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ML-AutoResearch: Training Machine Learning Research Agents with Automatically Generated Environments

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Abstract

With the advent of AI agents, automated scientific discovery is becoming an increasingly plausible goal. However, training agents to autonomously execute the engineering-heavy labor of machine learning (ML) research requires massive, process-level supervision. Existing static benchmarks omit critical intermediate steps such as debugging and incremental reasoning, and manual data collection is prohibitively expensive. To overcome this data bottleneck, we introduce ML-AutoResearch (ML-AR), a scalable pipeline for automatically generating synthetic, end-to-end ML research tasks. Each task defines a complete research cycle, including problem specification, dataset selection, baseline implementation, and iterative improvement. To ensure realism and executability, tasks are grounded in real-world datasets and refined via an automated self-debugging procedure without requiring human supervision. We construct a large-scale dataset of teacher trajectories on these synthetic tasks to train student agents via supervised fine-tuning. We evaluate the resulting agents across 3 diverse ML research benchmarks. Our comprehensive experiments across 2 distinct model families and 3 model sizes demonstrate that training on ML-AR trajectories yields consistent and significant capability gains. Fine-tuning improves the Aggregation Under the Performance (AUP) by up to 9% and substantially boosts overall pass rates, highlighting robust out-of-domain generalization.

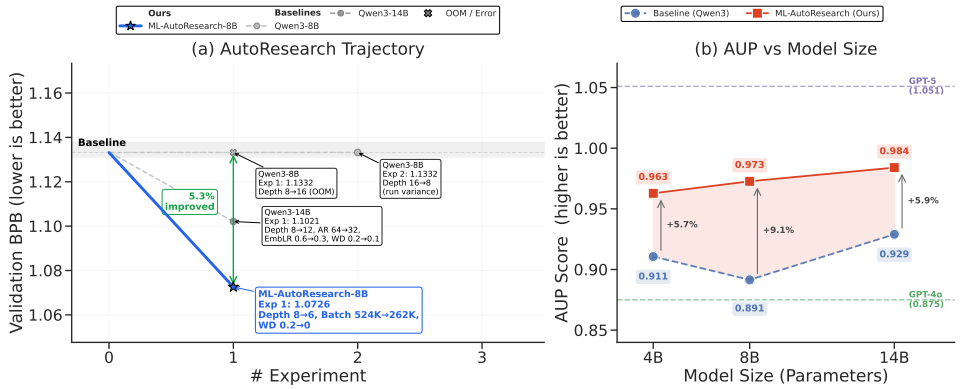


Figure 1: **Generalizability of ML-AutoResearch Models.** Performance comparison with the base instruction model across the MLGym and AutoResearch benchmarks.

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1 Introduction

One of the longstanding goals of artificial intelligence is to enable autonomous scientific discovery. Recently, automating AI research has shifted from a long-term academic vision to an immediate industry focal point, driven by advanced coding capabilities that allow AI systems to reliably execute the engineering-heavy labor of machine learning development. Building autonomous systems to drive end-to-end AI R&D is now a central pursuit for frontier laboratories, with academic prototypes like AI Scientist Lu et al. [2024], Co-Scientist Gottweis et al. [2025], and AlphaEvolve Novikov et al. [2025] demonstrating early success. Although current large language models (LLMs) have internalized vast amounts of ML theory and programming knowledge Brown et al. [2020], Touvron et al. [2023], static comprehension alone is insufficient. Effective research requires the ability to iteratively act, evaluate, and refine decisions over extended horizons.

However, training capable ML agents to operate autonomously is fundamentally challenging. ML research is an open-ended, long-horizon endeavor requiring deep domain expertise, complex library-specific coding, and robust error recovery. Consequently, teaching an agent to navigate this space requires massive, diverse, and process-level supervision in the form of step-by-step reasoning and interaction traces. A central bottleneck in the field is the absence of such data. Gathering it manually is prohibitively expensive, and existing human-authored benchmarks expose only a handful of curated tasks, failing to provide the scale and diversity needed for stable agentic supervised fine-tuning.

Existing approaches to training coding and ML agents typically rely on static artifacts such as completed papers, code repositories, or static benchmarks Yang et al. [2024], Nathani et al. [2025]. These resources capture final outcomes but critically omit the intermediate steps essential for learning: failed experiments, debugging cycles, and incremental reasoning. While related efforts in agent training and tool use highlight the importance of interaction Yao et al. [2022], Schick et al. [2023], they lack scalable methods to generate diverse, process-level training data. As a result, agents trained on these signals struggle to translate static knowledge into effective, multi-step problem solving.

To address this limitation, we introduce **ML-AutoResearch (ML-AR)**, a scalable pipeline for generating synthetic ML research tasks together with rich agentic trajectories. Each generated task instantiates an end-to-end research cycle, including problem formulation, dataset selection, baseline implementation, and iterative improvement. The pipeline grounds tasks in real-world datasets through external verification and improves reliability via an automated self-debugging loop. Importantly, ML-AR is compatible with the task-agnostic SWE-agent framework Yang et al. [2025b], enabling the generation of diverse research scenarios across domains with minimal manual effort.

We evaluate our approach on MLGym Nathani et al. [2025], MLAgentBench Huang et al. [2023], and AutoResearch, comprehensive benchmarks for ML agents comprising diverse tasks that require improving baseline implementations within a fixed interaction budget. In this setting, agents iteratively modify code, run experiments, and revise solutions based on execution feedback. From 1,000 sampled topics, ML-AR produces 555 verified task environments and approximately 34K teacher trajectories, which are filtered to 17K high-quality examples. The verified environments are not uniformly easy for GPT-5: it never improves the baseline on 195 tasks (35.1%) and produces no valid solution on 72 tasks (13.0%), indicating that the task pool spans its capability boundary. Across three evaluation seeds, fine-tuning Qwen3-4B, Qwen3-8B, and Qwen3-14B models Yang et al. [2025a] improves mean MLGym AUP by 5.7%, 9.1%, and 5.9%, respectively. Mixing additional GPT-5.4 trajectories into the 14B training set further raises its AUP by 7.0% over the baseline model. ML-AR also improves normalized MLAgentBench performance at every model size and transfers to AutoResearch. Finally, replacing GPT-5 with Qwen3-32B for trajectory generation still improves 8B and 14B students, showing that useful training trajectories are not specific to a proprietary teacher. Our primary contributions are summarized as follows:

- We propose ML-AutoResearch, a scalable pipeline for generating synthetic, end-to-end ML research tasks grounded in real-world data without human supervision, including tasks that remain challenging for GPT-5.

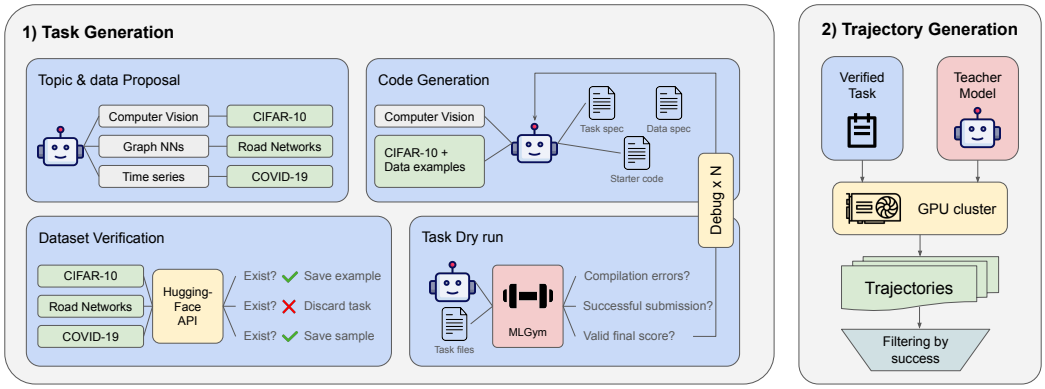


Figure 2: **Overview of the ML-AutoResearch framework**. **Stage 1:** Generate diverse research topic ideas. **Stage 2:** Verify each research topic by identifying a corresponding real-world dataset and discard topics for which no suitable dataset exists. **Stage 3:** Generate baseline code and evaluation pipelines for agents to solve the machine learning tasks. **Stage 4:** Execute tasks on a computational cluster, collect interaction trajectories, and select the best-performing trajectories.

- We construct a large dataset of agentic trajectories that capture iterative research behavior, including debugging and refinement over long horizons.
- We demonstrate consistent gains across two model families and three diverse ML benchmarks, including when Qwen3-32B replaces GPT-5 as the trajectory-generation teacher.

2 Related Work

Recent work has increasingly explored the use of LLM-based agents to automate scientific research, ranging from ideation to end-to-end paper generation. Systems like AI Co-Scientist Gottweis et al. [2025] and Bit-Flip O'Neill et al. [2025] focus heavily on generating novel hypotheses, while frameworks such as The AI Scientist Lu et al. [2024] attempt full hypothesis-to-paper research loops. However, downstream studies reveal a pronounced ideation-execution gap, where models propose novel ideas but struggle to reliably implement them Si et al. [2025], Siegel et al. [2024]. To measure these execution capabilities, several benchmarks have been introduced, including MLE-Bench for Kaggle-style engineering Chan et al. [2024], PaperBench for paper replication Starace et al. [2025], and long-horizon environments like MLAgentBench, MLGym, and MLRC-Bench Huang et al. [2023], Nathani et al. [2025], Zhang et al. [2025], Chen et al. [2025]. These evaluations consistently show that while agents can navigate established pipelines, they struggle with robust planning and genuinely novel method discovery over long horizons.

To address these execution shortcomings, there is a growing need for scalable methods to generate process-level training data. Because human-authored benchmarks are too small for stable agentic fine-tuning, recent efforts have turned to synthetic data generation. In software engineering, for example, SWE-Smith scales task generation by synthesizing test-breaking instances across Python codebases to improve downstream agent performance Yang et al. [2025b]. Similarly, automated loops have been used to generate targeted optimization tasks, such as NanoGPT speedruns Zhao et al. [2025]. Our work, ML-AutoResearch, builds directly upon these paradigms. By algorithmically synthesizing and verifying end-to-end ML research tasks, we provide the massive, process-level supervision required to bridge the execution gap and improve autonomous discovery on rigorous benchmarks like MLGym and MLAgentBench.

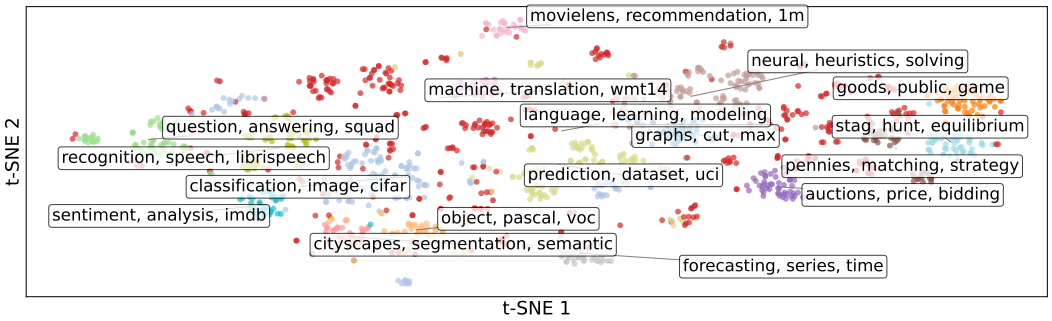


Figure 3: **Demonstration of Research Topic Diversity.** Overview of the diversity of topics generated during topic sampling.

3 ML-AutoResearch Framework

Machine learning (ML) agents hold the potential to accelerate scientific discovery by autonomously conducting ML workflows through code editors and command-line interfaces. However, training these agents is fundamentally challenging. Navigating open-ended, long-horizon ML research requires deep domain expertise and robust error recovery, demanding massive, diverse, process-level supervision for supervised fine-tuning (SFT). A central bottleneck in the field is the absence of such data: manual collection is prohibitively expensive, and existing human-authored benchmarks expose only a handful of curated tasks, failing to provide the necessary scale.

Inspired by recent successes in synthetic data generation, we hypothesize that the vast repositories of open-source datasets can be transformed into an infinite curriculum of structured ML tasks. Our core insight is to utilize a highly capable "teacher" LLM as an automated environment architect to dynamically synthesize high-quality, executable ML research environments at scale without human annotation. To this end, we introduce ML-AutoResearch (ML-AR), an end-to-end pipeline organized into three phases: (1) environment synthesis, which proposes tasks grounded in real-world datasets, (2) environment verification, which filters out ill-posed tasks via a teacher-driven self-debugging loop, and (3) trajectory generation and filtering, which curates large-scale agent rollouts for downstream training. We first formalize the problem setting and then describe each phase in detail. An overview is given in Figure 2.

