AVIARY: TRAINING LANGUAGE AGENTS ON CHALLENGING SCIENTIFIC TASKS

Anonymous authors
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ABSTRACT

Solving complex real-world tasks requires cycles of actions and observations. This is particularly true in science, where tasks require many cycles of hypothesis, experimentation, and analysis. Language agents hold promise for automating intellectual tasks in science because they can interact with tools via natural language or code. However, their flexibility creates conceptual and practical challenges for software implementations, since agents may comprise non-standard components such as internal reasoning, planning, tool usage, as well as the inherent stochasticity of temperature-sampled language models. Here, we introduce Aviary, an extensible gymnasium for language agents. We formalize agents as policies solving language-grounded partially observable Markov decision processes, which we term language decision processes. We then implement five environments, including three challenging scientific environments: (1) manipulating DNA constructs for molecular cloning, (2) answering research questions by accessing scientific literature, and (3) engineering protein stability. These environments were selected for their focus on multi-step reasoning and their relevance to contemporary biology research. Finally, with online training and inference-time compute scaling, we show that language agents based on open-source, non-frontier LLMs can match and exceed both frontier LLM agents and human experts on multiple tasks at up to 100x lower inference cost.

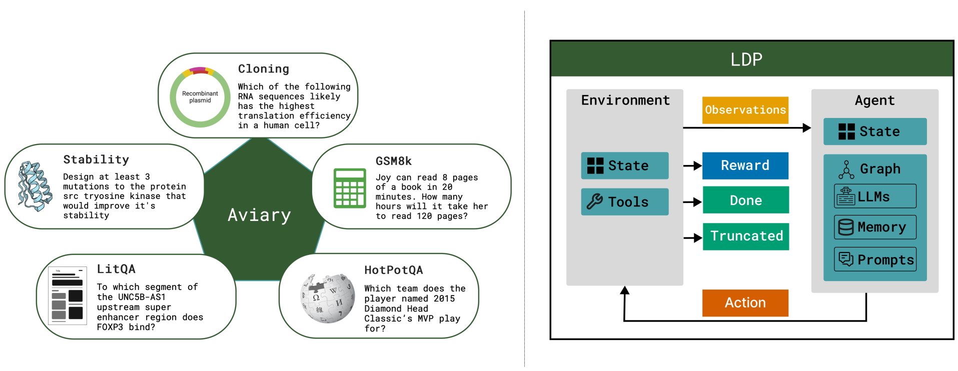

Figure 1: An overview of the five implemented Aviary environments and the language decision process (LDP) framework. The term language decision process here jointly refers to our theoretical description of the class of problems solved by language agents, as well as a software framework for implementing language agents based on a stochastic computation graph that enables training of language agent components such as LLM weights, prompts, memories, and LLM sampling parameters such as temperature.

1 INTRODUCTION

Language agents (Mialon et al., 2023; Xi et al., 2023; Gao et al., 2023; Sumers et al., 2024) are AI agents (Russell & Norvig, 2016) that integrate LLMs (Brown et al., 2020; Achiam et al., 2023; Bowman, 2023) as core components. LLMs excel at zero-shot generalization (Zeng et al., 2023a;

Szot et al., 2024), providing a notable advantage over traditional AI agents, such as those based on handcrafted rules or reinforcement learning, which often struggle to generalize to new environments (Lake et al., 2017). While LLMs can exhibit flawed reasoning and logic when used in isolation (Creswell et al., 2023; Frieder et al., 2024b;a), constructing a language agent by grounding LLMs in an environment with observational feedback can mitigate these issues. Early work on language agents used LLMs to directly output actions in the external environment (Brohan et al., 2023; Huang et al., 2022; Dasgupta et al., 2022), while more recently, language agents have been augmented with internal reasoning (Yao et al., 2023; Shinn et al., 2024) and planning procedures (Hao et al., 2023; Yao et al., 2024), as well as long-term memory storage (Park et al., 2023; Wang et al., 2024a).

An emergent research challenge is to pose a theoretical description of the learning problem solved by language agents (Sumers et al., 2024; Zhuge et al., 2024) and to develop efficient methods to optimize the components of a language agent (Zhuge et al., 2024; Yuksekgonul et al., 2024; Cheng et al., 2024). Here, we define common language agent tasks as language decision processes (LDPs) and frame language agents as stochastic computation graphs (Schulman et al., 2015) that may be trained to solve LDPs. We show that pre-existing agents (Yao et al., 2023; Shinn et al., 2024; Yao et al., 2024) can be implemented within our stochastic computation graph framework and introduce a simple and extensible software package named LDP that enables modular interchange of environments, agents, and optimizers, simplifying experimentation across a variety of settings.

In the problems we consider, we use the term optimization of language agents in the reinforcement sense to encompass procedures that yield iterative improvement of the language agent over time through feedback from an environment. An example of one such optimization algorithm is expert iteration (EI) (Anthony et al., 2017; Anthony, 2021; Havrilla et al., 2024) which achieves learning through successive rounds of supervised fine-tuning on (self-) generated trajectories from a progressively stronger language agent.

In what follows, we introduce our definition of an environment, a language decision process, and optimization of agents within a stochastic computation graph. We recast popular benchmarks such as GSM8K (Cobbe et al., 2021) and HOTPOTQA (Yang et al., 2018) as environments and integrate three scientific environments related to challenging tasks in the natural sciences. The scientific environments are (1) DNA construct engineering, where the task is to answer questions pertaining to molecular cloning (Laurent et al., 2024), (2) scientific literature question answering, where the task is to answer a multiple choice question by finding a specific passage from the scientific literature (Lála et al., 2023; Skarlinski et al., 2024), and (3) protein design, where the goal is to propose mutations to improve the stability of a given protein sequence (Gao et al., 2020; Khakzad et al., 2023). On the DNA construct design and scientific literature question answering environments, we demonstrate that language agents based on the small, open-source `Llama-3.1-8B-Instruct` model, when trained with expert iteration and using inference-time majority vote sampling, can exceed the performance of both human experts and frontier LLMs.

The environment framework described in this work, Aviary, is available at the anonymous GitHub link aviary and the stochastic computation graph framework together with language agent implementations and training code is available at the link ldp. The relationship between the Aviary and LDP frameworks is illustrated in Figure 1.

2 Related Work

Language Agent Formalisms Although language agents have achieved impressive empirical performance across a range of applications (Mialon et al., 2023; Skarlinski et al., 2024; Huang et al., 2024a), there is still no universally agreed upon theoretical framework for defining a language agent. In terms of conceptual models, the cognitive architectures for language agents (CoALA) framework (Sumers et al., 2024), inspired by ideas from production systems and cognitive architectures, taxonomizes agents according to their information storage (working and long-term memories), decision-making procedures e.g. planning, and action space (divided into internal and external actions). Similarly, in Weng (2023), the author describes language agents as consisting of memory, planning, and tool usage components. Theoretically, many works represent language agents as partially observable Markov decision processes (POMDPs) (Carta et al., 2023; Christianos et al., 2023; Wen et al., 2024b;a; Nguyen et al., 2024; Zhai et al., 2024; Song et al., 2024) yet differ in their treatment of the action space e.g. in Christianos et al. (2023) the authors partition the action space into internal and external actions in a similar fashion to CoALA where internal actions are a family of functions that operate on the agent's memory and external actions elicit an interaction with the environment. By contrast, in Wen et al. (2024b) the authors do not make a distinction between internal and external actions. In Chen et al. (2024c) the authors introduce a general framework for studying the design and analysis of LLM-based algorithms based on a computational graph where they assume LLM nodes are stateless, leaving consideration of aspects of language agents such as memory to future work.

