intentions, respectively.

Similarly, to evaluate the alignment with *environmental dynamics*, we build an ablated environment without the implementation of the personalized reranking algorithms, and define the alignment gap with environmental dynamics $G_{\rm ED}$:

$$\mathbf{G}_{\rm ED} = (R_{\rm full} - R_{\rm ED})/R_{\rm full} \times 100\%,\tag{2}$$

with $R_{\rm ED}$ as the reward of an agent in the ablated environment that excludes the personalized reranking algorithms.

4.4 RESULTS AND DISCUSSIONS

The performances of different methods in all the metrics are shown in Table 2. According to the results, Our framework achieves the top unified performance among all the methods, with the best balance between task completion performance and measures of different alignment sources.

LATS achieves the highest average reward, and Reflexion obtains the top success rate. This is because they both employ trial-and-error approaches with multiple rounds of interactions. However, the money and time costs of the two methods are significantly higher than other methods, suggesting their weaknesses in aligning with the *self-constraints* of agents. To be specific, Reflexion incurs a cost over $5 \times$ in time and $3 \times$ in money compared to other methods, while LATS, in contrast with other methods, entails a cost exceeding $100 \times$ in time and nearly $200 \times$ in money.

ReAct-SC achieves a comparable average reward and success rate (SR) with ReAct. This might be attributed to the complexity of our retrofitted environment, where even more runs of sampling are

required in ReAct-SC to vote for better actions. In addition, The incorporation of self-consistency in ReAct-SC requires more calls of the API of the proprietary foundation model, resulting in approximately three times the cost of money compared to ReAct. The time cost of ReAct and ReAct-SC is nearly identical. This is because we only document the endurance within the interactive environment (the time of API requests is neglected), and at the same time, ReAct might exhibit similar planning abilities as ReAct-SC. Finally, Our framework achieves the top performance in averaged rewards and success rates, which underscores the significance of the principles of UA^2 .

As for the alignment gap, the results of $G_{\rm HI}$ and $G_{\rm ED}$ in Table 2 indicate that almost all baselines possess the gap above 10% in terms of aligning with humans or the complex environment. Notably, our method demonstrates a significantly lower $G_{\rm HI}$ than other methods, which might benefit from its capacity to adapt to diverse human intentions by intra-task experience generalization with the structured memory. In contrast, LATS demonstrates a relatively low $G_{\rm ED}$ of 14.3%. This is because of the accumulation of trials from the exhaustive sampling in the environment, which meanwhile limits its practical applicability. For comparison, neither $G_{\rm HI}$ nor $G_{\rm ED}$ of Reflexion is satisfactory, which might indicate that the mechanism of the self-reflection is inferior to other techniques in this setting. These results highlight the need for agent techniques following the principles of UA^2 .

5 ACTIONABLE INSIGHTS

Envisioning the future of autonomous agents powered by foundation models in real-world applications, in this section, we provide insights on the next steps of research from UA^2 .

Synergizing agents with alignment research. Alignment research aims to steer a model to follow instructions faithfully. To achieve unified alignment in an agent system, techniques in the field of alignment research can be helpful to the foundation model agents in following the principles of UA^2 . For instance, humans can leverage ideas like Constitutional AI (Bai et al., 2022) to integrate the principles of unified alignment into the objectives of the agents.

Constructing realistic agent benchmarks. While appreciating the existing efforts on the benchmark construction for agents, we advocate for more realistic simulation and sandbox design reflecting the intricate scenarios with nuanced logistics and details. As shown in our proof-of-concept studies, the principles of UA^2 are also helpful in the design of the benchmark. Taking UA^2 into account, the gap between agents and realistic human demands and interactive environment can be revealed more faithfully, laying the foundation for the next breakthrough of agent techniques.

Developing holistic evaluations for agents. Existing research on agents mainly uses the final success of task completion as the evaluation metric. In our work, we propose the principles of unified alignment for agents, suggesting the proficiency of agents can be reflected by the quality of alignment with *human intentions, environmental dynamics,* and *self-constraints.* Given this, the dissection of the performance of agents is necessary for the development of agent techniques, since an analysis of alignment gaps with different roles indicates the direction of improvement for agents. This suggests the importance of holistic evaluations for the development of autonomous agents.

Toward self-evolving agents through continual alignment. While the sources of alignment have been categorized by UA^2 , it requires the elaborated design of agent methods that carefully balance the different alignment sources in a unified manner. Envisioning agents with next-level autonomy, we expect the agents to self-evolve through lifelong interaction with humans and the environment with continual alignment. In this vein, agents improve themselves with better use and efficiency, leading to general problem-solving abilities in complex, real-world scenarios.

6 CONCLUSION

In this work, we propose the principles of unified alignment for agents with *human intentions, environmental dynamics*, and *self-constraints*. We start by recognizing the three components in a working system of agents: agents, humans, and environment, then state the necessity of agents to align with the three roles in a unified manner and propose the principles of UA^2 . We demonstrate the significance of UA^2 by literature review and proof-of-concept studies. Eventually, we shed light on the impact of UA^2 on the future of agent research with enhanced general problem-solving abilities.