3.1 Problem Statement

We consider an agent that interacts with an ML research environment in the SWE-agent interaction format adopted by MLGym. A task is a tuple $T = (q, d, \mathcal{C}, \mathcal{V})$, where q is a natural-language specification of a machine learning problem, d is a dataset descriptor, $\mathcal{C}$ is a collection of starter and helper code files providing a baseline implementation, and $\mathcal{V}$ is an evaluation procedure that maps any candidate submission to a scalar score $s \in \mathbb{R}$. Given T, an agent π interacts with an execution environment $\mathcal{E}_T$ for at most H rounds; at round t it observes a context o_t (file contents, previous tool outputs, evaluator feedback) and produces a reasoning trace and an action $(h_t, a_t) \sim \pi(\cdot \mid o_{\leq t}, a_{<t})$, where a_t may inspect or edit files, run shell commands inside a sandboxed virtual environment, or submit a candidate solution; multiple submissions are permitted within the budget H. The interaction yields a trajectory $\tau = (o_0, h_1, a_1, o_1, \ldots, h_{H'}, a_{H'}, o_{H'})$ with $H' \leq H$, whose performance on T is summarized by the best score $s^\star(\tau, T) = \max_{a_t \in \tau:\,\text{submission}} \mathcal{V}(a_t)$. We assume access to a strong teacher policy π_{T} (in our case GPT-5) and aim to train a student policy π_θ via maximum-likelihood imitation of teacher trajectories,

$$\min_\theta \; \mathbb{E}_{T \sim p(T)} \, \mathbb{E}_{\tau \sim p_{\pi_{\mathrm{T}}}(\tau \mid T)} \left[-\sum_{t=1}^{H'} \log \pi_\theta\big(h_t,\, a_t \mid o_{\leq t},\, a_{<t}\big) \right], \tag{1}$$

Restricted to trajectories that pass the filter described in Section 3.4, optimizing Eq. 1 requires a large and diverse task distribution $p(T)$. However, human-curated benchmarks cover only a limited set of tasks, making them insufficient for stable agentic SFT. To address this, ML-AutoResearch constructs $p(T)$ algorithmically by inducing a distribution $\widehat{p}(T) = p(T \mid \pi_{\mathrm{T}}, \mathcal{H})$ over executable, dataset-grounded ML research tasks using the teacher π_{T} and the HuggingFace dataset hub $\mathcal{H}$. This induced distribution serves as a surrogate for $p(T)$ in Eq. 1, and is used to sample, verify, and generate trajectories.

Algorithm 1 Self-debugging verification loop for a candidate task T_i.

Input: candidate T_i, teacher π_{T}, max iterations K, debug probability p_{debug}
for $j = 1, \ldots, K$ **do**
  Execute π_{T} on T_i in $\mathcal{E}_{T_i}$, collect error log ε_j
  if $\varepsilon_j = \varnothing$ **then**
    return T_i ▷ verified
  end if
  Sample $u \sim \mathrm{Uniform}(0, 1)$
  Regeneration step
  if $u < p_{\mathrm{debug}}$ **then**
    Regenerate $\mathcal{C}_i \sim \pi_{\mathrm{T}}(\mathcal{C} \mid q_i, d_i, \varepsilon_j)$ ▷ repair
  else
    Regenerate $\mathcal{C}_i \sim \pi_{\mathrm{T}}(\mathcal{C} \mid q_i, d_i)$ ▷ restart
  end if
end for
return discard

3.2 Phase 1: Environment Synthesis

The first phase samples candidate tasks from $\widehat{p}(T)$. To encourage breadth without sacrificing executability, we factor task generation into three conditional steps that are each implemented as a structured prompt to the teacher π_{T}.

Stage 1: Topic sampling. We first draw a set of N machine learning topics $\mathcal{Z} = \{z_1, \ldots, z_N\} \sim \pi_{\mathrm{T}}(z)$, where each z_i is a short natural-language descriptor of a research area (e.g. contrastive sentence embedding, multi-agent matrix games, tabular anomaly detection). To promote diversity we sample topics in batches and include previously sampled topics in the prompt as exclusions (See Figure 3). Topics serve as the only source of stochasticity in the pipeline; everything downstream is conditioned on the chosen z_i.

Stage 2: Task and dataset proposal. For each topic z_i, the teacher proposes a task description q_i together with a candidate dataset name $\tilde{d}_i$, drawn jointly as $(q_i, \tilde{d}_i) \sim \pi_{\mathrm{T}}(\cdot \mid z_i)$. We then ground $\tilde{d}_i$ in a real-world artifact by issuing a query to the HuggingFace search API and selecting the closest match $d_i \in \mathcal{H}$. If the match score falls below a fixed similarity threshold, the task is discarded; if it succeeds, we enrich d_i with a small set of example rows fetched from HuggingFace, which allows the teacher to write code that respects the actual schema of the data. Topics that do not require a dataset (e.g. game-theoretic environments) bypass this grounding step and proceed with $d_i = \varnothing$.

Stage 3: Configuration and starter-code generation. Conditioned on the grounded pair (q_i, d_i), the teacher synthesizes the remaining components of the task as $(\mathcal{C}_i, \mathcal{V}_i, \kappa_i) \sim \pi_{\mathrm{T}}(\cdot \mid q_i, d_i)$, where $\mathcal{C}_i$ is the starter and helper code, $\mathcal{V}_i$ is an evaluation script, and κ_i is a configuration file describing how MLGym should mount the task (entry points, time limits, metric direction). The output of Phase 1 is a candidate task $T_i = (q_i, d_i, \mathcal{C}_i, \mathcal{V}_i)$ together with κ_i, which is passed to Phase 2 for verification.

3.3 Phase 2: Environment Verification

Because every step of Phase 1 may introduce errors, naively running an agent on a candidate T_i is unreliable: code may fail to compile, datasets may not match the assumed schema, or

GPT-5 outcome across rollouts	Tasks	Share
Consistently improves baseline	175	31.5%
Improves in some rollouts	185	33.3%
Valid, but never improves	123	22.2%
No valid solution	72	13.0%
Total verified tasks	555	100.0%

Table 1: **Difficulty distribution of verified tasks.** Outcomes are measured across up to 256 GPT-5 trajectories per task. The distribution spans tasks that GPT-5 improves reliably, improves only intermittently, or cannot improve or solve.

the evaluator may be ill-defined. We therefore subject each candidate to a teacher-driven verification loop that explicitly tests end-to-end executability before the task is admitted to $\widehat{p}(T)$.

Concretely, we plug T_i into MLGym and run a single rollout of the teacher π_{T} for at most H rounds. Let $E_i \in \{0, 1\}$ indicate whether the rollout produced an exception or a non-finite evaluator score. If $E_i = 0$, we accept T_i together with the resulting baseline trajectory and admit it to the verified task pool $\widehat{\mathcal{T}}$. Phase 2 tests only whether the environment executes end to end and returns a finite score; it does not require the teacher to outperform the baseline. Baseline improvement is considered only during Phase 3 trajectory filtering. If $E_i = 1$, we initiate a self-debugging loop, summarized in Algorithm 1.

The probability p_{debug} trades off two failure modes: pure repair ($p_{\mathrm{debug}} = 1$) tends to lock onto a flawed code skeleton, whereas pure restart ($p_{\mathrm{debug}} = 0$) discards potentially useful partial progress. In practice we find that intermediate values strike a good balance and noticeably increase the yield of verified tasks per topic. Critically, the entire verification phase requires no human input and parallelizes trivially across tasks, so the size of $\widehat{\mathcal{T}}$ scales with available compute rather than with annotation budget.

Verification yield and task difficulty. Of 1,000 sampled topics, 914 passed dataset validation and entered Phase 2; 86 were removed because no valid dataset was found. Of these candidates, 555 passed environment verification (60.7%), while 359 were discarded because repeated debugging did not produce an executable environment or valid configuration. Table 1 characterizes the verified tasks using up to 256 GPT-5 trajectories per task. GPT-5 improved the baseline at least once on 360/555 tasks (64.9%) and produced a valid solution on 483/555 tasks (87.0%). The substantial mass in both intermittent-success and unsuccessful categories shows that verification retains tasks spanning the teacher's capability boundary rather than only tasks it reliably improves.

3.4 Phase 3: Trajectory Generation and Filtering

Given the verified task pool $\widehat{\mathcal{T}}$, the final phase produces the trajectory dataset that drives the SFT objective in Eq. 1.

Large-scale sampling. For each verified task $T_i \in \widehat{\mathcal{T}}$ we draw K independent teacher trajectories $\tau_i^{(k)} \sim p_{\pi_{\mathrm{T}}}(\tau \mid T_i)$ for $k = 1, \ldots, K$, by running π_{T} in $\mathcal{E}_{T_i}$ on an HPC cluster, with one GPU allocated per concurrent rollout. We target $K = 256$ per task; however, because the pipeline is unsupervised, individual tasks can fail intermittently due to evaluator timeouts, file-system contention, or container instabilities, so the realized number of successful rollouts $K_i \leq K$ varies across tasks.

Trajectory filtering. After sampling raw rollouts, we select high-quality trajectories to construct the supervised fine-tuning dataset using two performance-based strategies. First, Z-score sampling computes $z_i^{(k)} = (s_i^{(k)} - \mu_i)/\sigma_i$ and discards trajectories below a threshold z_{th}. Second, successful experience selection retains only trajectories that outperform the baseline. We further filter trajectories to those under 32,768 tokens to ensure complete

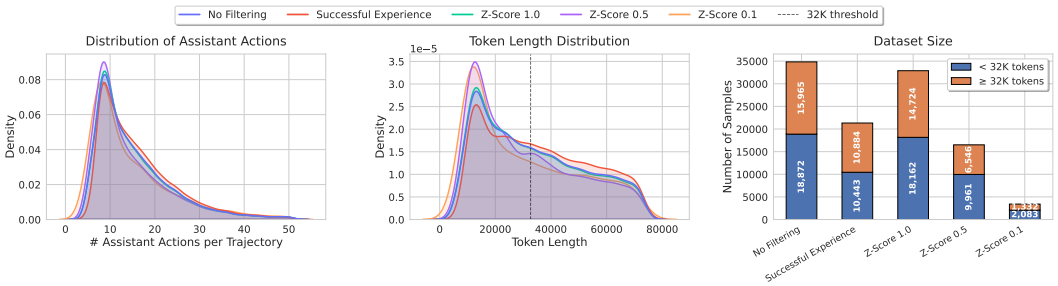


Figure 4: **Dataset Statistics.** Overview of the training set constructed by the ML-AutoResearch framework across different settings.

Model	Qwen3	ML-AR	Rel. gain
4B	$0.9107_{\pm 0.0099}$	$0.9628_{\pm 0.0237}$	+5.7%
8B	$0.8915_{\pm 0.0371}$	$0.9727_{\pm 0.0656}$	+9.1%
14B	$0.9290_{\pm 0.0204}$	$0.9840_{\pm 0.0364}$	+5.9%

Table 2: **Three-seed MLGym evaluation.** Mean AUP and standard deviation across evaluation seeds 42, 123, and 456.

Model	Qwen3	ML-AR	Abs. gain
4B	$0.000_{\pm 0.000}$	$0.101_{\pm 0.100}$	+0.101
8B	$0.044_{\pm 0.077}$	$0.215_{\pm 0.212}$	+0.171
14B	$0.126_{\pm 0.127}$	$0.420_{\pm 0.193}$	+0.294

Table 3: **Three-seed MLAgentBench evaluation.** Mean normalized score and standard deviation across seeds 42, 123, and 456.

reasoning within the context window. The final dataset $\mathcal{D}_{\text{SFT}}$ consists of all $(T_i, \tau_i^{(k)})$ pairs that satisfy these criteria. Statistical details are shown in Figure 4.

4 Experiments

In this section, we evaluate the ML-AutoResearch (ML-AR) framework across three diverse benchmarks to demonstrate its generalizability and scaling properties across different sizes and families of Qwen models.

Models and Environments. We utilize Qwen3-4B, Qwen3-8B, Qwen3-14B, and Qwen2.5-3B-Instruct as base models, fine-tuning them on the synthetic trajectory dataset generated by our ML-AutoResearch pipeline. We benchmark these fine-tuned student models against their respective un-tuned base models, as well as against frontier proprietary models, specifically GPT-4o and GPT-5.

Benchmarks. We evaluate the models on three comprehensive benchmarks: MLGym, AutoResearch, and MLAgentBench, which collectively span a wide spectrum of machine learning research tasks. Specifically, **MLGym** provides a broad evaluation suite with a strong emphasis on reinforcement learning environments, while also covering general ML engineering tasks. **AutoResearch** focuses on iterative research and optimization workflows, tasking the agent to tune a Small Language Model (SLM) to achieve a low validation bits-per-byte (`val_bpb`) metric. Finally, **MLAgentBench** offers a complementary suite of diverse, open-ended machine learning design and debugging tasks. For further details regarding the benchmark configurations and evaluation metrics, refer to Appendix A.1.

4.1 Main Results

ML-AutoResearch improves aggregate MLGym performance across model sizes. We reevaluate each base and ML-AR checkpoint using evaluation seeds 42, 123, and 456. As shown in Table 2, mean AUP improves by 5.7%, 9.1%, and 5.9% at 4B, 8B, and 14B, respectively. The gains persist across all three model sizes, although performance remains heterogeneous across individual tasks. Independent training-seed experiments further yield mean AUP gains of 4.4% at 8B and 4.0% at 14B (Appendix A.3).

Model	Best-run AUP	Gain over base
Qwen3-14B	1.0555	—
Original ML-AR-14B	1.0740	+1.8%
ML-AR-14B-Mixed	**1.1297**	+7.0%

Table 4: **Effect of additional data at 14B.** Seed-42 best-run AUP. ML-AR-14B-Mixed combines the original GPT-5 trajectories with additional GPT-5.4 trajectories and improves by 5.2% over the original ML-AR-14B.