Language Agent Optimization Frameworks Optimization of language agents may entail the learning of prompts, parametrized tools, LLM weights, inference hyperparameters, as well as more exotic parameters such as edges between nodes in computation graphs. Frameworks such as LangChain (Chase, 2022) and LlamaIndex (Liu, 2022) support manual optimization of prompts via human editing. Optimizers such as EcoOptiGen (Wang et al., 2023a) leverage black-box optimization schemes to learn LLM inference hyperparameters. Prompt optimization comprises the optimization of white-box LLMs and black-box LLMs (API-based models that cannot be differentiated through). In white-box prompt optimization (Shin et al., 2020; Li & Liang, 2021; Jia et al., 2022; Chen et al., 2022) numerical gradients can be taken over soft prompts (Qin & Eisner, 2021), the embedding representation of the text-based 'hard' prompt. In black-box prompt optimization a multitude of techniques have been applied to overcome the absence of gradients (Guo et al., 2024a; Ma et al., 2024a; Zhang et al., 2024; Cheng et al., 2023; Yang et al., 2024; Lin et al., 2024a; Hu et al., 2024b; Wu et al., 2024c; Lin et al., 2024b; Chen et al., 2024b; Zhou et al., 2023; Pryzant et al., 2023; Sabbatella et al., 2024; Chen et al., 2023b; Wang et al., 2024c; Mañas et al., 2024; Do et al., 2023; Sordoni et al., 2024; Sabbatella et al., 2023; Wen et al., 2024c; Ye et al., 2023; Wu et al., 2024a). Tool learning (Qu et al., 2024; Schick et al., 2024) can be attempted through in-context demonstrations (Qin et al., 2023) or by finetuning LLM weights on example demonstrations of appropriate tool usage (Havrilla et al., 2024; Yin et al., 2024) using techniques such as expert iteration (Anthony et al., 2017; Anthony, 2021). We discuss further related work on language agent optimization frameworks and benchmarks in Appendix D.

Our principal contributions are: (1) A precise definition of language decision processes (LDPs) for language agent tasks that encompass many proposed agent architectures as stochastic computation graphs. (2) We introduce Aviary, a gym framework that emphasizes multi-step reasoning and tool usage featuring five gym implementations (including three for scientific tasks). (3) We demonstrate that non-frontier LLMs, trained online with inference time sampling, can match or exceed the performance of frontier models on these tasks with a modest compute budget. (4) We release Aviary and our LDP framework as open-source software libraries to enable broader use and experimentation.

3 Methodology

Below we describe novel aspects of our methodology in Aviary and LDP. In Appendix B we provide background on pre-existing methods such as behavior cloning, expert iteration, and inference compute scaling that we employ for our experiments. Appendix F includes an example of an Aviary environment and rollout with an LDP agent.

3.1 Language Decision Processes

A language decision process (LDP) is a Partially-Observable Markov Decision Process (POMDP) (Åström, 1965) whose action and observation spaces are represented in natural language. More concretely, a LDP can be defined using the tuple $(\mathcal{V}, \mathcal{S}, \mathcal{A}, \mathcal{O}, T, Z, R, \gamma)$. Here, $\mathcal{V}$ is a non-empty alphabet[1], $\mathcal{S}$ is the state space, $\mathcal{A} \subseteq \mathcal{V}^*$ is the action space[2], $T(s'|s,a) : \mathcal{S} \times \mathcal{A} \mapsto \mathcal{P}(\mathcal{S})$ is the transition function, $R(s,a) : \mathcal{S} \times \mathcal{A} \mapsto \mathcal{P}(\mathbb{R})$ is the reward function, $\mathcal{O} \subseteq \mathcal{V}^*$ is the observation space, $Z(o|s') : \mathcal{S} \times \mathcal{A} \mapsto \mathcal{P}(\mathcal{O})$ is the observation function[3], and $\gamma \in [0,1]$ is the discount factor.

[1]In all LDPs we consider, $\mathcal{V}$ is the set of unicode characters, since Aviary is implemented in Python 3.

[2]Where $\mathcal{V}^* \stackrel{\text{def}}{=} \bigcup_{n=0}^{\infty} \mathcal{V}^n$ is the Kleene closure of a set $\mathcal{V}$ (Kleene, 1956; Meister et al., 2023).

[3]In all LDPs we consider, a state $s' \in \mathcal{S}$ uniquely defines an observation $o \in \mathcal{O}$. Unless otherwise specified, we omit the observation function Z.

Unlike traditional reinforcement learning agents, feedback for language agents is "grounded" in the sense that environment observations must be converted to text (Wu et al., 2024b). As such, the alphabet $\mathcal{V}$ is an important component of the LDP definition and follows other works (Carta et al., 2023; Wen et al., 2024b;a). The solution to an LDP is a policy $\pi_\theta : \mathcal{O} \mapsto \mathcal{A}$, where θ denotes the set of policy parameters we wish to learn. The parameter set θ is abstract and encapsulates any optimizable parameter of the language agent that may impact the action chosen such as LLM weights, inference hyperparameters such as temperature, as well as parametrized procedures such as internal reasoning.

In contrast to previous works which demarcate between internal and external actions (Sumers et al., 2024; Christianos et al., 2023), where internal actions include reasoning and memory retrieval, in our problem framing we consider the action space to strictly constitute interactions with the external environment, allowing our parameter set θ to subsume optimizable procedures that are internal to the language agent such as memory retrieval and internal reasoning. Practically, it is worth noting that the complexity of our environments is such that we do not expect to obtain the globally optimal π_θ^*. Our more modest goal is to be able to optimize θ in a direction that improves π_θ over time.

In all environments we consider, observations are deterministic functions of the state and so the reader may assume $Z = 1$ henceforth. For example, the environment may involve code execution where the observation consists of side-effects of the code. In this case, the state $\mathcal{S}$ includes all information necessary to induce the Markov property of the transition function such as the file system, package versions, environment variables, and hardware. However, the observation is simply the output message of the executed code.

3.2 Stochastic Computation Graphs

In the general case, a language agent may include both stochastic and deterministic operations. We build on the formalism of stochastic computation graphs (SCG) (Schulman et al., 2015): directed, acyclic graphs with nodes corresponding to computations and edges corresponding to arguments.

A deterministic node v corresponds to a function f_v, and the node's output $o(v)$ is defined as:

$$o(v) = f_v(\{o(w) \,|\, w \in \text{parents}(v)\}). \tag{1}$$

A stochastic node u is a distribution p_u, with output:

$$o(u) \sim p_u(\,\cdot \,|\, \{o(w) \,|\, w \in \text{parents}(v)\}). \tag{2}$$

Note that inputs to the SCG are treated as constant, deterministic nodes; outputs are leaf nodes.

A language agent's policy is an SCG with a string input (the observation) and string output (the action). Language agent architectures can easily be expressed as SCGs by combining deterministic and stochastic nodes. The SCGs of some common agents are provided in Appendix A.

4 Environments

Here, we provide an overview of the environments implemented in Aviary. Further details may be found in Appendix C.

4.1 GSM8K

The GSM8K environment is based on the GSM8K dataset introduced in Cobbe et al. (2021), which consists of linguistically diverse grade school math word problems designed to assess multi-step mathematical reasoning. The dataset comprises a train set (7,473 questions) and a test set (1,319). The environment exposes a calculator tool.

4.2 HotpotQA

The HotpotQA environment is based on the HotpotQA dataset introduced in Yang et al. (2018), which was subsequently extended to a language agent environment in Yao et al. (2023). The dataset comprises 112,779 question-answer pairs. We evaluate agent performance on the 7,405 question eval subset. The environment provides tools to search for and extract information from Wikipedia articles.

4.3 PaperQA

PaperQA (Lála et al., 2023; Skarlinski et al., 2024) was developed for literature research and question answering. By pairing agentic retrieval augmented generation with reranking and contextual summarization, PaperQA attained superhuman-level precision and human-level accuracy on the LitQA2 dataset (Laurent et al., 2024).

We refactored PaperQA into an Aviary environment, modifying the toolset as needed. We modified the `paper_search` tool to center on local storage of PDF, text, and HTML files and omitted the `citation_traversal` tool for this local setting. A `complete` tool was added to support agents that require at least one tool selection, and allow the agent to declare if the answer addresses all parts of the question.

For the sake of comparison against Skarlinski et al. (2024), we obtained LitQA2's private test questions through correspondence with the authors[4], and used an 80\20 split on the 199 public questions for train and eval splits.

4.4 Molecular Cloning

Molecular cloning is a fundamental technique for manipulating DNA in biomedical science, enabling basic research into gene function, transgenic models, and recombinant proteins (Bertero et al., 2017; Sharma et al., 2014). The molecular cloning process results in a DNA "construct," which is a general term for DNA that encodes for the desired biologic molecule or genes.

The molecular cloning environment comprises the main tools used by laboratory scientists: (1) an annotation tool for predicting the function of plasmid segments (2) a natural language search tool that retrieves sequences given text, and (3) tools required to plan protocols. A complete list of tools is provided in Appendix C.

The specific tasks used for evaluation come from the SeqQA benchmark (Laurent et al., 2024), which consists of textbook-style multiple-choice questions on molecular cloning. The SeqQA train set comprises 500 questions from Laurent et al. (2024) as well as 150 new test questions we introduce specifically for the Aviary SeqQA environment[5].