BROADER IMPACT

The prosperity of autonomous agents with foundation models has posed exciting avenues for future research toward the automatic execution of daily tasks for humans. In our work, we advocate for the unified alignment of agents (UA^2) with humans, the environment, and the agents themselves simultaneously. To align with humans means to improve the understanding of *human intentions*, and especially safety concerns, to provide better assistance. By doing so, the agents also need to align with the environment to enhance the awareness of *environmental dynamics*, so that the agents can be cautious about whether the next actions could be malicious or destructive. The agents should also align with themselves in terms of *self-constraints*, adhering to the running cost of money, time, battery, etc. In our work, we conduct proof-of-concept studies by introducing realistic features, such as human profiles, personalized reranking algorithms, and runtime cost counters into the original WebShop. While the results have proved the essence of UA^2 , we plan to experiment with extra alignment factors in the future, including safety concerns from human intentions, temporal variation and random events from the environment, as well as other types of self-constraints.

Our work covers the principles for agents to follow, and we expect the future of agents with narrowed alignment gaps in a unified manner. We also expect the construction of more realistic sandboxes or simulators as the testbeds for agents, where both the capability and safety of agents can be better studied and improved under realistic settings. Eventually, our principles of unified alignment for agents lay the foundation for the next-level agents more intelligent and more responsible.

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A ENVIRONMENT CONSTRUCTION IN SECTION 4.1

In this section, We introduce the realistic features we introduce into the original WebShop in detail. Note that as we aim to conduct *proof-of-concept* studies, the features are implemented for the purpose of *reflecting the three lines of alignment only*. We also anticipate realistic configurations and more nuanced logistics in a dedicated benchmark in the future.

A.1 TASK DESIGN IN THE RETROFITTED WEBSHOP

Different from the precise human instructions in the original WebShop environment, we design tasks to reflect the necessity of agents to align with *human intentions*. In reality, different human users own unique preferences about the properties and categories of shopping items. Such preferences form the profile of a user, which dominates their authentic intentions in the stream of shopping instructions. As it is not always easy for human users to explicitly write down the precise instructions for all their shopping intentions, the agent should assist humans by continually inferring human intentions.

Given this, we configure 10 different users, each possessing a basic preference (described in text) that corresponds with a certain hidden attribute of items. For example, for the hidden attribute cruelty-free, we design the corresponding basic human profile sentence to be I cannot care enough for the cute creatures in this world. We follow the reward computation rules in the original WebShop, therefore the match of hidden attributes is essential to the final reward. We equip each user with a group of 50 consecutive artificially constructed instructions. In all the instructions of the group, the aforementioned profile sentence always appears.

The specific instruction for the purchase of this round falls into three cases:

- The basic preference of the user should be considered. An example in this category reads: i am interested in a 60 count of toner that is suitable for sensitive skin, and price lower than 50.00 dollars. For this instruction, the expected item to be found contains two hidden attributes: sensitive skin according to the task instruction, and cruelty-free according to the user profile.
- The basic preference of the user does not need to be considered. An example in this category reads: i am looking for a nightstand that is easy to install. Our motivation for this case is that the users with whatever preferences always need to buy some specific items, which can be irrelevant to their profiles. In this example, the underlying hidden attributes contain just the task-related easy install.
- The basic preference of the user should be considered, *and* an extra preference should be recognized according to the recent instruction histories. An example in this category reads: Based on my purchase preference from history, help me to buy eco friendly face towels. And the corresponding instruction history for this example is listed in the following Table 3. It should be inferred according to the history that the hidden attribute (as the invisible intention) that frequently appears in recent instructions are sensitive skin. We design the order of the instruction group so that such to-be-inferred attributes appear at least five times more than other attribute consists of the cruelty-free according to the user profile, the eco friendly according to the description in the textual instruction, and also the sensitive skin that is to be tracked and inferred from history.

Most of the task instructions in the former two groups are selected from the crowdsourced instructions, whose corresponding ground-truth items are labeled with the hidden attributes of both the basic user preference and the task-related instruction. We artificially rewrite the instructions in the third category by introducing indicating words like Based on my purchase from the history. In the 10 groups of 50 consecutive instructions, the statistics of the three categories is 298/97/105 for the first/second/third category, approximately 3:1:1. The task completion performances of all agent techniques should be tested on the 10 groups of 50 instructions each, with the overall averaged reward and success rate reported. In the ablated version of the retrofitted environment for the calculation of $R_{\rm HI}$ and $G_{\rm HI}$ in Section 4.3, all the hidden attributes about the basic user profiles (*e.g.*, the cruelty free) and the preferences to be inferred (*e.g.*, the sensitive skin) are excluded from the reward computation. Table 3: The instruction history for the instruction example: *Based on my purchase preference from history, help me to buy eco friendly face towels.*

The following instruction history is listed in reverse chronological order:

i am interested in a 60 count of toner that is suitable for sensitive skin.

i am looking for a sulfate & paraben free shampoo that is also suitable for my sensitive skin.

i want some hand cream for dry and sensitive hands in a grapefruit scent.

i need men's non toxic deororizing body spray for sensitive skin. get the 2pack 3.4 ounce size.

get me a body scrub to remove dead skin. pick a 3.4 fl oz pack that is meant for sensitive skin.

i need low rise boot cut pants in grey color.

buy me some paraben free coconut oil lip balm for my sensitive skin.

i'm looking for some juicy watermelon lip gloss that is paraben and oil free and suitable for sensitive skin. i need soaps for dry and sensitive skin that are made with argan oil.

i'm looking to buy a body wash that has tea tree oil as an ingredient that would work well for sensitive skin.