Size	Model	Per-seed AUP			Mean AUP	Rel. gain
		42	123	456		
8B	Qwen3	1.5755	0.6331	0.8523	$1.0203_{\pm 0.4027}$	–
8B	ML-AR	1.7464	0.5522	0.8529	$1.0505_{\pm 0.5072}$	+3.0%
14B	Qwen3	1.7129	0.6218	0.9121	$1.0823_{\pm 0.4614}$	–
14B	ML-AR	1.7403	0.6353	0.9764	$1.1173_{\pm 0.4620}$	+3.2%

Table 5: **Open-weight trajectory teacher.** MLGym AUP by evaluation seed and aggregate performance after fine-tuning on trajectories generated by Qwen3-32B. The verified task environments are held fixed.

Additional trajectory data improves the 14B model. For the final 14B model, we mix additional GPT-5.4 trajectories with the original GPT-5 trajectory dataset. Under the seed-42 best-run protocol, this ML-AR-14B-Mixed model reaches an AUP of 1.1297, improving by 7.0% over Qwen3-14B and by 5.2% over the original ML-AR-14B (Table 4). We therefore use ML-AR-14B-Mixed as the primary 14B model in subsequent results and retain the original ML-AR-14B only for this data-scaling comparison. These best-run values are separate from the three-seed means in Table 2.

Open-weight trajectory generation also improves student models. To test whether the training gains depend specifically on GPT-5-generated behavior, we use Qwen3-32B to generate trajectories on the same 555 verified environments. Qwen3-32B generates 6K trajectories, of which 2.1K remain after filtering. Across three evaluation seeds, models trained on these trajectories improve mean MLGym AUP by 3.0% at 8B and 3.2% at 14B (Table 5). This experiment replaces the trajectory-generation teacher only; task synthesis and verification still use GPT-5. Full setup and task-level results appear in Appendix A.4.

ML-AutoResearch transfers to MLAgentBench. Across evaluation seeds 42, 123, and 456, ML-AR improves mean normalized performance at every model size (Table 3). The absolute gains are 0.101, 0.171, and 0.294 at 4B, 8B, and 14B, respectively, with the largest transfer gain at 14B. These results span different codebases, objectives, and evaluators from the synthetic training environments.

ML-AutoResearch-tuned models reliably discover superior solutions on the first attempt. To further demonstrate the out-of-domain generalizability of the model, we evaluated the ML-AR tuned agents on the AutoResearch benchmark. In this setting, the agent is provided with the training script of a small language model, alongside configurations and resource constraints, and must autonomously discover optimal hyperparameters to surpass a baseline metric. Our results demonstrate that the ML-AutoResearch model, upon analyzing the training code and initial observations, consistently proposes superior hyperparameter configurations on its first attempt. In particular, the tuned models achieve a 5% improvement on the `val_bpb` metric compared to baselines (See Figure 1). This zero-shot capability to parse execution contexts and immediately produce performance-enhancing modifications highlights the robust, creative reasoning unlocked by our framework.

Training tasks have limited overlap with evaluation tasks. We compare synthetic task names and descriptions against MLGym and MLAgentBench and find no shared 8-grams. We then encode each task with `nvidia/llama-embed-nemotron-8b` and compute pairwise cosine similarities. Average train–test similarity is below 0.30; only 6 of 555 synthetic

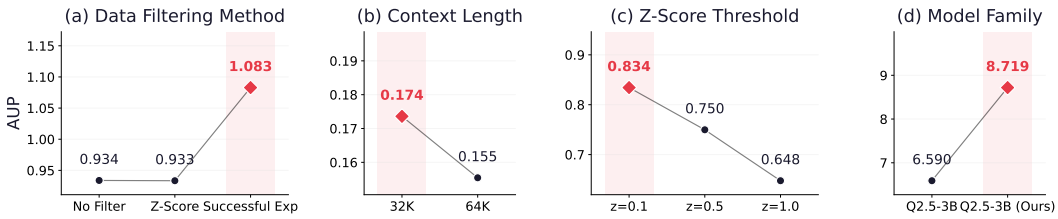


Figure 5: **Ablation Studies Comparison.** Performance comparison of ML-AutoResearch agents across different settings. Refer to A.5 for additional details.

Similarity threshold	MLGym	MLAgentBench	Combined
> 0.6	6/555 (1.1%)	0/555 (0.0%)	6/555 (1.1%)
> 0.7	0/555 (0.0%)	0/555 (0.0%)	0/555 (0.0%)

Table 6: **Semantic train–test similarity.** Number of synthetic tasks whose maximum cosine similarity to an evaluation task exceeds each threshold. Task descriptions are encoded with `nvidia/llama-embed-nemotron-8b`.

tasks (1.1%) have maximum similarity above 0.60, all with MLGym, and none exceed 0.70 (Table 6). Trajectories from the six tasks account for less than 0.9% of the training set. Although familiarity with the MLGym interaction format may still contribute to performance, transfer to MLAgentBench and the structurally distinct AutoResearch workflow suggests that interface alignment is not the sole explanation for the gains.

4.2 Ablation Studies

We present ablations on trajectory length, data filtering, and base model architectures to quantify their impact on the ML-AutoResearch framework.

Training Data Selection Mechanisms. To construct the final training dataset from candidate rollouts, we compared three selection mechanisms: (1) an unfiltered baseline, (2) Z-score sampling (discarding trajectories below a standardized performance threshold), and (3) successful experience selection (retaining only trajectories outperforming the baseline implementation). As Figure 5(a) shows, successful experience selection performs best by explicitly eliminating noisy, suboptimal executions. Z-score sampling improves upon the baseline but still admits some degenerate trajectories, highlighting the necessity of strict, performance-aligned curation.

Trajectory Integrity vs. Dataset Size. Because ∼35% of raw trajectories exceed our 32,768-token limit, we compared training Qwen3-4B on strictly complete trajectories versus a dataset that truncates over-length rollouts. Despite providing fewer training samples, training exclusively on complete trajectories consistently outperformed the truncated variant (Figure 5(b)). Preserving full temporal and causal coherence is thus more critical for effective credit assignment than artificially inflating dataset size.

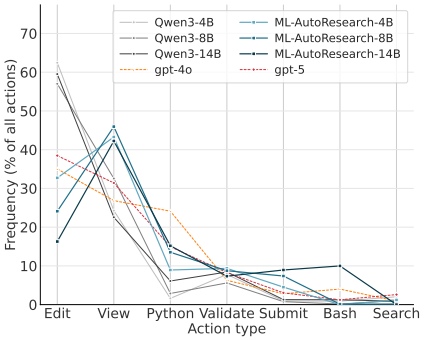


Figure 6: **Distribution of Action Types.** Comparison of the distribution of different action types across agents.

Sensitivity to Filtering Thresholds. Evaluating varying Z-score thresholds ($z \in \{0.1, 0.5, 1.0\}$) reveals that a stricter threshold of $z = 0.1$ achieves the best empirical results (Figure 5(c)). Lowering the threshold increases dataset size but admits noisier trajectories, reinforcing that a smaller, high-signal dataset is vastly preferable for agentic fine-tuning.

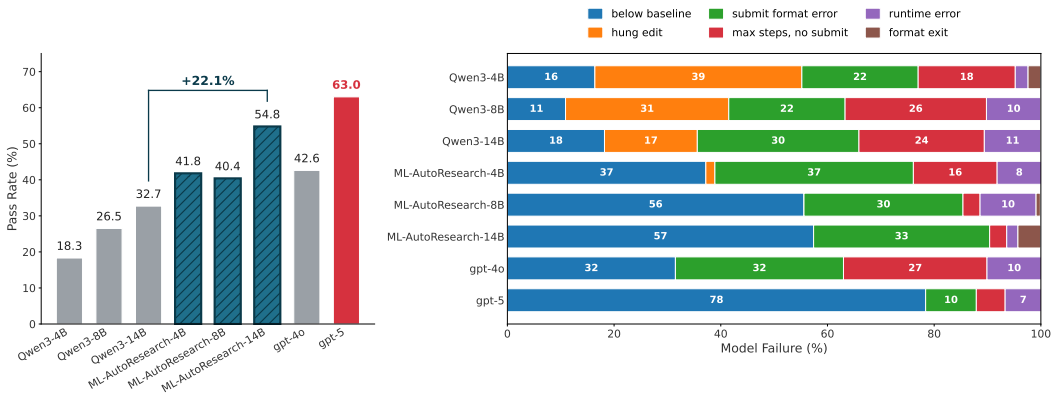


Figure 7: **Analysis Results.** Left: Comparison of ML-AutoResearch performance with other models based on pass rate, indicating how often agents outperform baseline results. Right: Overview of error categories across different agents.

Generalization Across Model Families. To confirm that ML-AutoResearch is model-agnostic, we applied our synthetic fine-tuning pipeline to an alternative architecture family, Qwen2.5-3B-Instruct. Evaluated on MLGym (Figure 5 (d)), the ML-AR tuned variant demonstrated consistent and significant performance improvements over its base model. This establishes that our data generation and filtering approach effectively transfers across different base model families and parameter scales.

4.3 Error Analysis

To understand behavioral differences, we categorized terminal failures into six classes (Figure 7). Baseline models predominantly fall into editing loops, repeatedly applying ineffective code changes until they exhaust their limits. In contrast, ML-AutoResearch tuned models successfully escape these degenerate loops to explore alternative strategies. Consequently, the primary failure mode for our agents shifts to submission format errors, reflecting occasional struggles with strict MLGym schemas.

While frontier models also avoid editing loops, they frequently fail by scoring below the baseline. This highlights a lack of exploratory creativity to design high-performing solutions, a bottleneck ML-AutoResearch-tuned models specifically overcome. Additionally, runtime errors from failing to debug written code constitute a small fraction of failures. The incidence of unrecovered runtime errors decreases further in our ML-AutoResearch-14B model, demonstrating that scaling the framework yields highly robust debugging capabilities.

5 Conclusion

We introduced ML-AutoResearch (ML-AR), a scalable framework for generating executable ML research tasks and process-level training trajectories. From 1,000 sampled topics, ML-AR produces 555 verified environments; 34K teacher trajectories are then filtered to 17K high-quality examples for supervised fine-tuning. Three-seed MLGym evaluation shows mean AUP gains of 5.7%, 9.1%, and 5.9% at 4B, 8B, and 14B, respectively, while additional mixed GPT-5/GPT-5.4 data raises the 14B model's best-run AUP by 7.0% over its instruction-tuned baseline. Improvements on MLAgentBench and AutoResearch further indicate that the learned process of experimentation, debugging, and feedback-driven refinement transfers beyond the primary evaluation environment.

Limitations Our training objective is supervised imitation, so ML-AR teaches feedback-driven execution and refinement rather than explicitly optimizing exploration or scientific novelty; reinforcement learning on the generated environments is a natural next step. The task-generation and verification stages remain mediated by GPT-5. Although an open-weight trajectory teacher also improves downstream performance (Appendix). Finally, generating

and evaluating long-horizon trajectories requires substantial compute. Broader impacts are discussed in the appendix under the "Broader impacts" subsection.

References

Tom Brown, Benjamin Mann, Nick Ryder, Melanie Subbiah, Jared D Kaplan, Prafulla Dhariwal, Arvind Neelakantan, Pranav Shyam, Girish Sastry, Amanda Askell, et al. Language models are few-shot learners. *Advances in neural information processing systems*, 33:1877–1901, 2020.

Jun Shern Chan, Neil Chowdhury, Oliver Jaffe, James Aung, Dane Sherburn, Evan Mays, Giulio Starace, Kevin Liu, Leon Maksin, Tejal Patwardhan, et al. Mle-bench: Evaluating machine learning agents on machine learning engineering. *arXiv preprint arXiv:2410.07095*, 2024.

Hui Chen, Miao Xiong, Yujie Lu, Wei Han, Ailin Deng, Yufei He, Jiaying Wu, Yibo Li, Yue Liu, and Bryan Hooi. Mlr-bench: Evaluating ai agents on open-ended machine learning research. *arXiv preprint arXiv:2505.19955*, 2025.

Juraj Gottweis, Wei-Hung Weng, Alexander Daryin, Tao Tu, Anil Palepu, Petar Sirkovic, Artiom Myaskovsky, Felix Weissenberger, Keran Rong, Ryutaro Tanno, et al. Towards an ai co-scientist. *arXiv preprint arXiv:2502.18864*, 2025.

Qian Huang, Jian Vora, Percy Liang, and Jure Leskovec. Mlagentbench: Evaluating language agents on machine learning experimentation. *arXiv preprint arXiv:2310.03302*, 2023.

Chris Lu, Cong Lu, Robert Tjarko Lange, Jakob Foerster, Jeff Clune, and David Ha. The ai scientist: Towards fully automated open-ended scientific discovery. *arXiv preprint arXiv:2408.06292*, 2024.

Deepak Nathani, Lovish Madaan, Nicholas Roberts, Nikolay Bashlykov, Ajay Menon, Vincent Moens, Amar Budhiraja, Despoina Magka, Vladislav Vorotilov, Gaurav Chaurasia, et al. Mlgym: A new framework and benchmark for advancing ai research agents. *arXiv preprint arXiv:2502.14499*, 2025.

Alexander Novikov, Ngân Vũ, Marvin Eisenberger, Emilien Dupont, Po-Sen Huang, Adam Zsolt Wagner, Sergey Shirobokov, Borislav Kozlovskii, Francisco JR Ruiz, Abbas Mehrabian, et al. Alphaevolve: A coding agent for scientific and algorithmic discovery. *arXiv preprint arXiv:2506.13131*, 2025.