4.5 Protein Stability

We introduce the protein stability environment as a sandbox for training agents to integrate knowledge from physics-based models, biochemical principles, and pre-trained protein models, with the potential to leverage experimental results. We assess the language agent's performance on forty proteins randomly selected from the megascale protein stability dataset, excluding any that are mentioned in the text of Tsuboyama et al. (2023). Proposed mutations are evaluated using the Rosetta cart_ddg protocol (Frenz et al., 2020). Note that we only perform inference time evaluation of language agents on the protein stability task and as such, we do not maintain a train set.

5 Experiments

We assess the capabilities of tool-equipped language agents to solve problems in the aforementioned environments. We subsequently explore behavior cloning and expert iteration (described in Appendix B) to train agents on specific tasks in environments. Finally, we explore the effect of majority vote sampling at inference-time.

An overview of the models and their performance is provided in Figure 2. The trained (described below) and frontier language models versions are `claude-3-5-sonnet-20241022`, `gpt-4o-08-06`, and `Llama-3.1-8B-Instruct`. Our agents are:

[4]The test set is private to prevent leakage to frontier models. The test split may be made available to the reviewers upon request pending permission from the original authors.

[5]These questions are maintained in a private repository to prevent test set leakage to frontier LLMs and can be made available to the reviewers upon request.

- Zero-shot Claude 3.5 Sonnet: The LLM is prompted to solve the tasks without access to the environment. No example output or formatting instructions are given.
- Claude 3.5 Sonnet agent: A language agent prompted to call environment tools until the task is solved. It uses the Anthropic API tool-calling schema (Anthropic, 2024).
- LDP-trained language agent: An LDP agent trained to solve tasks using environment tools. This can either be based on fine-tuned GPT-4o (GSM8K, HOTPOTQA) or Llama-3.1-8B-Instruct (SeqQA, LitQA2).
- Majority voting: We sample 32 trajectories from an agent using their consensus as the task solution. For protein stability, we do oracle-verification/pass@k, as in protein engineering one typically tests a batch and only keeps the most successful (Brown et al., 2024).

The set of existing benchmarks and closed-source models were chosen to demonstrate the flexibility of the Aviary software. Claude 3.5 Sonnet was the best frontier LLM across tasks, and was thus used as the benchmark for comparison. With the exception of GSM8K, all agents improve over the zero-shot baseline when given access to the environment. In the case of GSM8K, we hypothesize that a sequence of calculator calls (with no intermediate reasoning) is out-of-distribution with respect to the LLMs' training data, which also contains math word problems. This is consistent with recent findings (Mirzadeh et al., 2024), where modifying elements of the original questions or adding irrelevant information caused performance degradation, as such changes similarly introduce a distribution shift.

Training LDP agents improves performance over untrained agents of the same architecture. On challenging tasks (SeqQA, LitQA2), a relatively small model (Llama-3.1-8B-Instruct) can be trained to match performance of a much larger frontier model (Claude 3.5 Sonnet). Majority voting yields a further large gain at the cost of increased inference compute. The protein stability task sees a large improvement for pass@16, which is a well-known effect for oracle-verified problems(Brown et al., 2024). These results are described in detail below.

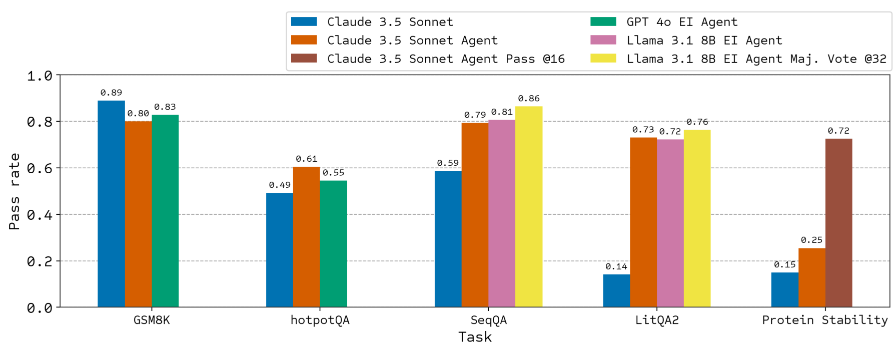

Figure 2: Ability of LLMs and language agents to solve tasks using Aviary environments. All LDP-trained agents are optimized using behavior cloning and expert iteration. For GSM8K and HOTPOTQA, EI is performed on GPT-4o; SeqQA and LitQA2 use Llama-3.1-8B-Instruct (see subsection 5.1). The difference in GSM8K zero-shot reported here (89%) vs Anthropic benchmarks (Anthropic, 2024) (96.5%) is likely because Anthropic's use of chain-of-thought prompting, which we did not use. All agents are rolled out on the environment for a maximum of 10 steps, with the exception of PaperQA (18 steps) and protein stability (20).

5.1 Behavior Cloning and Expert Iteration

Using LDP, we train language agents in the environments described in section 4. Since these environments are challenging, expert iteration initially rejects the majority of trajectories, leading to very slow learning. We therefore begin with behavior cloning, using high-quality trajectories collected by rejection-sampling from a larger LLM. Once the language agent can solve a reasonable fraction of training problems, we switch to expert iteration. All experiments are conducted with Llama-3.1-8B-Instruct (Grattafiori et al., 2024) as the base language model, using Nvidia A100 GPUs.

In Figure 3A, we show the results of training an agent (Llama-3.1-8B EI) to solve SeqQA tasks using the molecular cloning environment. Expert iteration is seeded with 2841 valid trajectories (behavior cloning), followed by 8 further EI epochs. Behavior cloning provides a large initial jump in performance, with a further 14% (absolute) improvement from EI. In Appendix E we study the distribution of trajectories explored by a trained language agent.

In Figure 3B, we show the results of a similar procedure applied to LitQA2 questions in the PaperQA environment. In this case, the untrained Llama-3.1-8B agent has non-trivial performance (30% accuracy), but still significantly improves from behavior cloning (430 trajectories). We aimed to focus training on the more difficult LitQA2 questions, so during expert iteration, we sample trajectories from each task in the dataset with probability:

$$P(\text{task } k) = \frac{w_k}{\sum_j w_j}; \quad w_k = M \cdot (1 - f^k_{\text{pass}}), \tag{3}$$

where f^k_{pass} is a moving average of task k's pass rate as the agent is trained and M is a scaling factor (set to 20). With this, EI produces a small improvement beyond behavior cloning, up to 72% on the test set.

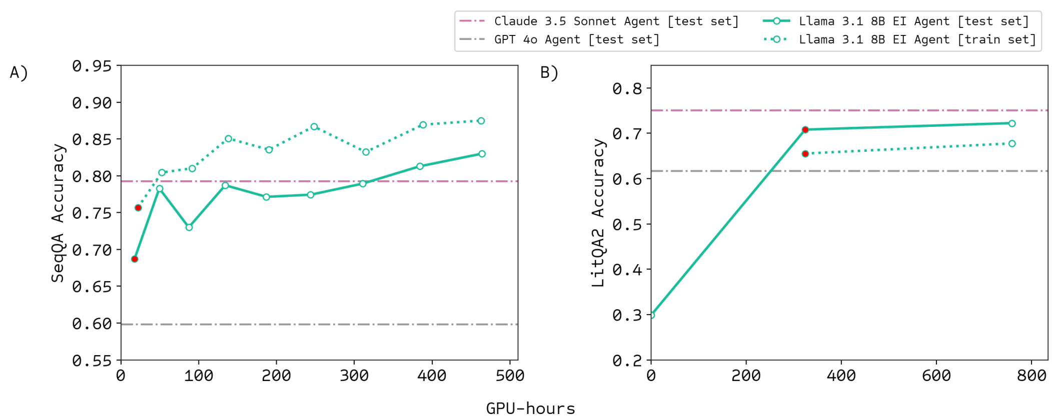

Figure 3: Training language agents to solve (A) SeqQA tasks using the molecular cloning environment and (B) LitQA2 questions using the PaperQA environment. The first epoch (red points) is behavior cloning, followed by expert iteration. These experiments use multiple workers to asynchronously collect trajectories and train the model, so `GPU-hours` measures the total time spent sampling and training. An untrained Llama-3.1-8B agent solves 1% of SeqQA tasks, so we omit the data point at `GPU-hours=0` in panel A.