A.2 PERSONALIZED RERANKING ALGORITHMS

A.2.1 OVERVIEW

To narrow the gap with realistic online shopping scenarios, we implement personalized reranking algorithms in WebShop. With the reranking algorithms, the search results of the shopping item list are re-ordered according to the click histories of the users. Specifically, on top of the Pyserini (Lin et al., 2021) search engine used in the original Webshop, we integrate a Collaborative Filtering (CF) (Sarwar et al., 2001) algorithm and a Determinantal Point Process (DPP) based algorithm (Chen et al., 2018) for fine-grained personalized re-ranking. The DPP-based algorithm provides the reranking weights based on the historical actions of the agent itself, while the CF-based algorithm provides the reranking weights based on the similarity with other users. The two sets of weights by the two algorithms are eventually linearly averaged with the coefficient of 0.2 for DPP-based weights and 0.8 for CF-based weights. Driven by the reranking algorithms, the environment is constantly evolving with user actions, which could better reflect the complexity of realistic environmental dynamics. In the ablated version of the retrofitted environment for the calculation of $R_{\rm ED}$ and $G_{\rm ED}$ in Section 4.3, the two algorithms are disabled.

Algorithms 1 and 2 brief the collaborative filtering and DPP-based reranking, respectively.

Algorithm 1 User-Based Collaborative Filtering
Input: Prime user-item rating matrix R , User Click Through Rate U , Top-n items I
Output: CF reranking score of top-n items Y
1: for each prime user i do
2: for $j \in \mathbf{I}$ do
3: $\mathbf{M}_{i,j} = \mathbf{R}_{i,j}$
4: end for
5: end for
6: for each prime user i do
7: /* Calculate the intersection of items contained in the current agent and prime users */
8: $P = \mathbf{U} \cap \mathbf{R}_i$
9: $\mathbf{S}_i = \frac{\sum_{p \in P} (\mathbf{R}_{i,p} - \overline{\mathbf{R}}_i) (\mathbf{U}_p - \overline{\mathbf{U}})}{\sqrt{\sum_{p \in P} (\mathbf{R}_{i,p} - \overline{\mathbf{R}}_i)^2} \sqrt{\sum_{p \in P} (\mathbf{U}_p - \overline{\mathbf{U}})^2}}$
$\sqrt{\sum_{p \in P} (\mathbf{R}_{i,p} - \overline{\mathbf{R}}_i)^2} \sqrt{\sum_{p \in P} (\mathbf{U}_p - \overline{\mathbf{U}})^2}$
10: end for
11: $\mathbf{Y} = \mathbf{SM} / \sum \mathbf{S}_i$

In the implementation of the CF-based algorithm, we first employed ChatGPT (gpt-3.5-turbo-1106) as an assistant to simulate 30 different users and gather their preference data for collaborative filtering (detailed in Appendix A.2.2). During the shopping process, we record the click-through rates (CTR) of the agent on every item. We then re-rank the item list of the search results according to the agent's CTR and its Pearson correlation between the simulated user preferences.

Algorithm 2 Deterministic Point Process Based Reranking (Chen et al., 2018)

Input: Item score vector **I**, Item similarity matrix **S**, Top K **Output:** DPP-based reranking score of top-n items Y_q 1: $\mathbf{c}_i = [], d_i^2 = \mathbf{L}_{ii}, j = \arg \max_{i \in \mathbb{Z}} \log(d_i^2), Y_q = \{j\}$ 2: $\mathbf{L} = \operatorname{diag}(\mathbf{I}) \mathbf{S} \operatorname{diag}(\mathbf{I})$ 3: while $|Y_q| < K$ do for $i \in Z \setminus Y_g$ do 4: $e_i = (\mathbf{L}_{ji} - \langle \mathbf{c}_j, \mathbf{c}_i \rangle)/d_j$ 5: $\mathbf{c}_i = \mathbf{c}_i \| e_i$ $d_i^2 = d_i^2 - e_i^2$ 6: 7: end for 8: $j = \arg\max_{i \in Z \setminus Y_q} \log(d_i^2), Y_q = Y_q \cup \{j\}$ 9: 10: end while

A.2.2 USER BEHAVIOR SIMULATION

We employed ChatGPT to design 30 different roles, simulating the process of shopping and gathering the ranking results for 50 products for each role, the prompts are shown in Table 4. The collected data will be used to simulate user behavior for simulating the dynamic environment similar to recommendation systems with changeable displayed items for different users and behaviors. The information of 30 roles is shown in Table 5 and Table 6. Note that these roles are completely generated by ChatGPT, including their genders and other information. In this work, we construct the 30 roles to obtain the set of preference weights for only the purpose of introducing the reranking mechanisms into the environment. We plan to refine the construction of the profiles with a broader coverage of demographic groups in the future.