Charles O'Neill, Tirthankar Ghosal, Roberta Răileanu, Mike Walmsley, Thang Bui, Kevin Schawinski, and Ioana Ciucă. Sparks of science: Hypothesis generation using structured paper data. *arXiv preprint arXiv:2504.12976*, 2025.

Timo Schick, Jane Dwivedi-Yu, Roberto Dessì, Roberta Raileanu, Maria Lomeli, Eric Hambro, Luke Zettlemoyer, Nicola Cancedda, and Thomas Scialom. Toolformer: Language models can teach themselves to use tools. *Advances in neural information processing systems*, 36: 68539–68551, 2023.

Chenglei Si, Tatsunori Hashimoto, and Diyi Yang. The ideation-execution gap: Execution outcomes of llm-generated versus human research ideas. *arXiv preprint arXiv:2506.20803*, 2025.

Zachary S Siegel, Sayash Kapoor, Nitya Nagdir, Benedikt Stroebl, and Arvind Narayanan. Core-bench: Fostering the credibility of published research through a computational reproducibility agent benchmark. *arXiv preprint arXiv:2409.11363*, 2024.

Giulio Starace, Oliver Jaffe, Dane Sherburn, James Aung, Jun Shern Chan, Leon Maksin, Rachel Dias, Evan Mays, Benjamin Kinsella, Wyatt Thompson, Johannes Heidecke, Amelia Glaese, and Tejal Patwardhan. Paperbench: Evaluating AI's ability to replicate AI research. In *Forty-second International Conference on Machine Learning*, 2025. URL `https://openreview.net/forum?id=xF5PuTLPbn`.

Hugo Touvron, Thibaut Lavril, Gautier Izacard, Xavier Martinet, Marie-Anne Lachaux, Timothée Lacroix, Baptiste Rozière, Naman Goyal, Eric Hambro, Faisal Azhar, et al. Llama: Open and efficient foundation language models. *arXiv preprint arXiv:2302.13971*, 2023.

An Yang, Anfeng Li, Baosong Yang, Beichen Zhang, Binyuan Hui, Bo Zheng, Bowen Yu, Chang Gao, Chengen Huang, Chenxu Lv, et al. Qwen3 technical report. *arXiv preprint arXiv:2505.09388*, 2025a.

John Yang, Carlos E Jimenez, Alexander Wettig, Kilian Lieret, Shunyu Yao, Karthik Narasimhan, and Ofir Press. Swe-agent: Agent-computer interfaces enable automated software engineering. *Advances in Neural Information Processing Systems*, 37:50528–50652, 2024.

John Yang, Kilian Lieret, Carlos E Jimenez, Alexander Wettig, Kabir Khandpur, Yanzhe Zhang, Binyuan Hui, Ofir Press, Ludwig Schmidt, and Diyi Yang. Swe-smith: Scaling data for software engineering agents. *arXiv preprint arXiv:2504.21798*, 2025b.

Shunyu Yao, Jeffrey Zhao, Dian Yu, Nan Du, Izhak Shafran, Karthik Narasimhan, and Yuan Cao. React: Synergizing reasoning and acting in language models. *arXiv preprint arXiv:2210.03629*, 2022.

Yunxiang Zhang, Muhammad Khalifa, Shitanshu Bhushan, Lajanugen Murphy, Jaekyeom Kim, Moontae Lee, Honglak Lee, and Lu Wang. Mlrc-bench: Can language agents solve machine learning research challenges? *arXiv preprint arXiv:2504.09702*, 2025.

Bingchen Zhao, Despoina Magka, Minqi Jiang, Xian Li, Roberta Raileanu, Tatiana Shavrina, Jean-Christophe Gagnon-Audet, Kelvin Niu, Shagun Sodhani, Michael Shvartsman, et al. The automated llm speedrunning benchmark: Reproducing nanogpt improvements. *arXiv preprint arXiv:2506.22419*, 2025.

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A Appendix

A.1 Benchmarks Details

MLGym benchmark (13 subtasks). We evaluate on the 13-task MLGym suite spanning supervised learning, self-supervised learning, reinforcement learning, algorithmic reasoning, and game theory. The subtasks are: *House Price Prediction*, *Image Classification (CIFAR-10)*, *Image Classification (Fashion-MNIST)*, *Image Captioning (MS-COCO)*, *Natural Language Inference (MNLI)*, *Language Modeling (FineWeb)*, *MetaMaze Navigation*, *MountainCar Continuous*, *Breakout MinAtar*, *3-SAT*, *Prisoner's Dilemma*, *Battle of Sexes*, and *Colonel Blotto*.

Each MLGym subtask uses its task-native evaluator to produce a scalar score, with directionality (maximize/minimize) defined per task by the benchmark configuration. Following benchmark convention, we report both (i) whether an agent beats the provided baseline (pass-style success) and (ii) aggregate trajectory quality via AUP over intermediate submissions.

MLAgentBench benchmark (reported subtasks and metrics). For MLAgentBench, we report the following subtasks and their native evaluation metrics: *CIFAR-10* (Accuracy, ↑), *IMDb* (Accuracy, ↑), *House Price Prediction* (MAE, ↓), *ogbn-arxiv* (Accuracy, ↑), *Vectorization* (runtime sec, ↓), *Spaceship Titanic* (Accuracy, ↑), *AMP Parkinsons* (SMAPE, ↓), *LLaMA Inference* (sec/token, ↓), and *Feedback Prize* (MCRMSE, ↓). Metrics are computed by the task evaluator and compared by direction-aware best-attempt performance.

A.2 Multi-Seed Evaluation Details

Table 7 reports the complete per-task MLGym results for the primary three-seed reevaluation. ML-AR generally improves execution reliability, converting many invalid base-model runs into valid solutions, while outcomes remain heterogeneous: for example, the 4B MNLI and 14B Breakout results regress. Table 8 reports task-level three-seed MLAgentBench results, and Table 9 provides the seed-level normalized scores underlying the aggregate results in Table 3.

Task	Metric	Qwen3-4B	ML-AR-4B	Qwen3-8B	ML-AR-8B	Qwen3-14B	ML-AR-14B
CIFAR-10	Accuracy (↑)	$0.000_{\pm 0.000}$ [0/3]	$0.000_{\pm 0.000}$ [0/3]	$0.000_{\pm 0.000}$ [0/3]	$0.667_{\pm 0.577}$ [2/3]	$0.243_{\pm 0.421}$ [1/3]	$0.667_{\pm 0.577}$ [2/3]
Battle of Sexes	Avg. reward (↑)	$1.445_{\pm 0.002}$ [3/3]	$1.804_{\pm 0.002}$ [3/3]	$1.445_{\pm 0.002}$ [3/3]	$1.759_{\pm 0.265}$ [3/3]	$1.446_{\pm 0.001}$ [3/3]	$1.870_{\pm 0.113}$ [3/3]
Prisoners Dilemma	Avg. reward (↑)	$2.629_{\pm 0.005}$ [3/3]	$3.388_{\pm 0.002}$ [3/3]	$2.624_{\pm 0.010}$ [3/3]	$2.635_{\pm 0.002}$ [3/3]	$2.633_{\pm 0.003}$ [3/3]	$2.638_{\pm 0.003}$ [3/3]
Blotto	Avg. reward (↑)	$0.208_{\pm 0.074}$ [3/3]	$0.662_{\pm 0.473}$ [3/3]	$0.096_{\pm 0.129}$ [3/3]	$0.334_{\pm 0.577}$ [3/3]	$0.340_{\pm 0.443}$ [3/3]	$0.111_{\pm 0.126}$ [3/3]
House Price	R^2 (↑)	$0.596_{\pm 0.517}$ [2/3]	$0.880_{\pm 0.000}$ [3/3]	$0.899_{\pm 0.010}$ [3/3]	$0.914_{\pm 0.002}$ [3/3]	$0.908_{\pm 0.011}$ [3/3]	$0.918_{\pm 0.002}$ [3/3]
Fashion MNIST	Accuracy (↑)	$0.000_{\pm 0.000}$ [0/3]	$0.000_{\pm 0.000}$ [0/3]	$0.000_{\pm 0.000}$ [0/3]	$0.672_{\pm 0.497}$ [3/3]	$0.000_{\pm 0.000}$ [0/3]	$0.977_{\pm 0.040}$ [3/3]
MS-COCO	BLEU (↑)	$0.008_{\pm 0.014}$ [1/3]	$0.280_{\pm 0.000}$ [3/3]	$0.323_{\pm 0.006}$ [3/3]	$0.535_{\pm 0.404}$ [3/3]	$0.297_{\pm 0.018}$ [3/3]	$0.760_{\pm 0.416}$ [3/3]
MNLI	Accuracy (↑)	$0.834_{\pm 0.004}$ [3/3]	$0.537_{\pm 0.008}$ [3/3]	$0.000_{\pm 0.000}$ [0/3]	$0.766_{\pm 0.008}$ [3/3]	$0.557_{\pm 0.482}$ [2/3]	$0.735_{\pm 0.178}$ [3/3]
Language Modeling	Val. loss (↓)	$4.924_{\pm 0.006}$ [2/3]	$4.922_{\pm 0.001}$ [3/3]	$4.931_{\pm 0.000}$ [1/3]	$4.919_{\pm 0.004}$ [3/3]	$4.931_{\pm 0.000}$ [0/3]	$4.917_{\pm 0.002}$ [3/3]
Breakout	Avg. score (↑)	$0.000_{\pm 0.000}$ [0/3]	$41.233_{\pm 7.447}$ [3/3]	$0.000_{\pm 0.000}$ [0/3]	$29.970_{\pm 18.123}$ [3/3]	$48.137_{\pm 5.383}$ [3/3]	$39.793_{\pm 1.396}$ [3/3]
Mountain Car	Avg. reward (↑)	$0.000_{\pm 0.000}$ [0/3]	$49.830_{\pm 1.923}$ [3/3]	$16.240_{\pm 28.129}$ [1/3]	$52.050_{\pm 0.000}$ [3/3]	$29.321_{\pm 23.829}$ [3/3]	$50.940_{\pm 1.923}$ [3/3]
Meta Maze	Avg. return (↑)	$0.000_{\pm 0.000}$ [0/3]	$21.203_{\pm 3.837}$ [3/3]	$8.327_{\pm 14.422}$ [1/3]	$21.800_{\pm 2.803}$ [3/3]	$5.394_{\pm 4.680}$ [2/3]	$21.433_{\pm 3.223}$ [3/3]
3-SAT	Time (s) (↓)	$13.397_{\pm 0.578}$ [3/3]	$13.740_{\pm 0.667}$ [3/3]	$13.663_{\pm 0.356}$ [3/3]	$13.930_{\pm 0.451}$ [3/3]	$11.620_{\pm 0.061}$ [3/3]	$12.920_{\pm 0.713}$ [3/3]

Table 7: **Per-task three-seed MLGym results.** Values are mean and standard deviation across evaluation seeds 42, 123, and 456; brackets show the number of valid runs. Invalid runs follow the benchmark aggregation convention used in the rebuttal results. The 14B column evaluates the original ML-AR-14B checkpoint, not ML-AR-14B-Mixed.

Task	Qwen3-4B	ML-AR-4B	Qwen3-8B	ML-AR-8B	Qwen3-14B	ML-AR-14B
CIFAR-10	$0.000_{\pm 0.000}$	$0.171_{\pm 0.296}$	$0.221_{\pm 0.383}$	$0.418_{\pm 0.363}$	$0.274_{\pm 0.392}$	$0.867_{\pm 0.010}$
IMDb	$0.000_{\pm 0.000}$	$0.000_{\pm 0.000}$	$0.000_{\pm 0.000}$	$0.304_{\pm 0.527}$	$0.000_{\pm 0.000}$	$0.611_{\pm 0.529}$
ogbn-arxiv	$0.000_{\pm 0.000}$	$0.000_{\pm 0.000}$	$0.000_{\pm 0.000}$	$0.350_{\pm 0.304}$	$0.357_{\pm 0.310}$	$0.431_{\pm 0.221}$
Vectorization	$0.000_{\pm 0.000}$	$0.334_{\pm 0.577}$	$0.001_{\pm 0.001}$	$0.001_{\pm 0.002}$	$0.000_{\pm 0.000}$	$0.192_{\pm 0.332}$
BabyLM-fixed	∞	∞	∞	∞	∞	$6.03_{\pm 0.98}$ [2/3]†

Table 8: **Task-level three-seed MLAgentBench results.** Values are mean and standard deviation across evaluation seeds 42, 123, and 456. A dash indicates that the model did not solve BabyLM-fixed. †BabyLM-fixed reports evaluation loss (lower is better) and was solved in two of three runs; the other task columns report normalized performance (higher is better).

A.3 Robustness Across Training Seeds

We independently train the 8B and 14B models using seeds 42, 1234, and 5678 and evaluate each resulting checkpoint with three independent evaluation seeds. Table 10 reports mean AUP gains of 4.4% at 8B and 4.0% at 14B. This protocol measures sensitivity to training randomness and is distinct from the primary-checkpoint evaluation in Table 2. The 14B checkpoints use the original ML-AR dataset rather than the mixed GPT-5/GPT-5.4 dataset.