5.2 Inference Compute Scaling

We assess majority voting on two sets of multiple-choice tasks: SeqQA, and LitQA2, with the results in Figure 4. Majority voting generally affords large improvements, achieving ∼20 percentage points (p.p.) of accuracy gain. Figure 4B demonstrates that non-agentic LLMs benefit as well, with a ∼10 p.p. gain for zero-shot Claude.

Figure 4C shows that majority voting on LitQA2 with a Claude 3.5 Sonnet agent reaches 89% accuracy on the test set, significantly exceeding previously reported scores of 67% from Skarlinski et al. (2024) and the human performance reported in Laurent et al. (2024). The Llama-3.1-8B EI agent performs well, matching human and previously reported best at only a single sample. Three samples exceeds those marks, but cannot match the Sonnet agent if it also uses majority voting on more than one sample. Nevertheless, exceeding a frontier LLM in the single sample setting on unseen data with a small model is a surprising result.

Figure 4A shows that majority voting with the Llama-3.1-8B EI agent significantly exceeds a Claude 3.5 Sonnet agent across all sample counts. SeqQA is more structured than LitQA2, requiring more consistent and longer tool call sequences. The Llama-3.1-8B EI agent can be sampled from cheaply, and so we run 945 rollouts (Figure 4A inset). We observe improvement up to 100s of

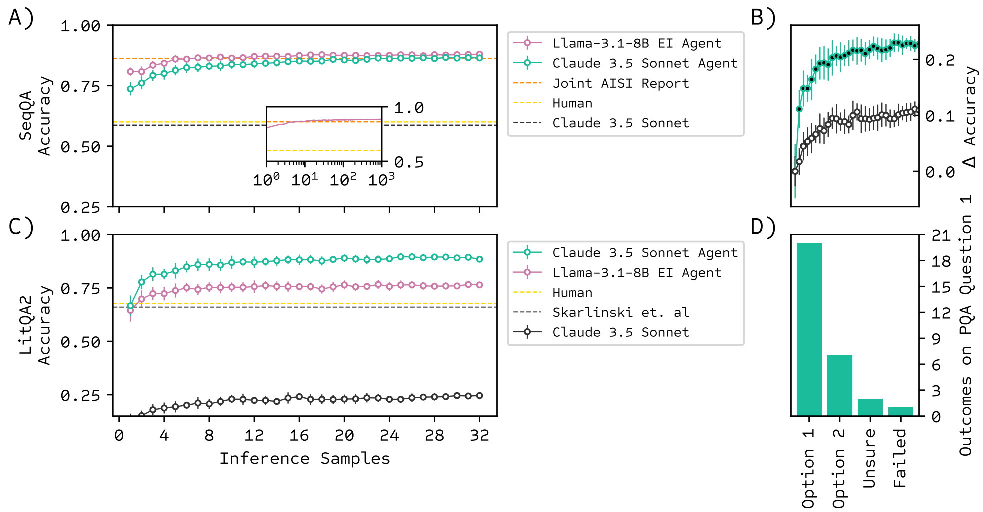

Figure 4: A) majority voting accuracy in SeqQA as a function of number of sampled trajectories. With 32 samples, performance exceeds previously-reported scaffolded agents (Joint AISI Report (US AI Safety Institute, 2024)). The "Claude 3.5 Sonnet" line refers to the zero-shot setting. The inset shows further gains from 0.86 to 0.89 from 32 to 945 samples. B) shows SeqQA improvement from majority voting with an LLM without tools vs. a language agent. C) majority voting accuracy on LitQA2. Both agents significantly exceed previously-measured human and agent performance (Skarlinski et al., 2024). Claude 3.5-Sonnet Agent plateaus at 90% accuracy. D) shows an example question voting on LitQA2 (question id `3e6d7a54`). Option 1 is the correct response, option 2 is incorrect, and failure is because the agent did not submit an answer prior to trajectory termination. Error bars are computed by bootstrap resampling.

samples, yielding a final accuracy of 89%. The highest previously reported result was from a joint technical report from the US and UK AI Safety Institutes on pre-deployment evaluation of `claude-3.5-sonnet-20241022` at 87% accuracy.

5.3 Inference Cost Scaling

The results of the previous sections demonstrate how the performance of different agents scales as training time and sampled trajectories are increased. In this section, we consider a more practical metric: inference cost. This becomes especially relevant in a high-throughput setting, in which agents are tasked to solve thousands of problems in parallel. We focus our comparison on the Claude 3.5 Sonnet agent versus the Llama-3.1-8B EI agent. At the time of writing, Claude 3.5 Sonnet's input tokens cost \$3/1M and output tokens cost \$15/1M [6]. We price Llama 3.1-8B inference at \$0.03/1M input and output tokens, typical in the LLM inference market[7], which we use as a reasonable estimate for EI-trained model inference. In Figure 5, we report performance and inference cost on SeqQA and LitQA2. While majority voting with the Claude 3.5 Sonnet agent clearly outperforms other settings, this requires $\mathcal{O}(\$1)$ per task. We reach the same SeqQA accuracy using the Llama-3.1-8B EI agent for 100x less cost. While this was not achievable for LitQA2, we note that majority voting with Llama-3.1-8B EI still exceeds single-rollout with Sonnet at 3x less cost.

6 Discussion and Limitations

We were motivated to design Aviary and LDP by (a) a need to implement language interfaces to complex scientific environments and (b) a need to optimize agents in these environments. In this work, we have focused on benchmark tasks that are easy to evaluate across five different environments. A surprising, but welcome outcome of our experiments is that trained agents based on relatively

[6] https://www.anthropic.com/pricing#anthropic-api
[7] https://lambdalabs.com/inference#pricing

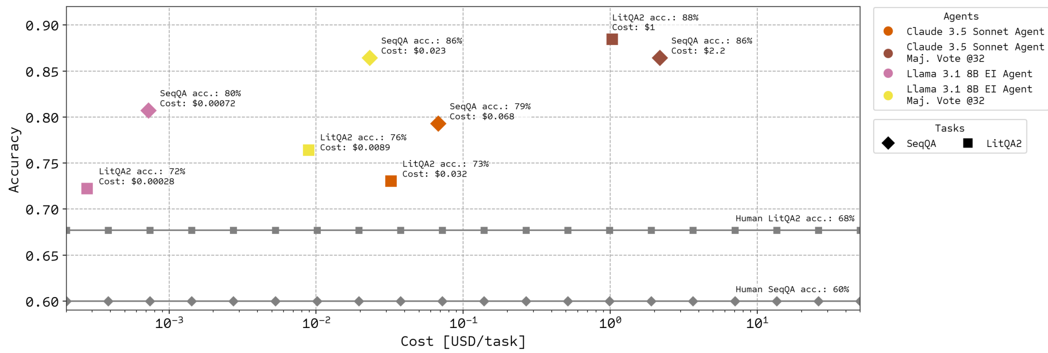

Figure 5: Accuracy vs. inference cost of two agents (Claude 3.5 Sonnet and `Llama-3.1-8B` EI) on the SeqQA and LitQA2 tasks. For both agents, the single-rollout and majority-voting settings are considered. Note that all inference settings here outperform human performance (reported in Skarlinski et al. (2024) and Laurent et al. (2024)).

small language models can compete with or even beat frontier model-based agents. While out of scope for this paper, we anticipate that future work can extend these conclusions by leveraging more sophisticated policy optimization methods (compared to EI) and inference-time scaling (compared to majority voting). To that end, we hope that LDP serves as a useful framework for experimenting with such algorithms.

Small, trained agents reduce inference costs substantially. For reference, our SeqQA tasks require 7-10 LLM calls (Figure 7) and cost $0.07 on average per trajectory with Claude 3.5 Sonnet and $0.00066 with `Llama-3.1-8B` EI. The human PhD contractors that represent the human data series in Figure 4 cost between $4 and $12 per question (see Laurent et al. (2024) for details). In summary, trained agents can exceed the accuracy of human and frontier models at 100x cheaper cost.

There are some limitations in this work. Several of our benchmarks are new or introduce new data and so we are intentionally gating access to the test sets to avoid leakage into pre-training corpora. Our human performance comparison comes with the caveat that human evaluators do not always have access to the exact same toolset. Laurent et al. (2024) gave incentives for correct answers, ample time, and only restricts the use of AI tools. Nevertheless, it is always possible that humans could have been given more expansive or precise technology for the task. Ultimately, the test of these language agents is their ability to make novel scientific discoveries and not simply to achieve high scores on benchmarks.