Table 4: The prompt for user behavior simulation using ChatGPT. We define roles (colored in green) and the query (colored in blue), asking for reranking items (colored in orange) given by the original Webshop. The generated results (colored in red) can serve as a simulation of user click behavior.

User Behavior Simulation /* Prompt */ Your name is [NAME] and here is your profile: Gender: [Gender] Age: [Age] Occupation: [Occupation] Shopping Habits: [Shopping Habits] You are searching for [Query] on a shopping website and obtain 50 results:

Id: [Id₁]; Description: [Desc₁]; Price: [Price₁] Id: [Id₂]; Description: [Desc₂]; Price: [Price₂]

Id: [Id₅₀]; Description: [Desc₅₀]; Price: [Price₅₀]

Please sort all 50 products according to your preferences using the format of "Id-Ranking".

/* Response */ [Id₁]-[Rank₁]; [Id₂]-[Rank₂]; ...; [Id₅₀]-[Rank₅₀];

Human Evaluation for the Ranking Results by ChatGPT. Furthermore, we conducted a human evaluation on the ranking results of ChatGPT, and the results in Table 7 show that the NDCG score of ChatGPT is 0.871, indicating that the simulation results are close to human ranking preferences.

Profile	Role #1	Role #2	Role #3	Role #4	Role #5
Name	Sarah	Juan	Lisa	Michael	Emma
Gender	Female	Male	Female	Male	Female
Age	32	21	40	45	55
Occupation	Software Engi-	College Student	Stay-at-home mom	Construction Man-	Retired
	neer			ager	Teacher
Habits	Sarah loves on-	Juan is pas-	Lisa prioritizes her	Michael is passion-	Emma is a
	line shopping	sionate about	family's health and	ate about home im-	avid reader an
	for the latest	fashion and	wellness. She shops	provement projects.	loves hostin
	gadgets and	enjoys shop-	for organic groceries,	He frequently visits	book clu
	tech accessories.	ping for trendy	supplements, and	hardware stores, re-	meetings. Sh
	She researches	clothing and	natural skincare	searches tools and	enjoys brows
	extensively, reads	accessories.	products. She also	materials, and en-	ing bookstore
	reviews, and	He follows	invests in fitness	joys renovating and	collecting li
	compares prices	fashion influ-	equipment and en-	enhancing his living	erary classic
	before making a	encers on social	joys trying new	space. He seeks	and explorin
	purchase. She's	media, visits	workout routines.	quality products for	various genre
	always on the	local boutiques,		long-term durabil-	She values rec
	lookout for the	and regularly		ity.	ommendations
	newest tech	updates his		10,1	from fello
	trends.	wardrobe to			book lovers.
	dends.	stay stylish on			book lovels.
		campus.			
Profile	Role #6	Role #7	Role #8	Role #9	Role #10
Name	Alex	Ryan	Maya	Daniel	Olivia
Gender	Non-binary	Male	Female	Male	Female
Age	27	35	28	50	42
Occupation	Etsy Shop Owner	Chef	Environmental Sci-	Pet Store Owner	Financial Ana
1	5 1		entist		lyst
Habits	Alex loves cre-	Ryan is pas-	Maya loves hik-	Daniel owns a	Ólivia love
	ating unique	sionate about	ing, camping, and	pet store and con-	finding th
	handmade items	cooking and	exploring nature.	stantly seeks out	best deals an
	and runs an on-	constantly	She invests in high-	pet-related products	discounts. Sh
	line store. They	seeks out new	quality outdoor	for his business.	enjoys usin
	actively seek	ingredients	gear, such as tents,	He actively sources	coupons, con
	out specialty	and culinary	hiking boots, and	pet food, toys,	paring price
	craft supplies,	tools. He enjoys	backpacks. She	grooming supplies,	and explorin
	materials, and	shopping at	actively researches	and accessories to	online pla
	tools to produce	local markets,	and reads reviews to	cater to various pet	forms to sav
	high-quality	specialty food	ensure durability and	owners' needs.	money on he
	products. They	stores, and on-	functionality.		purchases. Sh
	also enjoy attend-	line platforms	j.		values bot
	ing craft fairs and	for gourmet			quality an
	networking with	products. He			affordability.
	other artisans.	values quality			······································
		and freshness.			
Profile	Role #11	Role #12	Role #13	Role #14	Role #15
Name	Ahmed	Sophia	Carlos	Emily	Javier
Gender	Male	Female	Male	Female	Male
Age	38	25	30	27	34
Occupation	Physical Educa-	Social Media	Automotive Engi-	Environmental Ac-	Travel Blogge
n. 1 %	tion Teacher	Influencer	neer	tivist	T. ' '
Habits	Ahmed is pas-	Sophia is a	Carlos has a deep	Emily is focused	Javier love
	sionate about	beauty en-	interest in cars and	on sustainable	traveling an
	sports and fitness.	thusiast and	enjoys shopping for	living and seeks	exploring ne
	He shops for	creates content	automotive acces-	out eco-friendly	destinations.
	athletic apparel,	about cosmet-	sories, performance	products. She	He shops for
	sports equipment,	ics, skincare,	parts, and main-	shops for ethically	travel gea
	and supplements.	and makeup	tenance tools. He	sourced clothing,	luggage, ar
	He enjoys ex-	tutorials. She	actively researches	reusable items, and	outdoor ad
		actively seeks	and stays updated on	environmentally	cessories.
	ploring local		Ale a late of ante and a second a late	friendly household	He value
	sports stores and	out new beauty	the latest automobile		
	sports stores and stays updated on	out new beauty products, fol-	technology.	products.	lightweight
	sports stores and stays updated on the latest fitness	out new beauty products, fol- lows trends,			and durab
	sports stores and stays updated on	out new beauty products, fol- lows trends, and shares her			and durab products for h
	sports stores and stays updated on the latest fitness	out new beauty products, fol- lows trends, and shares her recommenda-			and durab
	sports stores and stays updated on the latest fitness	out new beauty products, fol- lows trends, and shares her			and durabl products for h