A.4 Open-Weight Trajectory Teacher

To test whether the trajectory-generation stage depends specifically on GPT-5 behavior, we replace GPT-5 with the open-weight Qwen3-32B model while holding the 555 verified task environments fixed. This experiment evaluates trajectory-teacher transfer only; it does not regenerate topics, datasets, or task environments with Qwen3-32B. The model generated 6K trajectories, of which approximately 3.9K were removed by the filtering pipeline, leaving 2.1K supervised fine-tuning examples. The aggregate result is reported in Table 5 in the main text. Table 11 gives the corresponding task-level results and valid-run counts, showing heterogeneous transfer despite positive aggregate gains. This provides initial evidence that downstream gains are not specific to GPT-5-generated trajectories, while leaving full open-weight environment synthesis for future work.

A.5 Details of Ablation Study Results

In this section, we provide detailed results of ablation studies across all tasks in the MLGym benchmark.

A.6 Broader impact

The development of autonomous machine learning agents presents significant dual-use characteristics, carrying both profound positive potential and notable risks of misuse.

Model	Mean score	Per-seed score		
		42	123	456
Qwen3-4B	$0.000_{\pm 0.000}$	0.000	0.000	0.000
ML-AR-4B	$0.101_{\pm 0.100}$	0.103	0.000	0.200
Qwen3-8B	$0.044_{\pm 0.077}$	0.000	0.133	0.000
ML-AR-8B	$0.215_{\pm 0.212}$	0.425	0.219	0.000
Qwen3-14B	$0.126_{\pm 0.127}$	0.124	0.000	0.254
ML-AR-14B	$0.420_{\pm 0.193}$	0.207	0.469	0.584

Table 9: **MLAgentBench results by evaluation seed.** Mean normalized score and standard deviation across evaluation seeds 42, 123, and 456, together with each seed-level score.

Model	Qwen3	ML-AR	Rel. gain
8B	$0.871_{\pm 0.012}$	$0.910_{\pm 0.040}$	+4.4%
14B	$0.904_{\pm 0.025}$	$0.940_{\pm 0.035}$	+4.0%

Table 10: **Robustness across training seeds.** Mean AUP across independently trained checkpoints using seeds 42, 1234, and 5678, with each checkpoint evaluated using three independent evaluation seeds. The 14B result uses the original ML-AR dataset rather than the mixed-data model.

Positive Societal Impacts. Frameworks like ML-AutoResearch (ML-AR) have the potential to democratize scientific discovery by automating the highly technical, engineering-heavy, and time-consuming aspects of ML research. By lowering the barrier to entry for developing and optimizing machine learning models, such systems can drastically reduce the cost of research and development. This acceleration allows human researchers to shift their focus away from tedious debugging and hyperparameter tuning, and toward high-level conceptual design, safety alignment, and solving complex societal challenges.

Negative Misuse Risks. Conversely, these advanced capabilities carry inherent risks. An agent capable of autonomously writing, debugging, and optimizing ML code could be repurposed by malicious actors to rapidly develop harmful AI systems. This includes accelerating the creation of advanced surveillance tools, generating highly convincing deepfakes, or automating the discovery of vulnerabilities for cyberattacks. Furthermore, the autonomous nature of these agents means that, without proper oversight, they might inadvertently optimize for proxy metrics that introduce severe biases, unfairness, or security flaws into deployed models.

Mitigations and Evaluation Context. To mitigate these risks during the development and evaluation phases, our work strictly confines agent execution to controlled, sandboxed environments such as the MLGym. This environment isolates the agents from the open internet, restricting them to well-defined datasets and scoped computational resources, thereby preventing the execution of arbitrary, unverified code on host machines. As autonomous ML research systems continue to scale, we strongly advocate for the continued use of secure sandboxing, rigorous alignment checks, and human-in-the-loop oversight before such agents are deployed in unconstrained, real-world settings.

A.7 Licenses and terms of use

We document licenses and terms for third-party assets used in this work in the following inventory.

All external assets are used under their respective licenses or terms of service.

Task	Metric	Qwen3-8B	ML-AR-8B	Qwen3-14B	ML-AR-14B
CIFAR-10	Accuracy (↑)	∞ [0/3]	∞ [0/3]	$0.730_{\pm 0.000}$ [1/3]	$0.733_{\pm 0.000}$ [1/3]
Battle of Sexes	Avg. reward (↑)	$1.445_{\pm 0.001}$ [3/3]	$1.424_{\pm 0.315}$ [3/3]	$1.445_{\pm 0.001}$ [3/3]	$1.804_{\pm 0.000}$ [3/3]
Prisoners Dilemma	Avg. reward (↑)	$2.624_{\pm 0.008}$ [3/3]	$2.802_{\pm 0.424}$ [3/3]	$2.633_{\pm 0.003}$ [3/3]	$2.971_{\pm 0.422}$ [3/3]
Blotto	Avg. reward (↑)	$0.096_{\pm 0.105}$ [3/3]	$0.227_{\pm 0.506}$ [3/3]	$0.340_{\pm 0.362}$ [3/3]	$0.199_{\pm 0.049}$ [3/3]
House Price	R^2 (↑)	$0.899_{\pm 0.007}$ [3/3]	$0.880_{\pm 0.000}$ [3/3]	$0.908_{\pm 0.009}$ [3/3]	$0.900_{\pm 0.001}$ [3/3]
Fashion MNIST	Accuracy (↑)	∞ [0/3]	∞ [0/3]	∞ [0/3]	$0.949_{\pm 0.000}$ [1/3]
MS-COCO	BLEU (↑)	$0.323_{\pm 0.005}$ [3/3]	$0.292_{\pm 0.017}$ [3/3]	$0.297_{\pm 0.015}$ [3/3]	$0.290_{\pm 0.014}$ [3/3]
MNLI	Accuracy (↑)	∞ [0/3]	∞ [0/3]	$0.835_{\pm 0.002}$ [2/3]	$0.835_{\pm 0.003}$ [3/3]
Language Modeling	Val. loss (↓)	$4.931_{\pm 0.000}$ [1/3]	$4.923_{\pm 0.000}$ [1/3]	∞ [0/3]	$4.927_{\pm 0.000}$ [1/3]
Breakout	Avg. score (↑)	∞ [0/3]	$36.631_{\pm 3.010}$ [2/3]	$48.135_{\pm 4.396}$ [3/3]	$50.138_{\pm 12.057}$ [3/3]
Mountain Car	Avg. reward (↑)	$48.717_{\pm 0.000}$ [1/3]	$46.040_{\pm 10.138}$ [2/3]	$29.318_{\pm 19.455}$ [3/3]	$45.592_{\pm 3.126}$ [2/3]
Meta Maze	Avg. return (↑)	$24.981_{\pm 0.000}$ [1/3]	∞ [0/3]	$8.091_{\pm 0.282}$ [2/3]	$21.732_{\pm 2.570}$ [3/3]
3-SAT	Time (s) (↓)	$13.665_{\pm 0.294}$ [3/3]	$11.973_{\pm 0.480}$ [3/3]	$11.621_{\pm 0.049}$ [3/3]	$12.740_{\pm 0.346}$ [3/3]

Table 11: **Per-task results with an open-weight trajectory teacher.** Values are mean and standard deviation over evaluation seeds 42, 123, and 456; brackets report valid runs. A dash denotes no valid solution. ML-AR students are trained on trajectories generated by Qwen3-32B over the fixed verified task pool.

Task	Metric	Z-score 0.1	Z-score 0.5	Z-score 1
CIFAR-10	Accuracy (↑)	1.0000	1.0000	0.1426
Battle of Sexes	Average Reward (↑)	1.4418	2.0000	2.0000
Prisoners Dilemma	Average Reward (↑)	5.0000	2.6312	2.6284
Blotto	Average Reward (↑)	0.2458	0.2502	0.0790
House Price Prediction	R^2 Score (↑)	0.9106	0.9246	0.9200
Fashion MNIST	Accuracy (↑)	1.0000	0.9277	1.0000
MS-COCO	BLEU Score (↑)	0.9000	0.2806	0.2806
MNLI	Validation Accuracy (↑)	46.1233	63.2705	50.4432
Language Modeling	Validation Loss (↓)	4.9170	4.9187	4.9159
Breakout	Average Score (↑)	70.7970	56.8625	43.8539
Mountain Car Continuous	Average Reward (↑)	56.3959	49.4486	74.8382
Meta Maze	Average Return (↑)	48.6188	20.4422	20.1750
3-SAT Heuristic	Wall-Clock Time (s) (↓)	17.3700	19.4300	18.3060

Table 12: Comparison across different Z-score filtering thresholds. Arrows indicate whether higher (↑) or lower (↓) values are better.

Task	Metric	No Filter	Z-score	Successful Experience
CIFAR-10	Accuracy (↑)	∞	0.1426	1.0000
Battle of Sexes	Average Reward (↑)	2.0000	2.0000	1.4453
Prisoners Dilemma	Average Reward (↑)	2.6283	2.6284	2.6324
Blotto	Average Reward (↑)	1.0000	0.0790	0.8631
House Price Prediction	R^2 Score (↑)	0.9246	0.9200	0.9274
Fashion MNIST	Accuracy (↑)	0.1000	1.0000	1.0000
MS-COCO	BLEU Score (↑)	0.2949	0.2806	0.3169
MNLI	Validation Accuracy (↑)	35.3337	50.4432	82.3943
Language Modeling	Validation Loss (↓)	4.9234	4.9159	4.9175
Breakout	Average Score (↑)	64.7484	43.8539	46.8381
Mountain Car Continuous	Average Reward (↑)	52.3536	74.8382	49.4486
Meta Maze	Average Return (↑)	22.3875	20.1750	23.8203
3-SAT Heuristic	Wall-Clock Time (s) (↓)	18.3470	18.3060	18.2600

Table 13: Comparison across filtering strategies. Arrows indicate whether higher (↑) or lower (↓) values are better.

A.8 Reproducibility and training details

We provide implementation-level details used for SFT runs in our internal training pipeline, including data construction, model optimization, filtering, and cluster compute settings.

Task	Metric	32k	64k
CIFAR-10	Accuracy (↑)	0.4977	0.4977
Battle of Sexes	Average Reward (↑)	1.8032	1.4405
Prisoners Dilemma	Average Reward (↑)	3.3925	2.3817
Blotto	Average Reward (↑)	1.0000	1.0000
House Price Prediction	R^2 Score (↑)	0.8800	0.8800
Fashion MNIST	Accuracy (↑)	0.8480	0.8480
MS-COCO	BLEU Score (↑)	0.2806	0.2806
MNLI	Validation Accuracy (↑)	54.2129	55.1707
Language Modeling	Validation Loss (↓)	4.9191	4.9222
Breakout	Average Score (↑)	46.8381	46.8381
Mountain Car Continuous	Average Reward (↑)	49.4486	49.4486
Meta Maze	Average Return (↑)	23.6078	23.8281
3-SAT Heuristic	Wall-Clock Time (s) (↓)	17.9490	17.8090

Table 14: Comparison across different context lengths. Arrows indicate whether higher (↑) or lower (↓) values are better.

Task	Metric	Qwen2.5-3B-Instruct	ML-AR-3B
CIFAR-10	Accuracy (↑)	∞	0.0996
Battle of Sexes	Average Reward (↑)	1.0304	1.4378
Prisoners Dilemma	Average Reward (↑)	2.3883	2.6225
Blotto	Average Reward (↑)	-0.2430	1.0000
House Price Prediction	R^2 Score (↑)	-4.1698	0.8800
Fashion MNIST	Accuracy (↑)	∞	∞
MS-COCO	BLEU Score (↑)	∞	0.2809
MNLI	Validation Accuracy (↑)	∞	∞
Language Modeling	Validation Loss (↓)	∞	∞
Breakout	Average Score (↑)	28.1272	∞
Mountain Car Continuous	Average Reward (↑)	∞	∞
Meta Maze	Average Return (↑)	∞	∞
3-SAT Heuristic	Wall-Clock Time (s) (↓)	18.0780	18.2730

Table 15: Comparison between Qwen2.5-3B-Instruct and ML-AR-3B. Arrows indicate whether higher (↑) or lower (↓) values are better.

A.9 Prompts used in the task generation pipeline

This appendix lists the core, non-redundant prompt texts used in the data generation pipeline.

A.9.1 Topic sampling prompt

```
You are an expert in machine learning research. Generate a list of 20 diverse
     and interesting machine learning research topics. Each topic should be a
     short phrase or sentence, suitable for use as a research challenge or
    task. Do not repeat topics from previous examples. Return the topics as a
     JSON array of strings.

Your output:
```

Asset class	Example assets in this work	Licenses/terms used	Notes
Datasets	Hugging Face datasets used for synthetic task generation and evaluation	Apache-2.0, MIT, CC0-1.0, CC-BY-4.0, CC-BY-SA-4.0, CC-BY-SA-3.0, CC-BY-SA-3.0+GFDL, BSD/BSD-3-Clause, CC-BY-NC-SA-4.0, CC-BY-NC-ND-4.0, AFL-3.0, ODC-BY, C-UDA	Per-dataset terms are respected and attributed
Open models	Qwen family student models	Qwen model licenses/terms from the corresponding model cards	Version-specific model terms apply
API models	GPT teacher/evaluator APIs	OpenAI API Terms of Use and associated service policies	API use only; no model weight redistribution
Benchmarks/codebases	MLGym, MLAgentBench, AutoResearch benchmark code	Repository-specific OSS licenses (including MIT/Apache-2.0/BSD-style where applicable)	We follow each repository's LICENSE file
Agent framework/-tools	SWE-agent and related tooling	Repository-specific OSS licenses (including MIT/Apache-2.0/BSD-style where applicable)	We follow each repository's LICENSE file

Table 16: Licenses and terms of use for external assets used in this work.