7 Conclusion

We have presented Aviary, a gymnasium for language agents. Aviary currently contains five environments, three of which focus on challenging scientific tasks. Language agents implemented in these environments exceed the performance of zero-shot frontier LLMs on the SeqQA, HOTPOTQA, LitQA2, and protein stability tasks. Language agents also exceed human performance on SeqQA and LitQA2.

We have introduced the language decision process (LDP) framework for formally describing language agent tasks and showed that language agents can be cast as stochastic computation graphs. Through behavior cloning, expert iteration, and inference-time sampling, we demonstrated that trained `Llama-3.1-8B` EI agents can match and exceed the performance of humans and frontier LLMs in the LitQA2 and SeqQA benchmarks at significantly lower cost. Thus, we have demonstrated that modest compute budgets and model sizes can be competitive at solving realistic scientific tasks. The reported trained `Llama-3.1-8B` EI agents are compute efficient and exceed human-level performance, enabling high-throughput automation of meaningful scientific tasks across biology.

Both the Aviary (`aviary`) and LDP (`ldp`) frameworks are open source and should serve as useful libraries for implementing environments and language agents.

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A Stochastic Computation Graphs for Selected Language Agent Architectures

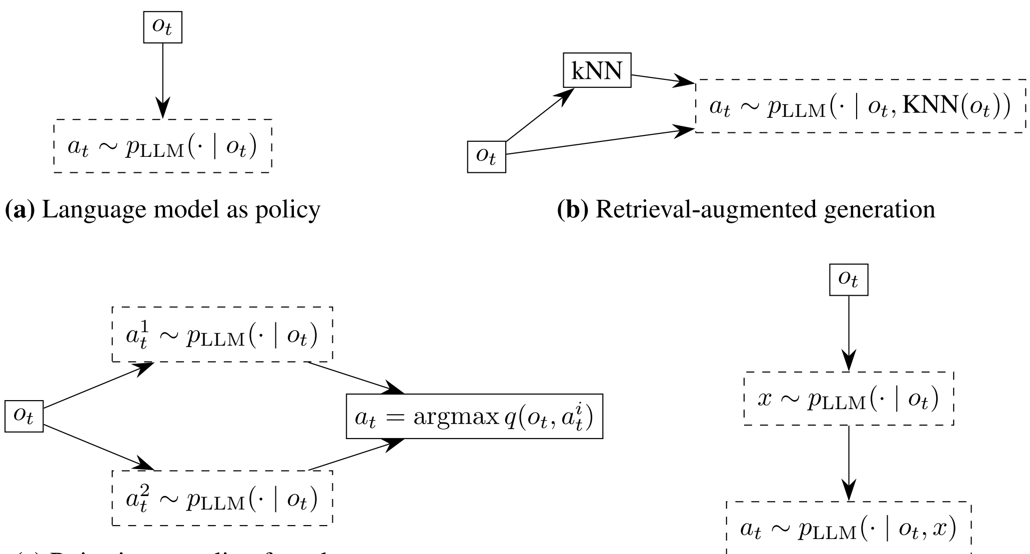
The SCGs of the following simple language agents are presented in Figure 6:

(a) Language model as policy: a single stochastic node corresponding to sampling from the language model.

(b) Retrieval-augmented generation (RAG): a deterministic node (document retrieval) leading to a stochastic node (LLM sampling).

(c) Rejection sampling from LLM: several stochastic nodes (LLM samples), all leading to a deterministic node (selecting the preferred sample).

(d) ReAct (Yao et al., 2023): two consecutive stochastic nodes, corresponding to sampling a reasoning string and an action (tool call).



(a) Language model as policy

(b) Retrieval-augmented generation

(c) Rejection sampling from language model

(d) ReAct

Figure 6: Simple language agent architectures represented as stochastic computation graphs. Deterministic nodes are solid rectangles; stochastic nodes are dashed. Note that we augment the graphs with a deterministic input node to indicate how the observation o_t is consumed.

B Training Methods

Below we describe commonly-used imitation learning (Widrow & Smith, 1964; Chambers & Michie, 1969; Pomerleau, 1988) methods employed to improve language agent performance on our environments. These training methods do not optimize the SCG graph directly, instead we optimize only the language model node in the SCG.

Behavior cloning (BC) BC (Michie et al., 1990; Bain & Sammut, 1995) refers to a general imitation learning technique that derives a policy by supervised learning on high quality trajectories termed expert demonstrations. In the context of language agents this is typically achieved by supervised fine-tuning (SFT) of an LLM on either human trajectories or trajectories generated from a stronger LLM (Christianos et al., 2023; Chen et al., 2023a; Zeng et al., 2023b; Yin et al., 2024; Song et al., 2024). In the context of our experiments, we use BC to initialize the trajectory buffer for an expert iteration loop on `Llama-3.1-8B-Instruct`, due to its inability to self-generate successful trajectories prior to training.

Expert iteration (EI) EI (Anthony et al., 2017; Anthony, 2021; Havrilla et al., 2024) performs behavior cloning in an iterative fashion, improving the demonstration data each iteration. The inputs to the EI algorithm are a base LLM represented as an initial policy π_0 and a trajectory buffer D_0, which may either be empty or consist of an initial set of demonstrations generated by a human expert or a stronger LLM. At each round of EI, first a batch B of trajectories are sampled from the current policy π_i (via rollout). Then these trajectories $\{\tau_i^{(j)}\}_{j=1}^{B}$ are filtered (the rejection sampling step (Yuan et al., 2023)) based on return R exceeding a threshold value ρ. The filtered trajectories are then appended to the trajectory buffer D_i and the current LLM, π_i, is fine-tuned on D_i using cross-entropy loss. Pseudocode for EI is provided in Algorithm 1.

Algorithm 1 Expert Iteration with Rejection Sampling Fine-Tuning

1: **Inputs**: initial policy π_0, iteration rounds N, batch size B, return threshold ρ, trajectory buffer D_0
2: **for** $i = 1, \dots N$ **do**
3: $\quad T_i \leftarrow \text{rollout}(\pi_{i-1})$
4: $\quad D_i \leftarrow D_{i-1} \cup \{(\tau_i^{(j)}, R_i^{(j)}) |\ \tau_i^{(j)} \in T_i, R_i^{(j)} > \rho, j = 1, \dots, B\}$ {Rejection sample trajectories}
5: $\quad \pi_i \leftarrow \text{SFT}(D_i)$ {SFT on updated trajectory buffer}
6: **end for**

Inference Compute Scaling Scaling inference-time compute to improve LLM performance is now a frequently-employed technique (Brown et al., 2024; Wang et al., 2023b). There are two common settings: oracle-verified (pass@k) and majority vote (consensus@k). As shown in Brown et al. (2024), if an oracle verifier can identify any correct solution – namely, if you can obtain just one correct answer among k – then it is possible to scale across multiple orders of magnitude. Without an oracle verifier, majority voting can be used (Wang et al., 2023b). Majority voting is simply the consensus response, which requires some natural binning of responses. Although oracle verification scales to very large numbers of completions (Li et al., 2022), majority voting plateaus more quickly than oracle verification (Brown et al., 2024). In this work, we omit any "unsure" or truncated trajectories (trajectories for which the agent did not submit an answer) from majority voting.

C ENVIRONMENT DETAILS

Below we expand on the details of the environments comprising Aviary including example questions, available tools, and their framing as instances of Language Decision Processes (LDPs). Environment details already mentioned in the main paper are repeated here for clarity. As a reminder, an LDP is defined as follows:

LDP $(\mathcal{V}, \mathcal{S}, \mathcal{A}, \mathcal{O}, T, Z, R, \gamma)$

- $\mathcal{V}$ is an alphabet, a non-empty set, consisting of tokens $w \in \mathcal{V}$.
- $\mathcal{S}$ is the state space.
- $\mathcal{A} \subseteq \mathcal{V}^*$ is the action space.[a]
- $T(s'|s, a) : \mathcal{S} \times \mathcal{A} \mapsto \mathcal{P}(\mathcal{S})$ is the transition function.
- $R(s, a) : \mathcal{S} \times \mathcal{A} \mapsto \mathcal{P}(\mathbb{R})$ is the reward function.
- $\mathcal{O} \subseteq \mathcal{V}^*$ is the observation space.
- $Z(o|s') : \mathcal{S} \times \mathcal{A} \mapsto \mathcal{P}(\mathcal{O})$ is the observation function.[b]
- $\gamma \in [0, 1]$ is the discount factor.