Table 5: The generated 30 different simulated users by using ChatGPT (part 1).

Profile	Role #16	Role #17	Role #18	Role #19	Role #20
Name	Lily	Oliver	Emma	Noah	Ava
Gender	Female	Male	Female	Male	Female
Age	29	19	52	65	45
Occupation	Marketing Man-	College Student	Antique Store Owner	Retired Engineer	Art Galler
1	ager	0	1	C	Owner
Habits	Lily recently	Oliver is pas-	Emma has a keen	Noah embraces	Ava is pas
	became a new	sionate about	interest in vintage	technology and	sionate abou
	parent and ac-	music and	items and actively	enjoys shopping for	art and ac
	tively shops for	loves shopping	seeks out antique	the latest gadgets,	tively collect
	baby products,	for musical	furniture, clothing,	smartphones, and	paintings,
	including cloth-	instruments,	and collectibles. She	smart home de-	sculptures, an
	ing, toys, and	equipment, and	enjoys visiting flea	vices. He actively	other fine an
	nursery essen-	vinyl records.	markets, estate sales,	seeks user-friendly	pieces. Sh
	tials. She seeks	He actively	and auctions to ex-	products and keeps	frequents an
	out trusted brands	explores local	pand her collection.	up with technologi-	fairs, galleries
	and prioritizes	music stores	I	cal advancements.	and auction
	safety and qual-	and online			to discove
	ity.	platforms for			new artists an
		unique finds.			expand he
		1			collection.
Profile	Role #21	Role #22	Role #23	Role #24	Role #25
Name	Max	Olivia	Liam	Sophia	Ethan
Gender	Male	Female	Male	Female	Male
Age	20	35	32	26	50
Occupation	College Student	Interior De- signer	Personal Trainer	Graphic Designer	Landscape An chitect
Habits	Max is an avid	Olivia special-	Liam is dedicated to	Sophia has a pas-	Ethan enjoy
	gamer and ac-	izes in creating	fitness and actively	sion for stationery	gardening an
	tively shops for	beautiful spaces	shops for workout	and actively shops	frequently
	the latest gam-	and frequently	apparel, equipment,	for notebooks,	shops fc
	ing consoles,	shops for fur-	and supplements.	pens, art supplies,	plants, seeds
	accessories, and	niture, decor,	He seeks out high-	and planners. She	gardening
	video games. He	and lighting	quality gear that	values aestheti-	tools, an
	stays updated on	fixtures. She	withstands intense	cally pleasing and	outdoor deco
	gaming news,	stays updated	training sessions and	functional products	He seeks ou
	follows esports	on design	recommends prod-	that inspire her	sustainable an
	tournaments, and	trends, visits	ucts to his clients.	creativity.	eco-friendly
	seeks out mer-	trade shows,			products that
	chandise from his	and sources			enhance hi
	favorite games.	unique pieces			garden.
		for her clients.			
Dancel		Tor her chems.			
Profile	Role #26	Role #27	Role #28	Role #29	Role #30
Name	Mia	Role #27 Noah	Isabella	James	Harper
Name Gender	Mia Female	Role #27 Noah Male	Isabella Female	James Male	Harper Female
Name Gender Age	Mia Female 38	Role #27 Noah Male 75	Isabella Female 30	James Male 35	Harper Female 23
Name Gender Age	Mia Female	Role #27 Noah Male	Isabella Female 30 Environmental Sci-	James Male	Harper Female 23 Vintage Cloth
Name Gender Age	Mia Female 38	Role #27 Noah Male 75	Isabella Female 30	James Male 35	Harper Female 23 Vintage Cloth ing Stor
Name Gender Age Occupation	Mia Female 38 CEO	Role #27 Noah Male 75 Retired Teacher	Isabella Female 30 Environmental Sci- entist	James Male 35 Stay-at-home dad	Harper Female 23 Vintage Cloth ing Stor Owner
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates	Role #27 Noah Male 75 Retired Teacher Noah prefers	Isabella Female 30 Environmental Sci- entist Isabella is committed	James Male 35 Stay-at-home dad James is a hands-	Harper Female 23 Vintage Cloth ing Stor Owner Harper has
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac-	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living	James Male 35 Stay-at-home dad James is a hands- on parent and fre-	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion,	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ-	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ-	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel shops for
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items.	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags,	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child-	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion fc vintage fashio and activel shops fc retro clothing
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries,	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel shops for retro clothing accessories,
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands,	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion fc vintage fashio and activel shops fc retro clothing accessories, and antiqu
Name Gender Age	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones,	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion fc vintage fashio and activel shops fc retro clothing accessories, and antiqu jewelry. Sh
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion events, and val-	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones, tablets, and	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning supplies. She values	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products that make parenting	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion fc vintage fashio and activel shops fc retro clothing accessories, and antiqu jewelry. Sh enjoys visitin
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion events, and val- ues premium	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones, tablets, and assistive tech-	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning supplies. She values products with min-	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion fc vintage fashio and activel shops fc retro clothing accessories, and antiqu jewelry. Sh enjoys visitin thrift store:
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion events, and val-	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones, tablets, and assistive tech- nology. He	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning supplies. She values products with min- imal environmental	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products that make parenting	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel shops for retro clothing accessories, and antiqu jewelry. Sh enjoys visitin thrift store: vintage mat
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion events, and val- ues premium	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones, tablets, and assistive tech- nology. He values products	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning supplies. She values products with min-	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products that make parenting	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel shops for retro clothing accessories, and antiqu jewelry. Sh enjoys visitin thrift store: vintage mai kets, and onlin
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion events, and val- ues premium	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones, tablets, and assistive tech- nology. He values products with clear in-	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning supplies. She values products with min- imal environmental	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products that make parenting	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel shops for retro clothing accessories, and antiqu jewelry. Sh enjoys visitin thrift stores vintage man kets, and onlin platforms for
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion events, and val- ues premium	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones, tablets, and assistive tech- nology. He values products with clear in- structions and	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning supplies. She values products with min- imal environmental	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products that make parenting	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel shops for retro clothing accessories, and antiqu jewelry. Sh enjoys visitin thrift stores vintage mai kets, and onlin
Name Gender Age Occupation	Mia Female 38 CEO Mia appreciates luxury and ac- tively shops for high-end fashion, accessories, and designer items. She seeks out exclusive brands, attends fashion events, and val- ues premium	Role #27 Noah Male 75 Retired Teacher Noah prefers simplicity when it comes to technology and shops for user-friendly devices, such as easy-to-use smartphones, tablets, and assistive tech- nology. He values products with clear in-	Isabella Female 30 Environmental Sci- entist Isabella is committed to sustainable living and actively shops for eco-friendly products, includ- ing reusable bags, zero-waste toiletries, and environmentally friendly cleaning supplies. She values products with min- imal environmental	James Male 35 Stay-at-home dad James is a hands- on parent and fre- quently shops for baby gear, includ- ing strollers, baby carriers, and child- proofing items. He seeks out functional and safe products that make parenting	Harper Female 23 Vintage Cloth ing Stor Owner Harper has passion for vintage fashio and activel shops for retro clothing accessories, and antiqu jewelry. Sh enjoys visitin thrift stores vintage man kets, and onlin platforms for