Item	Setting
Base models	Qwen3-4B, Qwen3-8B, Qwen3-14B
Tokenizer	Matching Qwen tokenizer for each base model
Optimizer	AdamW
Learning rate	1.0×10^{-5} (4B), 5.0×10^{-6} (8B), 2.0×10^{-5} (14B) on H100 configs
LR schedule	WarmupDecayLR with linear warmup; warmup steps 100 (4B/8B), 200 (14B)
Weight decay	1.0×10^{-4} (4B/8B), 1.0×10^{-1} (14B config)
Global batch size	64 (4B/8B), 32 (14B)
Micro-batch size/GPU	2 (4B/8B H100), 1 (14B H100)
Training length	1500 max steps (H100 configs)
Precision	BF16 enabled
Random seed	42
Sequence window	64k in current data build (`max_seq_len=65536`); trajectories above `max_seq_len+8192` are filtered out
Trajectory selection	Per-task metric-aware ranking; optional z-score filtering (`MLGYM_DROP_Z_THRESHOLD`, default 1.0) and top-percentile retention (`MLGYM_KEEP_TOP_PERCENTILE`)

Table 17: Training and data-construction settings used by the SFT pipeline.

A.10 Task proposal and dataset validation prompts

Task proposal prompts

```
You are an expert ML researcher create a training task for a junior
    researcher. Given a topic, generate a JSON object describing a machine
    learning task for that topic. The JSON must include:
- topic: the original topic
- metric: a suitable evaluation metric for the task
- description: a detailed description of the ML task
- dataset: a dataset name that can be matched to a huggingface dataset OR a
    simple search query for a public huggingface dataset (e.g., 'cifar10', '
```

```
    imdb', 'tiny imagenet'). Omit this field if the task does not require a
    dataset.

You have access to a tool that can search the HuggingFace datasets API to
    find suitable datasets based on your query. Please make sure the dataset
    exists on HuggingFace.

Here are some examples:

Topic: Image Classification
Output:
{"topic": "Image Classification", "metric": "Accuracy", "description": "
    Classify images into categories using a standard image classification
    dataset.", "dataset": "cifar10"}

Topic: Sentiment Analysis
Output:
{"topic": "Sentiment Analysis", "metric": "Accuracy", "description": "Predict
     the sentiment (positive/negative) of movie reviews.", "dataset": "imdb"}

Topic: Named Entity Recognition
Output:
{"topic": "Named Entity Recognition", "metric": "F1-score", "description": "
    Identify named entities in text using a standard NER dataset.", "dataset":
     "conll2003"}

Topic: Text Summarization
Output:
{"topic": "Text Summarization", "metric": "ROUGE score", "description": "
    Generate concise summaries of news articles.", "dataset": "cnn_dailymail"}


Topic: Machine Translation
Output:
{"topic": "Machine Translation", "metric": "BLEU", "description": "Translate
    sentences from English to German.", "dataset": "wmt14"}

Topic: Speech Command Recognition
Output:
{"topic": "Speech Command Recognition", "metric": "Accuracy", "description":
    "Classify spoken commands from audio clips.", "dataset": "google speech
    commands"}

Topic: Human Activity Recognition
Output:
{"topic": "Human Activity Recognition", "metric": "Accuracy", "description":
    "Classify human activities from wearable sensor data.", "dataset": "UCI
    HAR"}

Topic: {{topic}}
Output:
```

Dataset validation prompt

```
You may call the dataset search tool to validate or refine the dataset choice
     before producing the final JSON.
Rules:
- If you are unsure about the dataset name, call the tool with a short query.
- When confident, output ONLY the final JSON object (no surrounding prose)
    with required keys.
```

```
- Keys: topic, metric, description, optional dataset (string). If dataset
    provided, ensure it plausibly exists on HuggingFace.
- Avoid re-calling the tool if current results already contain a suitable
    dataset.
- You can modify the topic slightly to fit the available datasets.
```

Dataset Search Tool-Result Follow-Up Prompt

```
Search results for query '{query}': {json.dumps(results, ensure_ascii=False)}
Select one dataset id (or refine by calling the tool again) and output final
    JSON when ready.
```

JSON-Missing Nudge Prompt

```
I did not receive a valid JSON. Please either call the search tool or output
    the final JSON object now.
```

A.11 Task files generation prompt

Task files stage 1: config generation

````
Your objective is to create YAML config files for a machine learning task.
    You are given JSON input that describes the topic as well as the dataset
    you are working with. The first file is a task configuration file that
    describes the task, dataset, and submission format. The other files (
    usually one but can be multiple) are dataset configuration files that
    describe the datasets used in the task. Be creative and generate a task
    that is interesting and challenging for the agent to solve.

IMPORTANT OUTPUT FORMAT REQUIREMENT:
Return every file using markdown code blocks ONLY (no sentinel markers, no
    extra text) exactly like:
```lang
# relative/path/to/file
<file contents>
```

- The task is executed in a linux environment with Python 3.10 and the
    following packages preinstalled (generic_conda_requirements.txt):
 generic_conda_requirements.txt (preinstalled packages):
  numpy
  pandas
  scipy
  torch
  scikit-learn
  tqdm
  datasets
  gymnasium
  transformers[torch]
  datasets
  matplotlib
  torchvision

Here is the format for the input JSON.
```json
# input.json
{
````
````

````
  "topic": ...,
  "metric": ...,
  "description": ...,
  "dataset": {
    "id": ...,
    "features": [...],
    "examples": [...]
  }
}
```

Here is the format for the config files (showing expected file outputs using
    markdown code blocks):
```yaml
# tasks/task_id.yaml
id: # task id, will be used as the config file name as well. Recommend using
    snake_case.
name: # task name
description: # Description of the task that includes the task objective
    submission format requirements. You must include the string "{
    dataset_docs}", which reference the description in the dataset config
    file.
dataset_configs: # zero or more data config files described below.
task_entrypoint: # one of four values: CSVSubmissionTasks,
    ModelSubmissionTasks, LMSubmissionTasks, PythonSubmissionTasks
training_timeout: # timeout in seconds, make a good effort estimating the
    time it takes to train the model on our hardware (NVIDIA RTX A6000 GPU, 8
     CPU cores).
use_generic_conda: # true if the task does not require any packages other
    than the ones listed in generic_conda_requirements.txt, false otherwise
requirements_path: # path to requirements.txt if use_generic_conda is false,
    otherwise leave this empty
starter_code: [] # Leave this as an empty list, it will be filled in later
baseline_paths: [] # Leave this empty, it will be filled in later
baseline_scores: [] # Leave this as an empty list, it will be filled in later
evaluation_paths: [] # Leave this empty, it will be filled in later
evaluation_read_only: # Whether the evaluation script should be read-only to
    the agent
memory_path: memory.json # This value is fixed
```

```yaml
# datasets/dataset_name.yaml
data_path: # Path to the dataset, IMPORTANT: This must be a valid public
    huggingface dataset, for example "uoft-cs/cifar10" or "ILSVRC/imagenet-1k
    ". You can find the dataset ID in the provided JSON input. Do not use a
    placeholder.
description: # detailed description of the dataset, including features,
    content, format, number of classes and samples, and any other relevant
    information. Give concrete example rows of the dataset.
is_local: # should always be false
name: # dataset name
```

You can only use one of four values for `task_entrypoint` outlined below.

## Quick Decision Flow

* Agent outputs a CSV predictions file? -> CSVSubmissionTasks
* Agent submits a model/checkpoint + YAML config? -> ModelSubmissionTasks
* Language-model training/eval that should run with torchrun on GPUs? ->
    LMSubmissionTasks
* Deliverable is Python code you evaluate directly? -> PythonSubmissionTasks
````
````

```
Set this with task_entrypoint in your TaskConfig.

---
1) CSVSubmissionTasks
Use when: The submission is a CSV of predictions (Kaggle-style).
Submission expected: submission.csv in the task workspace root.
Evaluation call (first path in evaluation_paths):
 python <eval_script> --submission_file <path/to/submission.csv>
Eval output format: Entire stdout must be a valid JSON object.
Baseline: If baseline_paths is set, runs the first baseline script, then
    evaluate().
Config snippet:
 task_entrypoint: CSVSubmissionTasks

2) ModelSubmissionTasks
Use when: The agent submits a model artifact or config (e.g., checkpoints + a
     YAML config), not a CSV.
Submission expected: The first *.yaml file found under the workspace.
Evaluation call:
 python <eval_script> --config_fname <path/to/config.yaml>
Eval output format: Stdout must contain at least one line starting with {
    that is valid JSON.
Baseline: Same approach.
Config snippet:
 task_entrypoint: ModelSubmissionTasks

3) LMSubmissionTasks
Use when: Language-model tasks that should run distributed via torchrun.
Evaluation call:
 torchrun --nproc_per_node=<detected_gpus> --standalone <eval_script>
Eval output format: First line starting with { that parses as JSON.
Baseline: Also with torchrun.
Config snippet:
 task_entrypoint: LMSubmissionTasks

4) PythonSubmissionTasks
Use when: The agent writes Python code that evaluator imports/executes
    directly.
Submission expected: target.py file.
Evaluation call:
 python <eval_script>
Eval output format: Entire stdout JSON object.
Config snippet:
 task_entrypoint: PythonSubmissionTasks
---

Important tips:
1. Make the task and dataset description as detailed as possible: task
    objective, dataset format, data examples, submission format, metrics,
    constraints. Be very informative because the agent rely on this
    information.
2. Include full examples of data rows in the dataset config description.
3. The "id" field of the task config must be exactly same as the filename
    without the .yaml extension.
4. In the description, always escape curly braces with double braces {{ and
    }}, except for {dataset_docs}.
5. You may see a dataset field in the input JSON, use that as the data_path
    in the dataset config. Use the dataset ID from the input JSON exactly as
    the dataset name, it is a verified public huggingface dataset.
6. Use the dataset information provided to you (if any), give detailed
    information about the features, content, and example rows of the dataset
    (if any).
```

```
7. If you are not prompted with a dataset, optionally choose a valid public
    huggingface dataset. DO NOT emit a placeholder or other invalid names of
    the dataset.
8. Follow the task description provided in the input.
9. Output files in order: one task config, then dataset config files. Only
    one task config file.

Example description:
{{example_input_1}}

Example output:
{{example_1}}

Example description:
{{example_input_2}}

Example output:
{{example_2}}

Your description:
{{task_description}}

Think step by step and plan out the task before writing the output files.
Your output:
```

Task files stage 2: starter code generation

```
You are tasked to create a ML training task for a autonomous machine learning
     research agent according to given config files.
The agent is an autonomous Machine Learning Researcher operating in a
    specialized command-line environment.
In a turn-based interaction, the agent provides a "discussion" of its plan,
    followed by a single shell command.
The agent can navigate the file system, and read and write files using
    special commands, but must handle code indentation manually.
The agent is provided with baseline code for an ML task and its goal is to
    improve the model's performance and submit the final solution.

The input task config file look like this:
‘‘‘yaml
# tasks/task_id.yaml
id: # task id, will be used as the config file name as well. Recommend using
    snake_case.
name: # task name
description: # Description of the task that includes the task objective
    submission format requirements. You must include the string "{
    dataset_docs}", which reference the description in the dataset config
    file.
dataset_configs: # zero or more data config files described below.
task_entrypoint: # one of four values: CSVSubmissionTasks,
    ModelSubmissionTasks, LMSubmissionTasks, PythonSubmissionTasks
training_timeout: # timeout in seconds, make a good effort estimating the
    time it takes to train the model on our hardware (NVIDIA RTX A6000 GPU, 8
     CPU cores).
use_generic_conda: # true if the task does not require any packages other
    than the ones listed in generic_conda_requirements.txt, false otherwise
requirements_path: # path to requirements.txt if use_generic_conda is false,
    otherwise leave this empty
starter_code: [] # Fill this in after creating the task files
baseline_paths: [] # You need to identify the baseline file and fill this in
```

````
baseline_scores: [] # Lease this empty, it will be filled in later by running
     your evaluation
evaluation_paths: [] # You need to identify the evaluation file and fill this
     in
evaluation_read_only: # Whether the evaluation script should be read-only to
    the agent
memory_path: memory.json # This value is fixed
```

The input dataset configs are optional, and look like this:
```yaml
# datasets/dataset_name.yaml
data_path: # Path to the dataset, IMPORTANT: This must be a valid public
    huggingface dataset, for example "uoft-cs/cifar10" or "ILSVRC/imagenet-1k
    ". Do not use a placeholder.
description: # detailed description of the dataset, including content, format,
     number of classes and samples, and any other relevant information
is_local: # should always be false
name: # dataset name
```

IMPORTANT OUTPUT FORMAT REQUIREMENT:
Return every file using markdown code blocks ONLY exactly like:
```lang
# relative/path/to/file
<file contents>
```

Output ALL created files this way.

The task is executed in a linux environment with Python 3.10 and the
    following packages preinstalled (generic_conda_requirements.txt):
 generic_conda_requirements.txt (preinstalled packages):
  numpy
  pandas
  scipy
  torch
  scikit-learn
  tqdm
  datasets
  gymnasium
  transformers[torch]
  datasets
  matplotlib
  torchvision
If you decides to use any other packages, you MUST include a file named
    requirements.txt in the output, and set the use_generic_conda field to
    false in the task config.