[a] Where $\mathcal{V}^* \stackrel{\text{def}}{=} \bigcup_{n=0}^{\infty} \mathcal{V}^n$ is the Kleene closure of a set $\mathcal{V}$ (Kleene, 1956; Meister et al., 2023).
[b] In all POMDPs we consider, a state $s \in \mathcal{S}$ uniquely defines an observation $o \in \mathcal{O}$. Unless otherwise stated, we will omit Z.

C.1 GSM8K

The GSM8K environment is based on the GSM8K dataset introduced in Cobbe et al. (2021), which consists of linguistically diverse grade school math word problems designed to assess multi-step mathematical reasoning. The GSM8K dataset comprises a training set of 7,473 questions and a test set of 1,319 questions. The GSM8K environment is fully observable and hence reduces to the LDP $(\mathcal{V}, \mathcal{S}, \mathcal{A}, \mathcal{T}, R, \gamma)$.

Example Task: Weng earns $12 an hour for babysitting. Yesterday, she just did 50 minutes of babysitting. How much did she earn?

Tools:

1. Calculator[Expression]: Return the result of a numerical expression.
2. Submit[Answer]: Return the answer.

LDP:

- $\mathcal{V}$: Unicode characters.
- $\mathcal{S}$: GSM8K question, current step in the reasoning process.
- $\mathcal{A}$: {calculator, submit}.
- $\mathcal{T}$: The deterministic transition function.
- R : The reward function:

$$R = \begin{cases} 1 & \text{if the action submits a correct answer,} \\ -1 & \text{if the action is an invalid tool call,} \\ 0 & \text{otherwise.} \end{cases}$$

- γ : Takes on a value of 1.

C.2 HOTPOTQA

The HOTPOTQA environment is based on the HOTPOTQA dataset introduced in Yang et al. (2018), which was subsequently extended to a language agent environment in Yao et al. (2023). The HOTPOTQA dataset comprises 112,779 question-answer pairs. We run evals on the 7,405 eval subset of questions. In the HOTPOTQA environment, the agent is provided with a Wikipedia API and tasked with answering the questions. The agent is not provided with any context and the API supports full access to all articles and sections on Wikipedia.

Example Task: The Battle of Gettysburg was fought in which state and in which year?

Tools:

1. Search[Entity]: Search for an entity on Wikipedia. If a Wikipedia page exists, the first 5 sentences of the page are returned, otherwise the top-5 similar entities from the Wikipedia search engine are returned.
2. Lookup[Keyword]: Return the first sentence featuring the keyword in the current Wikipedia page, simulating Ctrl + F functionality in the web browser.
3. Finish[Answer]: Return the answer.

LDP:

- $\mathcal{V}$: Unicode characters.
- $\mathcal{S}$:{HOTPOTQA question, current Wikipedia page}.
- $\mathcal{A}$: {Search, Lookup, Finish}.
- $\mathcal{T}$: The deterministic transition function.
- R : The reward function:

$$R = \begin{cases} 1 & \text{if the action produces a correct answer,} \\ 0 & \text{otherwise.} \end{cases}$$

- $\mathcal{O}$: The current paragraph (following Search) or sentence (following Lookup) in the Wikipedia page.
- $\mathcal{Z}$: Is 1 in all cases as observations arise deterministically conditioned on the action taken.
- γ : Takes on a value of 1.

C.3 PaperQA

PaperQA2 (Lála et al., 2023; Skarlinski et al., 2024) is a language agent/environment pairing developed for scientific literature research and question answering. The environment exposes tools for full text literature search (`paper_search`), citation traversal (`citation_traversal`), reranking and contextual summarization (`gather_evidence`), and answer given ranked contextual summaries (`generate_answer`). This pairing demonstrated superhuman-level precision and human-level accuracy on version 2 of a multiple choice literature question and answering task, called LitQA2 (Laurent et al., 2024).

To implement this in Aviary, we refactored the agent/environment pairing into a standalone PaperQA environment. This environment is similar to the one used in PaperQA2, with three differences. First, to make it easy for the ML community to use, we modified the `paper_search` tool to center on local storage containing a set of PDF, text, and HTML files using tantivy (Inc., 2024). Second, the `citation_traversal` tool was omitted for this local setting. And third, a `complete` tool was added to allow the agent to declare if the answer addresses all parts of the question.

We evaluate agents on their ability to use the PaperQA environment to solve LitQA2 questions. LitQA2 features 248 questions, 199 of which are publicly available and the remaining 49 were held out as a test set. For the sake of comparison against Skarlinski et al. (2024) we obtain the private test set through correspondence with the authors[8]. The public dataset of 199 questions is randomly partitioned into an 80\20 split with 149 train questions and 40 eval questions.

To build the tantivy search indices, we (1) aggregated all paper search or citation traversal results from many PaperQA2 invocations, (2) binned the results corresponding to each LitQA2 question, and (3) combined bins based our train, evaluation, and test split LitQA2 questions. The end result is

[8]The test set is private to prevent test set leakage to frontier models. The test split may be made available to the reviewers upon request pending permission from the original authors.

18955 DOIs in the train split, 5457 DOIs in the evaluation split, and 5519 DOIs in the test split[9]. The large number of distractor papers in each split's index forms a learnable retrieval task for language agents. To avoid copyright infringement of the underlying papers, we only distribute the paper DOIs, and not the parsed texts used by the environment.

Finally, we note that our local PaperQA environment is capable of tasks beyond LitQA2. For example, it can do literature review writing and contradiction detection as reported in Skarlinski et al. (2024).

Example Task: Which base editor has been shown to be the most efficient for inducing the mutation K352E in CD45 in human T-cells?

A) ABE8e-NG
B) ABE8e–SpRY
C) SPACE-NG
D) ABE8e-SpG
E) Insufficient information to answer this question

Tools:

1. `paper_search(query: str, min_year: int | None, max_year: int | None)` - Full-text semantic search through a local search index.
2. `gather_evidence(question: str)` - Perform LLM reranking and contextual summarization given a question on `paper_search` results.
3. `gen_answer()` - Attempt to answer given the top ranked contextual summaries.
4. `complete(has_successful_answer: bool)` - Terminate using the last proposed answer, with the argument declaring whether the answer addressed all parts of the question.

LDP:

- $\mathcal{V}$: Unicode characters.
- $\mathcal{S}$:{paper chunks, metadata, ranked contextual summaries and final answer}.
- $\mathcal{A}$: {`paper_search`, `gather_evidence`, `gen_answer`, `complete`}.
- $\mathcal{T}$: Nondeterministic, as the `gather_evidence` and `gen_answer` tools rely on LLM completions.
- R :
$$\begin{cases} 1 & \text{correct answer,} \\ -1 & \text{incorrect answer,} \\ 0.1 & \text{unsure answer.} \end{cases}$$
- $\mathcal{O}$: Same as $\mathcal{S}$.
- $\mathcal{Z}$: Controlled by the stochasticity of LLM temperature sampling in `gather_evidence` and `gen_answer`.
- γ : Takes on a value of 0.9.

C.4 Molecular Cloning

Molecular cloning is a fundamental technique for manipulating DNA in biomedical science, enabling basic research into gene function, transgenic models, and recombinant proteins (Bertero et al., 2017; Sharma et al., 2014). The molecular cloning process results in a DNA "construct," which is a general term for DNA that encodes for the desired biologic molecule or genes. Molecular cloning involves assembling DNA fragments, ligating them into vectors, introducing the recombinant DNA into host organisms, and screening for desired clones (Bertero et al., 2017). The steps in molecular cloning are

[9]The train, evaluation, and test split DOIs can be made available to the reviewers upon request.

usually undertaken using a combination of human planning, specialized software, and databases of known purchasable components.

The molecular cloning environment comprises the main tools used by laboratory scientists: (1) an annotation tool for predicting the function of plasmid segments (2) a natural language search tool that retrieves sequences given text, and (3) tools required to plan protocols. Applications for protocol-specific tools include PCR primer design, ligation, codon optimization, Gibson or Golden gate assembly, and fetching genes from standard organisms. Many implementations use or are derived from the Go Poly library (Bebop, 2025). The annotation tools were built using MMSeqs2 (Steinegger & Söding, 2017).