Table 6: The generated 30 different simulated users by using ChatGPT (part 2).

Annotator	Query #1	Query #2	Query #3	Query #4	Query #5	Average.
#1	0.807	0.830	0.826	0.857	0.819	0.828
#2	0.823	0.908	0.871	0.798	0.814	0.843
#3	0.795	0.956	0.999	0.962	0.964	0.935
#4	0.927	0.896	0.974	0.931	0.763	0.898
#5	0.843	0.900	0.910	0.961	0.876	0.898
#7	0.836	0.934	0.883	0.860	0.915	0.885
#6	0.851	0.905	0.872	0.749	0.841	0.844
#8	0.798	0.824	0.920	0.764	0.877	0.837
Average.	0.835	0.894	0. 907	0.860	0.859	0.871

Table 7: NDCG@10 scores of the ranking results according to the results by ChatGPT and eight human evaluators.

A.3 RUNTIME ENVIRONMENT

To measure the expenses of the agents themselves we implement the runtime environment for the agent working system that tracks the temporal and monetary expenditures. We compute the monetary cost of each API call of the proprietary foundation models based on their official pricing. We also track the time consumption of the interaction between the agents and the environment. As the response of the website can be affected by networking issues, we leverage the following benchmarking measures for simplicity: In our environment construction, we documented all kinds of actions taking place in the environment and pre-calculated a static list of their estimated response delays. We also disregard the duration of API calls in the runtime environment as the tracked monetary cost also reflects the expense of API calls. With the runtime environment as a wrapper of the working system, humans can monitor the obedience of the agents to their self-constraints.