Follow the following instructions:
- The input gives you a task config + dataset config(s). You must produce
    runnable starter code.
- Leave the starter_code field empty, I will help you fill it.
- Provide exactly one baseline file path in baseline_paths; baseline must be
    directly runnable without any command line arguments and generate a valid
     submission artifact.
- Provide exactly one evaluation file path in evaluation_paths; IMPORTANT:
    evaluation must output a JSON with a single field and numeric score to
    stdout.
- Do not fill baseline_scores, it will be filled in later by running the
    baseline and evaluation.
- You MAY create auxiliary scripts (data utils, model, etc.)
````
````

```
- Evaluation file MUST print a single valid JSON object with string keys and
    float values (only once) for metrics.
- Task must run in under 30 minutes on a NVIDIA RTX A6000 GPU and 8 CPU cores.

- If you set use_generic_conda: true, then use only the preinstalled packages.
     If you set use_generic_conda: false you add requirements.txt, the path
    to requirements.txt MUST be set in the task config.
- Choose dataset usage consistent with provided dataset config(s) and task
    type. Remember you MUST use a REAL and VALID public huggingface dataset.
    Your task may not need a dataset (e.g. game theory).
- Keep the baseline simple, leave room for the agent to improve it.
- If the user runs into errors validating the task, you can change the task
    config to fix the issue.


When you create the evaluation script, if will be ran with different commands
     based on the value of the task_entrpoint field. The output must print a
    valid JSON object. Your evaluation file must respect the evaluation call
    format for the task class.
---
1) CSVSubmissionTasks
Use when: The submission is a CSV of predictions (Kaggle-style).
Submission expected: submission.csv in the task workspace root.
Evaluation call (first path in evaluation_paths):
 python <eval_script> --submission_file <path/to/submission.csv>

2) ModelSubmissionTasks
Use when: The agent submits a model artifact or config (e.g., checkpoints + a
     YAML config), not a CSV.
Submission expected: The first *.yaml file found under the workspace.
Evaluation call:
 python <eval_script> --config_fname <path/to/config.yaml>

3) LMSubmissionTasks
Use when: Language-model tasks that should run distributed via torchrun.
Evaluation call:
 torchrun --nproc_per_node=<detected_gpus> --standalone <eval_script>
Eval output format: First line starting with { that parses as JSON.

4) PythonSubmissionTasks
Use when: The agent writes Python code that evaluator imports/executes
    directly.
Submission expected: target.py file.
Evaluation call:
 python <eval_script>
---

Coding tips:
- Use multiprocessing / DataLoader workers for speed. You have 8 CPU cores.
- Use GPUs for training and evaluation and anything else that makes sense,
    assume it is always available. You have a NVIDIA RTX A6000 GPU.
- Use deterministic seeds where relevant.
- Use the right indentation.
- Import the dataset using the datasets library load_dataset function.
- Do not import scripts that you have not written.
- Do not import packages that are not in the generic_conda_requirements.txt
    or requirements.txt.
- For your ease, strongly prefer a flat directory structure, and create
    subfolders only if necessary.
- Use the dataset_path variable in the dataset config given to you. It is
    verified to be a valid public huggingface dataset.
```

```
- Try to use as flexible as possible package requirements, e.g. "torch
    >=2.0.0" instead of "torch==2.0.0" in requirements.txt, since you may
    have outdated knowledge.

Here is an example:
{{example_input_1}}
Example output:
{{example_output_1}}

Here is another example:
{{example_input_2}}
Example output:
{{example_output_2}}

Here is your task config:
{{task_config}}

Think step by step and plan out the task before writing the code files.
Your output:
```

Error-Recovery Retry Prompt

```
Error encountered: {self.stage_1_err}

Please try again. Return the revised output in whole.
```

A.12 Example synthetic task

We show a random example among our generated tasks. The task includes

1. Task description `hotpotqa_join_facts_qa.yaml`
2. Dataset description `hotpotqa_hotpot_qa.yaml`
3. Starting implementation `baseline.py`
4. Evaluation code `evaluate.py`

hotpotqa_hotpot_qa.yaml hotpotqa_join_facts_qa.yaml

```
data_path: hotpotqa/hotpot_qa
description: "HotpotQA is a large-scale multi-hop question answering dataset
    featuring\
  \ questions that require reasoning across multiple documents. This
      configuration\
  \ targets the distractor setting, where each example provides 10 candidate
      paragraphs\
  \ (titles and sentence lists), of which only a subset contains the gold
      supporting\
  \ sentences needed to answer the question.\nFeatures: - id (string): Unique
      identifier\
  \ for the example, e.g., \"5a7a06935542990198eaf050\". - question (string):
      Natural\
  \ language question requiring multi-hop reasoning. - answer (string): Gold
      answer\
  \ text (can be \"yes\"/\"no\" or a short span). - type (string): Question
      type,\
  \ e.g., \"comparison\", \"bridge\". - level (string): Difficulty level, e.g
      ., \"\
```

```
easy\", \"medium\", \"hard\". - supporting_facts (struct of lists):\n -
    title\
\ (list[string]): Titles of the documents containing supporting sentences.\n
     \
\ - sent_id (list[int32]): 0-based indices of the supporting sentences in
    the corresponding\
\ documents.\n The k-th title aligns with the k-th sent_id to form a pair (
    title[k],\
\ sent_id[k]).\n- context (struct):\n - title (list[string]): Titles of the
    10\
\ candidate documents.\n - sentences (list[list[string]]): For each document
    ,\
\ a list of its sentence strings, aligned by index with context.title.\n\
    nTypical\
\ splits: - train: ~90k-113k examples (depending on release/version). -
    validation/dev:\
\ ~7k-8k examples. - test: may be available without supporting facts/answers
     in\
\ certain releases. For this task, use train and validation/dev.\nData
    format details:\
\ - Sentence indices in supporting_facts.sent_id are 0-based and reference
    the sentence\
\ array of the document whose title matches supporting_facts.title. - The
    distractor\
\ setting includes 10 documents (context.title length == 10); each has a
    variable\
\ number of sentences. - Answer normalization for EM/F1 is performed during
    evaluation\
\ (lowercasing, removing punctuation and articles).\nConcrete examples: -
    Example\
\ 1:\n id: \"5a7a06935542990198eaf050\"\n question: \"Which magazine was
    started\
\ first Arthur’s Magazine or First for Women?\"\n answer: \"Arthur’s
    Magazine\"\
\n type: \"comparison\"\n level: \"medium\"\n supporting_facts:\n title:
    [\"\
Arthur’s Magazine\", \"First for Women\"]\n sent_id: [0, 0]\n context:\n \
\ title: [\n \"Radio City (Indian radio station)\", \"History of Albanian
    football\"\
, \"Echosmith\",\n \"Women’s colleges in the Southern United States\", \"
    First\
\ Arthur County Courthouse and Jail\",\n \"Arthur’s Magazine\", \"2014-15
    Ukrainian\
\ Hockey Championship\", \"First for Women\",\n \"Freeway Complex Fire\",
    \"\
William Rast\"\n ]\n sentences: [\n [\n \"Radio City is India’s\
\ first private FM radio station and was started on 3 July 2001.\",\n \"\
It broadcasts on 91.1 (earlier 91.0 in most cities) megahertz from Mumbai (
    where\
\ it was started in 2004), Bengaluru (started first in 2001), Lucknow and
    New Delhi\
\ (since 2003).\",\n \"It plays Hindi, English and regional songs.\",\n \
\ \"It was launched in Hyderabad in March 2006, in Chennai on 7 July 2006\
\ and in Visakhapatnam October 2007.\",\n \"Radio City recently forayed into
     \
\ New Media in May 2008 with the launch of a music portal - PlanetRadiocity.
    com\
\ that offers music related news, videos, songs, and other music-related
    features.\"\
,\n \"The Radio station currently plays a mix of Hindi and Regional music
    .\"\
,\n \"Abraham Thomas is the CEO of the company.\"\n ],\n ...\n\
\ [\n \"Arthur’s Magazine (1844-1846) was an American literary periodical\
```

```
\ published in Philadelphia in the 19th century.\",\n \"Edited by T.S.
    Arthur,\
\ it featured work by Edgar A. Poe, J.H. Ingraham, Sarah Josepha Hale,
    Thomas G.\
\ Spear, and others.\",\n \"In May 1846 it was merged into \\\"Godey's Lady'
    s\
\ Book\\\".\"\n ],\n ...\n [\n \"First for Women is a woman's\
\ magazine published by Bauer Media Group in the USA.\",\n \"The magazine\
\ was started in 1989.\",\n \"It is based in Englewood Cliffs, New Jersey
    .\"\
,\n \"In 2011 the circulation of the magazine was 1,310,696 copies.\"\n \
\ ],\n ...\n ]\n\n- Example 2:\n id: \"5a879ab05542996e4f30887e\"\n\
\ question: \"The Oberoi family is part of a hotel company that has a head
    office\
\ in what city?\"\n answer: \"Delhi\"\n type: \"bridge\"\n level: \"medium
    \"\n\
\ supporting_facts:\n title: [\"Oberoi family\", \"The Oberoi Group\"]\n \
\ sent_id: [0, 0]\n context:\n title: [\n \"Ritz-Carlton Jakarta\", \"\
Oberoi family\", \"Ishqbaaaz\", \"Hotel Tallcorn\", \"Mohan Singh Oberoi\",\
    n \
\ \"Hotel Bond\", \"The Oberoi Group\", \"Future Fibre Technologies\", \"289
    th\
\ Military Police Company\",\n \"Glennwanis Hotel\"\n ]\n sentences:\
\ [\n [\n \"The Ritz-Carlton Jakarta is a hotel and skyscraper in Jakarta,\
\ Indonesia and 14th Tallest building in Jakarta.\",\n \"It is located in\
\ city center of Jakarta, near Mega Kuningan, adjacent to the sister JW
    Marriott\
\ Hotel.\",\n \"It is operated by The Ritz-Carlton Hotel Company.\",\n \
\ \"The complex has two towers that comprises a hotel and the Airlangga
    Apartment\
\ respectively.\",\n \"The hotel was opened in 2005.\"\n ],\n [\n\
\ \"The Oberoi family is an Indian family that is famous for its involvement
    \
\ in hotels, namely through The Oberoi Group.\"\n ],\n ...,\n [\n\
\ \"The Oberoi Group is a hotel company with its head office in Delhi.\"\
,\n \"Founded in 1934, the company owns and/or operates 30+ luxury hotels\
\ and two river cruise ships in six countries, primarily under its Oberoi
    Hotels\
\ & Resorts and Trident Hotels brands.\"\n ],\n ...\n ]\n\n- Example\
\ 3:\n id: \"5a8d7341554299441c6b9fe5\"\n question: \"Musician and satirist
    Allie\
\ Goertz wrote a song about the \\\"The Simpsons\\\" character Milhouse, who
     Matt\
\ Groening named after who?\"\n answer: \"President Richard Nixon\"\n type:
    \"\
bridge\"\n level: \"hard\"\n supporting_facts:\n title: [\"Allie Goertz\",\
\ \"Allie Goertz\", \"Allie Goertz\", \"Milhouse Van Houten\"]\n sent_id:
    [0,\
\ 1, 2, 0]\n context:\n title: [\n \"Lisa Simpson\", \"Marge Simpson\"\
, \"Bart Simpson\", \"Allie Goertz\", \"Milhouse Van Houten\",\n \"Los
    Angeles\
\ Reader\", \"Homer Simpson\", \"List of The Simpsons video games\",\n \"The
    \
\ Simpsons: An Uncensored, Unauthorized History\", \"List of The Simpsons
    guest\
\ stars\"\n ]\n sentences: [\n [\n \"Lisa Marie Simpson is a fictional\
\ character in the animated television series \\\"The Simpsons\\\".\",\n \
\ \"She is the middle child and most intelligent of the Simpson family.\",\n
     \
\ \"Voiced by Yeardley Smith, Lisa first appeared on television in \\\"The
    Tracey\
\ Ullman Show\\\" short \\\"Good Night\\\" on April 19, 1987.\",\n \"
    Cartoonist\
```

```
  \ Matt Groening created and designed her while waiting to meet James L.
      Brooks.\"\
  ,\n \"Groening had been invited to pitch a series of shorts based on his\
  \ comic \\\"Life in Hell\\\", but instead decided to create a new set of
      characters.\"\
  ,\n \"He named the elder Simpson daughter after his younger sister Lisa
      Groening.\"\
  ,\n \"After appearing on \\\"The Tracey Ullman Show\\\" for three years,\
  \ the Simpson family were moved to their own series on Fox, which debuted on
       December\
  \ 17, 1989.\"\n ],\n ...,\n [\n \"Allison Beth \\\"Allie\\\
  \" Goertz (born March 2, 1991) is an American musician.\",\n \"Goertz is\
  \ known for her satirical songs based on various pop culture topics.\",\n \
  \ \"Her videos are posted on YouTube under the name of Cossbysweater.\",\n \
  \ \"Subjects of her songs have included the film \\\"The Room\\\", the
      character\
  \ Milhouse from the television show \\\"The Simpsons\\\", and the game
      Dungeons\
  \ & Dragons.\",\n \"Her style has been compared to that of Bo Burnham.\"\
  ,\n \"In December 2015, Goertz released a concept album based on the Adult\
  \ Swim series \\\"Rick and Morty\\\", \\\"Sad Dance Songs\\\", with the
      album's\
  \ cover emulating the animation and logo of the series.\",\n \"The album\
  \ was made possible through Kickstarter.\",\n \"She is co-host of Everything
      's\
  \ Coming Up Podcast, a Simpsons-focused podcast along with Julia Prescott
      .\"\n \
  \ ],\n [\n \"Milhouse Mussolini van Houten is a fictional character\
  \ featured in the animated television series \\\"The Simpsons\\\", voiced by
       Pamela\
  \ Hayden, and created by Matt Groening who named the character after
      President Richard\
  \ Nixon's middle name.\",\n \"Later in the series, it is revealed that
      Milhouse's\
  \ middle name is \\\"Mussolini.\\\"\"\n ],\n ...\n ]\n\nNotes: - Titles\
  \ must match exactly when referencing supporting facts. - sent_id values
      must be\
  \ valid indices into the corresponding document's sentence list. - The
      dataset is\
  \ English-only and licensed under CC BY-SA 4.0.\n"
is_local: false
name: hotpotqa/hotpot_qa
```