The specific tasks used for evaluation come from the SeqQA benchmark (Laurent et al., 2024), which consists of textbook-style multiple-choice questions broken down into 15 subtasks designed to cover diverse properties of DNA, RNA, and protein sequences, as well as common tasks in molecular biology workflows such as restriction digests and polymerase chain reactions (PCR). The SeqQA train set comprises 500 questions from Laurent et al. (2024) as well as 150 new test questions we introduce specifically for the Aviary SeqQA environment[10]. The SeqQA task is solvable using only a subset of the tools, and the tools have *not* been engineered specifically for the conventions of SeqQA. For example, SeqQA questions assume 1-indexing, but the tools are 0-indexed and thus the language agent needs to learn to convert indices. Another example illustrating that that the tools are not engineered specifically for SeqQA is that SeqQA only considers coding open reading frames, but the tools may consider both reading frames.

In the molecular cloning environment, it is worth nothing that the combination of tools for manipulating DNA constructs, annotating sequences or plasmids, and searching for DNA components in databases facilitates tasks beyond SeqQA. The environment also supports working with "CloningScenarios," which is a multiple-choice benchmark for working with DNA constructs derived from real laboratory notebooks (Laurent et al., 2024). One can also perform more normative plasmid tasks, an example prompt being, "Clone the given protein [protein] into [plasmid] to express in yeast with a GFP fusion (check annotations above, plus GFP in correct relative orientation)."

Example Task:

Which of the following RNA sequences contains an ORF that is most likely to have high translation efficiency in a human cell?

A) [RNA sequence 1]
B) [RNA sequence 2]
C) [RNA sequence 3]
D) [RNA sequence 4]
E) Insufficient information to answer this question

Tools:

1. `search(query: str)` - Search Plasmid and NCBI nucleotide databases.
2. `annotate(sequence: Sequence)` - Annotate proteins, ORFs, restriction sites in a DNA sequence.
3. `gibson(sequences: list[Sequence])` - Simulate gibson assembly.
4. `goldengate(sequences: list[Sequence], enzyme: str)` - Simulate golden gate assembly.
5. `simulate_pcr(sequence: Sequence, forward_primer: Sequence | None, forward_primer_name: str | None)` - Simulate polymerase chain reaction.
6. `optimize_translation(sequence: Sequence, cg_content: int, codon_table: int, min_repeat_length: int)` - Codon optimization.
7. `separate(sequences: list[Sequence])` - Simulate gel electrophoresis.

[10]These questions are maintained in a private repository to prevent test set leakage to frontier LLMs and can be made available to the reviewers upon request.

8. `enzyme_cut(sequence: Sequence, enzyme: str)` - Simulate restriction digest.
9. `search(query: str)` - Search Plasmid and NCBI nucleotide databases.
10. `annotate(sequence: Sequence)` - Annotate proteins, ORFs, restriction sites in a DNA sequence.
11. `gibson(sequences: list[Sequence])` - Simulate gibson assembly.
12. `goldengate(sequences: list[Sequence], enzyme: str)` - Simulate golden gate assembly.
13. `simulate_pcr(sequence: Sequence, forward_primer: Sequence | None, forward_primer_name: str | None)` - Simulate polymerase chain reaction. Primers can be sequence (by ref) or name of enzyme or sequence value.
14. `optimize_translation(sequence: Sequence, cg_content: int, codon_table: int, min_repeat_length: int)` - Codon optimization.
15. `separate(sequences: list[Sequence])` - Simulate gel electrophoresis.
16. `enzyme_cut(sequence: Sequence, enzyme: str)` - Simulate restriction digest.
17. `find_sequence_overlap(sequence1: Sequence, sequence2: Sequence, reverse: bool)` - Find overlapping regions between two sequences.
18. `find_orfs(sequence: Sequence, min_length: int, codon_table: int, strand: int)` - Find open reading frames in a DNA sequence.
19. `design_primers(sequence: Sequence, target_tm: float, forward_overhang_name: str, reverse_overhang_name: str)` - Design PCR primers for a sequence.
20. `merge(sequences: list[Sequence])` - Combine multiple sequences, needed to do assembly simulation.
21. `add(sequence1: Sequence, sequence2: Sequence)` - Add two sequences together.

Tools Continued:

22. `slice_sequence(sequence: Sequence, start: int, end: int, name: str)` - Extract a subsequence.
23. `view_translation(sequence: Sequence)` - View the amino acid translation of a DNA sequence.
24. `view_sequence_stats(sequence: Sequence)` - View sequence statistics.
25. `view_restriction_sites(sequence: Sequence)` - View restriction enzyme cut sites.
26. `view_sequence(sequence: Sequence)` - View the raw sequence.
27. `submit_answer(answer: str)`

LDP:

- $\mathcal{V}$: Unicode characters.
- $\mathcal{S}$: A set of reference DNA sequences, provided by the task or obtained from previous actions. A protocol with the steps taken so far. Current reward.
- $\mathcal{A}$: A text sequence generated using the vocabulary, which should specify a tool to use and its parameters, though not all sequences will necessarily form valid or usable actions.
- $\mathcal{T}$: A transition function that executes the selected action and as a result can add more reference DNA sequences, extend the protocol, or propose a final answer.
- R :
$$\begin{cases} 1 & \text{correct answer,} \\ -1 & \text{incorrect answer,} \\ 0.1 & \text{unsure answer.} \end{cases}$$
- $\mathcal{O}$: A list of names and statistics of sequences in $\mathcal{S}$.
- $\mathcal{Z}$: 1.0 in all cases as observations arise deterministically from the state.
- γ : Takes on a value of 1.0.

C.5 Protein Stability

Engineering proteins with increased stability is a crucial task in protein engineering, with broad applications in enzyme engineering and drug design (Sheldon & Woodley, 2018). Protein engineering remains challenging, however, due to the complex interplay of sequence, structure, and biological factors (Goldenzweig & Fleishman, 2018). Integrating sequence and structure-based methods, including tools such as Rosetta, affords a more comprehensive pipeline for improving protein stability (Laimer et al., 2015).

We introduce the protein stability environment as a framework for training agents that can effectively integrate knowledge from physics-based models, biochemical principles, and pre-trained protein models with the potential to leverage experimental results to improve protein stability. The protein stability environment consists of tools commonly used by human experts for analyzing protein sequences and structures, including (1) a biochemical description tool to identify residue bond types, (2) a sequence property tool to calculate molecular weight, aromaticity, instability index, isoelectric point, sequence charge, and hydropathy, (3) a secondary structure annotation tool, and (4) a Rosetta-based tool to calculate the aggregation propensity scores per residue (Lauer et al., 2012). We assess the language agent's performance on 40 proteins randomly selected from the megascale protein stability dataset, excluding any that are mentioned in the text of Tsuboyama et al. (2023). Proposed mutations are evaluated using the Rosetta cart_ddg protocol (Frenz et al., 2020). Note that we only perform inference time evaluation of language agents on the protein stability task and as such, we do not maintain a train set.

Prior work on utilizing LLMs for protein design include 310.ai (2024), which introduced a chat-based interface for protein design, and ProtAgents (Ghafarollahi & Buehler, 2024), a multi-agent platform for protein design that integrates deep learning models trained on protein structure data (Ingraham et al., 2023; Wu et al., 2022) with physics-based simulations. LLMs have also proven effective as biological sequence optimizers (Chen et al., 2024a).

Example Task: Design at least 3 mutations and a maximum of 7 mutations to the protein sequence MKVMIRKTATGHSAYVAKKDLEELIVEMENPALWGGKVTLANGWQLEL-PAMAADTPLPITVEARKL that would improve its stability. The sequence of this protein is provided in the text file located at {input_txt_path}, and the structure of the protein can be found in the PDB file located at {input_pdb_path}.