Specifically, we estimate the response delay of each action in the interactive environment by artificially sampling actions, trying them out, and then recording the delays. After gathering the delay statistics for each action, we fit the data with a uniform distribution, and use the expected value to reflect the estimated time for the action. Such estimated time is static, and is leveraged to benchmark the time cost in the experiments. The estimated time for all the actions is listed in the Table 8.

Action	Time (s)
reset	0.1874
search	0.5966
click[Instruction History]	0.2645
click[Back to Search]	0.1197
click[Next >]	0.2693
click[< Prev]	0.2545
click[Descriptions]	0.2401
click[Features]	0.2167
click[Reviews]	0.1275
click[Buy Now]	0.1920
click[other valid tag]	0.2896
think	0.0000
Invalid Action	0.3234
Average	0.2370

Table 8: Estimated time for different actions.

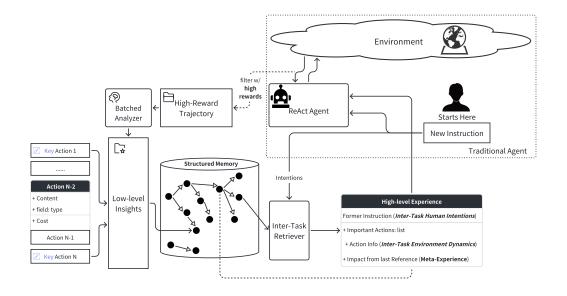


Figure 5: The details of our agent design that follows the principles of UA^2 . Compared to traditional ReACT agents, we append structured experience as the long-term memory: By filtering and analyzing raw trajectories, we extracted key actions from prior successes as low-level insights in reasoning/action paths. By retrieving reference low-level insights under the same user, we can find the high-level experience under most similar user instructions, expressing similar human intentions. Agents are able to understand human intentions and environment dynamics by extrapolating key actions from a similar, prior task.

B EXPERIMENTS

B.1 DESCRIPTIONS ON AGENT DESIGN WITH THE PRINCIPLES OF UA²

From Section 3.2, we identify three core capacities essential to agents and how they are related to the alignment principles. However, the trade-off between stronger capacities and fulfilling these principles makes it challenging to design a universally satisfactory method. Instead, to make the very first attempt, we consider improving well-known techniques to satisfy most principles.

We introduce structured memory for unified alignment principles for agents (UA^2) , as depicted in Figure 5, on top of the original ReAct (Yao et al., 2022b) agent.

Definition B.1. Trajectory is a list of actions (a_i) and observations (o_i) that agents have observed from environment (\mathcal{E}) after each action: $\mathcal{T} = \{a_i, o_i\}_{i=1}^n, o_i = \mathcal{E}(\{a_k\}_{k=1}^i).$

After filtering high-reward trajectories (Definition B.1) under human intentions from the given instruction q and temporal environment conditions (\mathcal{E}), we utilize a batched analyzer (Cheng et al., 2023) that tags key actions from the whole trajectory within one API call. Thus we integrate insights from environment dynamics with low costs compared to Reflexion (Shinn et al., 2023) and LATS (Zhou et al., 2023a).

Definition B.2. Key actions (a_i^*) are those having a positive impact on the efficiency or efficacy of task completion. We obtain the key actions $\mathcal{T}_q^* = \{a_i^*\}_{i=1}^m$ each time the agent completes a task.

Definition B.3. Low-level insights is a list of key actions (a_i^*) under a given instruction (q): $\mathcal{T}_q^* = \{a_i^*\}_{i=1}^m$. On top of this, structured experiences at *t*-th query are formed by a set of paired previous instructions and key actions: $\mathcal{S} = \{(q, \mathcal{T}_q^*) : q \in \mathcal{Q}_{t-1}\}$, where \mathcal{Q}_{t-1} denotes the set of previous instructions before *t*-th query.

Thus, we enhance agents' memory by mapping low-level insights with corresponding instructions of previous tasks, which formulates a structured memory (S) (Definition B.3). It is worth noting that

we construct the structured memory under each user, which allows agents to comprehend human intention from prior instructions. When a new instruction is given, denoted as q_{given} , a reference containing high-level experience under the instruction q_r could be retrieved by simply calculating the most similar instructions from its memory using *BM25* (Robertson et al., 2009) scoring: $\mathcal{T}_{q_r}^* \in S$, $q_r = \operatorname{argmax}_{q \in \mathcal{Q}} \{BM25(q, q_{given})\}$.

The retrieved high-level experience acts as a plan across tasks which guides the agent towards the goal accurately and rapidly, also reducing costs of time and money. After completing a task under the environment, the agent analyzes the new trajectory as well as the experience learned from the former reference, termed "meta-experience". We then record the new insights adjacent to the former reference. Also, we copy the "meta-experience" in the attachment to the former reference, which could be retrieved for upcoming tasks.