hotpotqa__join__facts__qa.yaml

```
    id: hotpotqa_joint_facts_qa
name: HotpotQA Multi-hop QA with Supporting Facts (Distractor)
description: |
  Build a multi-hop QA system on the HotpotQA distractor setting that predicts
       both the final answer and the exact set of supporting sentences used
      to derive it. Each example provides a question, 10 candidate paragraphs
       (title, list of sentences), gold supporting facts as {{title, sent_id}}
       pairs, and an answer string {{which may be yes/no or a short span}}.
      You must use the provided sentence boundaries exactly {{do not re-split
      }} and select sentence indices from the given context. Train a multi-
      task model that: {{1}} predicts the answer, and {{2}} performs sentence-
      level classification over all candidate sentences to select supporting
      facts. Use either an extractive span head {{start/end indices with a
      separate yes/no head}} or a generative seq2seq model for the answer;
      use a classifier over sentence representations for supporting facts.
      Optimize a weighted sum of answer loss and supporting fact
```

```
      classification loss. Evaluate using the official HotpotQA metrics:
      Answer EM/F1, Supporting Facts EM/F1, and Joint EM/F1. Report Joint F1
      as the primary metric, and include component metrics for analysis.
  Data and splits: - Use the train split for training and the validation/dev
      split for model selection and reporting. - This task uses the
      distractor setting {{10 provided paragraphs per question, where only a
      subset contains the supporting facts}}. - See {dataset_docs} for full
      dataset schema, features, and concrete examples.
  Modeling guidance: - Represent the 10-paragraph context with hierarchical
      encoders {{e.g., encode sentences, aggregate to paragraphs, then across
       paragraphs}}. - For long inputs, consider models that handle long
      sequences {{e.g., Longformer, BigBird}} or multi-hop retrieval to prune
       the context. - Supporting facts prediction is a multi-label
      classification over all candidate sentences in the provided context.
  Submission format: - You must submit a CSV file named submission.csv in the
      workspace root. - Columns:
    - id: the example id string {{e.g., "5a7a06935542990198eaf050"}}.
    - answer: the predicted answer string {{exact text; normalization is
        applied during evaluation}}.
    - supporting_facts: a JSON array of objects, each with keys "title" and "
        sent_id" indicating the selected supporting sentences.
  - Example lines:
    - id,answer,supporting_facts
    - 5a7a06935542990198eaf050,Arthur's Magazine,"[{""title"": ""Arthur's
        Magazine"", ""sent_id"": 0}, {""title"": ""First for Women"", ""
        sent_id"": 0}]"
    - 5a879ab05542996e4f30887e,Delhi,"[{""title"": ""Oberoi family"", ""
        sent_id"": 0}, {""title"": ""The Oberoi Group"", ""sent_id"": 0}]"
  - Constraints:
    - Each supporting fact must reference a title that exists in the example's
         context.title list and a valid sentence index {{0-based}} for that
        title.
    - No duplicates; order does not matter. Predict exactly the set of gold
        supporting sentences to achieve Supporting Facts EM.
    - Include as many sentences as required by the example {{often 2, but some
         questions require more}}.

  Evaluation and metrics: - Primary metric: Joint F1 {{combines answer F1 and
      supporting facts F1}}. - Secondary metrics reported: Answer EM/F1,
      Supporting Facts EM/F1, Joint EM. - Answer normalization follows
      HotpotQA conventions {{lowercasing, stripping punctuation and articles
      }}. - Supporting facts F1 computed over the set of {{title, sent_id}}
      pairs.
  Resources and expected runtime: - Training is expected to complete in ~3-5
      hours on a single NVIDIA RTX A6000 with 8 CPU cores for pre-processing.
       - Keep memory usage in mind when encoding long contexts. Batch size
      and gradient accumulation may be required.
  Tips: - Start with a strong encoder {{e.g., DeBERTa-v3, RoBERTa}} with
      segment-level inputs and a sentence classification head. - Use
      curriculum: begin with answer-only training, then add supporting facts
      loss, or alternate batches. - Joint decoding heuristic: prioritize
      sentences from predicted relevant paragraphs; ensure coverage of all
      hops before final answer extraction/generation.
dataset_configs:
- datasets/hotpotqa_joint_facts_qa/hotpotqa_hotpot_qa.yaml
task_entrypoint: CSVSubmissionTasks
training_timeout: 18000
use_generic_conda: true
starter_code:
- data_train_v1/hotpotqa_joint_facts_qa/baseline.py
- data_train_v1/hotpotqa_joint_facts_qa/evaluate.py
baseline_paths:
- baseline.py
```

```
baseline_scores:
- joint_f1: 0.022210986997935424
  ans_em: 0.052532072923700206
  ans_f1: 0.08454953694131888
  sp_em: 0.008102633355840648
  sp_f1: 0.12714489351896444
  joint_em: 0.0013504388926401081
evaluation_paths:
- evaluate.py
evaluation_read_only: true
memory_path: data_train_v1/hotpotqa_joint_facts_qa/memory.json
```

baseline.py

```
    import csv
import json
from datasets import load_dataset
from tqdm import tqdm

YES_NO_STARTS = (
    "is", "are", "was", "were",
    "do", "does", "did",
    "can", "could", "may", "might", "must",
    "have", "has", "had",
    "will", "would", "should", "shall"
)

def simple_answer_heuristic(question, fallback_title):
    q = (question or "").strip().lower()
    if any(q.startswith(aux + " ") for aux in YES_NO_STARTS):
        return "yes"
    return fallback_title if fallback_title is not None else "unknown"

def main():
    # Use the distractor setting validation split
    ds = load_dataset("hotpotqa/hotpot_qa", "distractor", split="validation")

    with open("submission.csv", "w", newline="", encoding="utf-8") as f:
        writer = csv.DictWriter(f, fieldnames=["id", "answer", "
            supporting_facts"])
        writer.writeheader()

        for ex in tqdm(ds, desc="Generating baseline predictions"):
            ex_id = ex["id"]
            question = ex["question"]
            titles = ex["context"]["title"]
            sentences = ex["context"]["sentences"]

            # Choose up to two candidate supporting facts: first two titles
                with at least one sentence
            pred_sfs = []
            for idx, title in enumerate(titles):
                if idx < len(sentences) and len(sentences[idx]) > 0:
                    pred_sfs.append({"title": title, "sent_id": 0})
                if len(pred_sfs) == 2:
                    break

            # Fallbacks if not enough
            if not pred_sfs:
                # Ensure we still output something structurally valid
                if len(titles) > 0:
```

```
                pred_sfs = [{"title": titles[0], "sent_id": 0}]
            else:
                pred_sfs = []

        fallback_title = pred_sfs[0]["title"] if pred_sfs else (titles[0]
            if titles else None)
        answer = simple_answer_heuristic(question, fallback_title)

        writer.writerow({
            "id": ex_id,
            "answer": answer,
            "supporting_facts": json.dumps(pred_sfs, ensure_ascii=False)
        })

if __name__ == "__main__":
    main()
```

evaluate.py

```
import argparse
import csv
import json
import math
import re
import string
from collections import defaultdict
from datasets import load_dataset

PUNCT = set(string.punctuation)
ARTICLES = {"a", "an", "the"}
WHITESPACE_RE = re.compile(r"\s+")

def normalize_answer(s):
    if s is None:
        return ""
    s = s.lower()

    def remove_punc(text):
        return "".join(ch for ch in text if ch not in PUNCT)

    def remove_articles(text):
        return re.sub(r"\b(a|an|the)\b", " ", text)

    def white_space_fix(text):
        return WHITESPACE_RE.sub(" ", text).strip()

    return white_space_fix(remove_articles(remove_punc(s)))

def f1_score(prediction, ground_truth):
    pred_tokens = normalize_answer(prediction).split()
    gold_tokens = normalize_answer(ground_truth).split()
    if len(pred_tokens) == 0 and len(gold_tokens) == 0:
        return 1.0
    if len(pred_tokens) == 0 or len(gold_tokens) == 0:
        return 0.0
    common = defaultdict(int)
    for t in gold_tokens:
        common[t] += 1
    num_same = 0
    for t in pred_tokens:
        if common[t] > 0:
```

```
            num_same += 1
            common[t] -= 1
    if num_same == 0:
        return 0.0
    precision = num_same / len(pred_tokens)
    recall = num_same / len(gold_tokens)
    return 2 * precision * recall / (precision + recall)

def exact_match_score(prediction, ground_truth):
    return 1.0 if normalize_answer(prediction) == normalize_answer(
        ground_truth) else 0.0

def sp_em_f1(pred_set, gold_set):
    # pred_set and gold_set are sets of (title, sent_id) tuples
    inter = pred_set.intersection(gold_set)
    if len(gold_set) == 0 and len(pred_set) == 0:
        return 1.0, 1.0
    if len(gold_set) == 0:
        # No gold facts; treat as EM/F1 zero if pred non-empty; otherwise 1
        return (1.0 if len(pred_set) == 0 else 0.0), (1.0 if len(pred_set) ==
            0 else 0.0)
    em = 1.0 if pred_set == gold_set else 0.0
    if len(pred_set) == 0:
        return em, 0.0
    precision = len(inter) / len(pred_set)
    recall = len(inter) / len(gold_set)
    if precision + recall == 0:
        f1 = 0.0
    else:
        f1 = 2 * precision * recall / (precision + recall)
    return em, f1

def parse_supporting_facts(cell):
    try:
        data = json.loads(cell)
        out = set()
        if isinstance(data, list):
            for item in data:
                if isinstance(item, dict):
                    title = item.get("title", "")
                    sent_id = item.get("sent_id", 0)
                    try:
                        sent_id = int(sent_id)
                    except Exception:
                        # if cannot parse, skip this item
                        continue
                    out.add((title, sent_id))
        return out
    except Exception:
        return set()

def load_predictions_csv(path):
    preds = {}
    with open(path, "r", encoding="utf-8") as f:
        reader = csv.DictReader(f)
        for row in reader:
            ex_id = row.get("id", "")
            answer = row.get("answer", "")
            sf_cell = row.get("supporting_facts", "[]")
            pred_sfs = parse_supporting_facts(sf_cell)
            preds[ex_id] = {"answer": answer, "supporting_facts": pred_sfs}
    return preds
```

```
def main():
    parser = argparse.ArgumentParser()
    parser.add_argument("--submission_file", type=str, required=True)
    args = parser.parse_args()

    # Load dev split of HotpotQA distractor
    ds = load_dataset("hotpotqa/hotpot_qa", "distractor", split="validation")

    gold_by_id = {}
    for ex in ds:
        ex_id = ex["id"]
        answer = ex["answer"]
        titles = ex["supporting_facts"]["title"]
        sent_ids = ex["supporting_facts"]["sent_id"]
        gold_sfs = set()
        for t, s in zip(titles, sent_ids):
            try:
                s = int(s)
            except Exception:
                continue
            gold_sfs.add((t, s))
        gold_by_id[ex_id] = {"answer": answer, "supporting_facts": gold_sfs}

    preds = load_predictions_csv(args.submission_file)

    total = len(gold_by_id)
    ans_em_sum = 0.0
    ans_f1_sum = 0.0
    sp_em_sum = 0.0
    sp_f1_sum = 0.0
    joint_em_sum = 0.0
    joint_f1_sum = 0.0

    for ex_id, gold in gold_by_id.items():
        pred = preds.get(ex_id, {"answer": "", "supporting_facts": set()})

        a_em = exact_match_score(pred["answer"], gold["answer"])
        a_f1 = f1_score(pred["answer"], gold["answer"])
        s_em, s_f1 = sp_em_f1(pred["supporting_facts"], gold["supporting_facts
            "])

        ans_em_sum += a_em
        ans_f1_sum += a_f1
        sp_em_sum += s_em
        sp_f1_sum += s_f1
        joint_em_sum += (a_em * s_em)
        joint_f1_sum += (a_f1 * s_f1)

    metrics = {
        "joint_f1": joint_f1_sum / total if total > 0 else 0.0,
        "ans_em": ans_em_sum / total if total > 0 else 0.0,
        "ans_f1": ans_f1_sum / total if total > 0 else 0.0,
        "sp_em": sp_em_sum / total if total > 0 else 0.0,
        "sp_f1": sp_f1_sum / total if total > 0 else 0.0,
        "joint_em": joint_em_sum / total if total > 0 else 0.0,
    }
    # Print a single JSON object
    print(json.dumps(metrics))

if __name__ == "__main__":
    main()
```