Tools:

1. `get_bond_types_between(residues: list[int], bond_type: str)` - Describes all instances of the specified bond type among a given list of residues as outlined in the function description.
2. `get_secondary_structure(pdb_string: str)` - Describes secondary structure elements found in the protein structure by residue.
3. `get_sequence_properties(mutations: list[str], return_wt: bool)` - Describes properties like instability index, molar extinction coefficient, fraction of charged residues, iso-electric point.
4. `get_distance_between_residues(mutation: list[str])` - Get pairwise distances between list of residues.
5. `get_residue_at_position(residues: list[int])` - Returns the residue present at a specific position and describes whether it is acidic or basic or charged, polar or aliphatic or aromatic.
6. `get_hydrophobicity_score(local_pdb_file: str)` - Calculates aggregation propensity by residue using Rosetta.
7. `get_mutant_protein_sequence(mutations: list[str])` - Returns the sequence of the protein after the mutations are applied to the sequence.
8. `complete(mutations: list[str])` - Terminate after proposing mutations to the protein sequence

LDP:

- $\mathcal{V}$: Unicode characters.
- $\mathcal{S}$: path to a .pdb file containing the protein structure renumbered from 1, path to a .txt file containing the protein sequence and list of mutations proposed.
- $\mathcal{A}$: {`get_bond_types_between`, `get_secondary_structure`, `get_sequence_properties`, `get_distance_between_residues`, `get_residue_at_position`, `get_hydrophobicity_score`, `get_mutant_protein_sequence`, `complete`}
- $\mathcal{T}$: A transition function that executes the selected action and as a result can update the proposed stabilizing mutations to the protein sequence.
- R :

$$\begin{cases} 1 & \text{if Rosetta } \Delta\Delta G < 0, \\ 0 & \text{otherwise.} \end{cases}$$

- $\mathcal{O}$: sequence or structure descriptions of wild type sequence or proposed mutations
- $\mathcal{Z}$: 1.0 in all cases as observations arise deterministically from the state.
- γ : Takes on a value of 1.0.

D FURTHER RELATED WORK

Below we discuss further related work on language agent optimization frameworks and benchmarks.

Language Agent Optimization Frameworks Continued Amongst methods that jointly optimize language agent components, the TextGrad framework (Yuksekgonul et al., 2024) backpropagates feedback received from an LLM. Zhou et al. (2024) also backpropagate textual feedback by creating natural language simulacra of weights, losses, and gradients. Hu et al. (2024a) uses a metaprompt to encourage an LLM to perform discrete optimization of an agent architecture. The OptoPrime optimizer in the Trace framework (Cheng et al., 2024) passes code execution traces and uses an LLM to perform updates. DSPy (Khattab et al., 2022; Singhvi et al., 2023; Khattab et al., 2024) parametrizes a computational graph for language agents and automatically generates useful demonstrations for in-context learning. In the multi-agent setting, GPTSwarm (Zhuge et al., 2024) introduces a computation graph and performs binary edge-level optimization and node-level optimization over prompts. Lastly, OpenR (Wang et al., 2024b) is a framework for LLM reinforcement learning and inference-time scaling, but is targeted at token-level optimization, not tool usage.

Language Agent Benchmarks Existing language agent benchmarks feature a broad range of applications including machine learning tasks (Huang et al., 2024b), data science (Guo et al., 2024b; Grosnit et al., 2024), data analysis (Hu et al., 2024c; Li et al., 2024), quantitative reasoning (Liu et al., 2024), and causal reasoning (Jin et al., 2023). In Aviary, we place particular focus on scientific tasks. Relevant work in this area has included DiscoveryBench, a benchmark for data-driven hypothesis generation (Majumder et al., 2024), ChemBench (Mirza et al., 2024) which focuses on chemistry tasks, BLADE (Gu et al., 2024) which is concerned with data-driven science, SciAgent (Ma et al., 2024b) a benchmark for scientific reasoning, DISCOVERYWORLD (Jansen et al., 2024) which concentrates on cycles of scientific discovery, and ScienceWorld (Wang et al., 2022) which is concerned with scientific reasoning. For a review focused on scientifically-relevant agents the reader is directed to Ramos et al. (2024). In Aviary, we focus on sequential decision-making tasks that necessitate multiple steps of agent-environment interactions. We construct environments from the pre-existing datasets such as GSM8K (Cobbe et al., 2021), HOTPOTQA (Yang et al., 2018), and LitQA2 (Skarlinski et al., 2024) by casting them as parametrizable tools manipulating an environment state.

E DISTRIBUTION OF TRAINED LANGUAGE AGENT TRAJECTORIES

In Figure 7, we study the distribution of SeqQA trajectories explored by a trained language agent in a Sankey diagram of the tool call patterns. The demonstration trajectories (all successful) heavily feature assembly simulations and are relatively long. The trained agent was initially cloned from the demonstrations, but through online learning discovered significantly different ways to solve SeqQA tasks. The agent's trajectories are generally shorter and less diverse, suggesting that self-training tends to converge on a subset of possible paths.

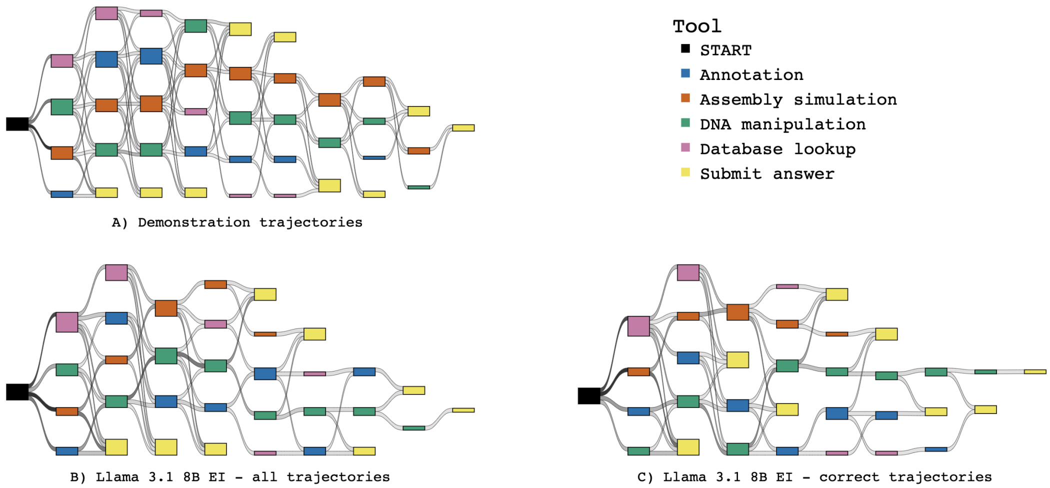


Figure 7: Patterns of tool calls across trajectories. Colored boxes represent different tool categories, and edges between boxes represent consecutive actions taken in a trajectory, with darker edges implying a greater number of trajectories. In panel (A), we show the demonstration trajectories used for behavior cloning. Panels (B) and (C) show the trajectories sampled from the `Llama-3.1-8B` EI agent after expert iteration.

F CODE EXAMPLES

Below is an example of a simple Aviary environment that maintains an integer counter. More realistic and complex examples are provided in the codebase and associated documentation.

```python
from collections import namedtuple
from aviary.core import Environment, Message, ToolRequestMessage, Tool

# State in this example is simply a counter
CounterEnvState = namedtuple('CounterEnvState', ['count'])

class CounterEnv(Environment[CounterEnvState]):
    """A simple env that allows an agent to modify a counter."""

    async def reset(self):
        self.state = CounterEnvState(count=0)
        self.tools = [
            # Parse signatures and docstrings
            # into Tool objects housing tool schemae
            Tool.from_function(self.incr),
            Tool.from_function(self.decr),
        ]
        return [Message(content=f"counter={self.state.count}")], self.tools

    async def step(self, action: ToolRequestMessage):
        obs = self.exec_tool_calls(action)
        reward = self.state.count ** 2
        # Returns observations, reward, done, truncated
        return obs, reward, reward < 0, False

    def incr(self):
        """Increment the counter."""
        self.state.count += 1
        return f"counter={self.state.count}"

    def decr(self):
        """Decrement the counter."""
        self.state.count -= 1
        return f"counter={self.state.count}"
```

Building on this, below is an example of a simple LDP agent illustrating how to sample trajectories in an environment.

```python
from ldp.agent import Agent
from ldp.graph import LLMCallOp
```

```python
from ldp.runners import RolloutManager

class AgentState:
    def __init__(self, messages, tools):
        self.messages = messages
        self.tools = tools

class SimpleAgent(Agent):
    def __init__(self, **kwargs):
        self.llm_call_op = LLMCallOp(**kwargs)

    async def init_state(self, tools):
        return AgentState([], tools)

    async def get_asv(self, agent_state, obs):
        action = await self.llm_call_op(
            config={"model": "gpt-4o", "temperature": 0.1},
            msgs=agent_state.messages + obs,
            tools=agent_state.tools,
        )
        new_state = AgentState(
            messages=agent_state.messages + obs + [action],
            tools=agent_state.tools,
        )
        # Return action, state, value (hence get_asv)
        return action, new_state, 0.0

agent = SimpleAgent(config={"model": "my_llm_endpoint"})
runner = RolloutManager(agent=agent)
trajectories = await runner.sample_trajectories(
    environment_factory=CounterEnv,
    batch_size=2,
)
```