B.2 IMPLEMENTATION DETAILS

We evaluate our method and baseline methods across all 10 users on our retrofitted Webshop, each comprising 50 tasks, except for LATS which is evaluated with only one user due to its high cost. All methods utilize gpt-3.5-turbo-instruct-0914 as the underlying model for their agents except for LATS where we utilize gpt-3.5-turbo-1106 to keep the same setting as the original paper. In executing each task, we limited the interaction with the web to a maximum of 15 steps per task, inclusive of any invalid actions.

B.3 DETAILS OF EXPERIMENTAL SETUPS

For ReAct, Reflexion, and our method, we set the temperature as 0.0. For ReAct-SC, we set the number of samples k to be 3 and the temperature to be 0.05. We also experiment with the family of chain-of-thought methods: CoT (Wei et al., 2022), CoT-L2M (Zhou et al., 2022), CoT-SC (Wang et al., 2022b). Since their performances in task completion are significantly less competitive than other methods (see the next section), we exclude them from the main experiments in Section 4.3, but include them here for reference. For CoT and CoT-L2M, we set the temperature as 0.0; and for CoT-SC, we set k = 3 and the temperature to be 0.05. To adhere to the same settings with (Zhou et al., 2023a), we set the temperature as 1.0, k as 5, the number of iterations n as 30 for LATS.

All methods were tested in each of the following three environments respectively:

- The fully retrofitted environment: configured exactly as described in Section 4.1.
- The ablated environment that excludes *human intentions*: Based on the fully retrofitted environment, the hidden attributes from the user profiles and to be inferred from purchase histories are not excluded from reward computation. The alignment gap with *human intentions* ($G_{\rm HI}$) can be identified by comparing the test performances therein with those in the fully retrofitted environment.
- The ablated environment that excludes *environmental dynamics*: The fully retrofitted environment with the re-ranking algorithms in Appendix A.2 disabled. The alignment gap with *environmental dynamics* ($G_{\rm ED}$) can be identified by comparing the test performances therein with those in the fully retrofitted environment.

B.4 RESULTS

We present the comparative results on our retrofitted WebShop in Figure 6, Figure 7, and Table 9. Note that due to the significantly lower reward and success rate of CoT-related methods compared to others, the relative differences $G_{\rm HI}$ and $G_{\rm ED}$ can be dominantly affected by stochastic issues, and are therefore not of reference and comparison value.

In each figure, the X-axis represents the alignment gap with *self-constraints*, and the Y-axis represents the performance. In terms of success rate, our proposed agent demonstrates comparable performance to Reflexion. To be specific, our approach places a greater emphasis on minimizing costs, whereas Reflexion prioritizes performance improvement. Our proposed agent, guided by the principles of UA^2 , achieves a good balance between reward and cost considerations, while there remain a substantial gap between our agent and the ultimate goal of an oracle agent.

Method	Reward \uparrow	SR (%) ↑	$G_{\mathrm{HI}}\left(\%\right)\downarrow$	$G_{\mathrm{ED}}\left(\%\right)\downarrow$	Time (s) \downarrow	Money (\$) \downarrow
СоТ	8.5	1.2	22.4	67.1	1.858	0.011
CoT-L2M	9.8	0.8	6.1	8.2	1.939	0.037
CoT-SC	11.8	1.4	32.2	-61.9	1.883	0.032
ReAct	50.3	8.0	11.7	14.9	1.716	0.013
ReAct-SC	49.9	7.4	14.4	14.6	1.720	0.039
Reflexion	44.4	13.8	22.5	25.7	5.539	0.045
LATS*	52.4	10.0	18.5	14.3	125.935	5.508
Ours	51.9	9.6	6.7	14.8	1.779	0.014

Table 9: Reward, success rate (SR), alignment gap with human intentions and environment dynamics, time and money cost result on our retrofitted WebShop. *LATS is tested on 1/10 subset of the entire task collection due to the significant cost.

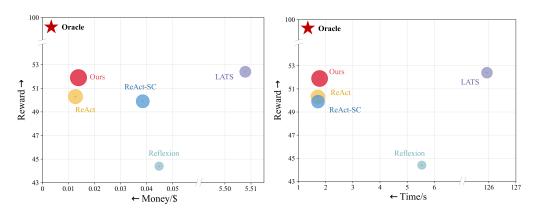


Figure 6: Agent's performance against the alignment gap with self-constraints tested on the retrofitted WebShop. The size of each circle represents the alignment gap with *human intentions* ($G_{\rm HI}$). The red star symbolizes our ultimate goal of developing an oracle agent capable of flaw-lessly completing complex tasks with minimal cost.

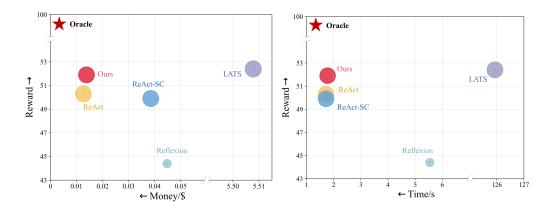


Figure 7: Agent's performance against the alignment gap with self-constraints tested on the retrofitted WebShop. The size of each circle represents the alignment gap with *environmental dynamics* (G_{ED}). The red star symbolizes our ultimate goal of developing an oracle agent capable of flawlessly completing complex tasks with minimal cost.