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011 012 013 014 015 016 017 018 019 020 021 022 023 024 025 026 027 028 029 030 We investigate the extent to which contemporary Large Language Models (LLMs) can engage in *exploration*, a core capability in reinforcement learning and decision making. We focus on native performance of existing LLMs, without training interventions. We deploy LLMs as agents in simple *multi-armed bandit* environments, specifying the environment description and interaction history entirely *in-context*, i.e., within the LLM prompt. We experiment with GPT-3.5, GPT-4, and LLAMA2, using a variety of prompt designs, and find that the models do not robustly engage in exploration without substantial interventions: i) Across all of our experiments, only one configuration resulted in satisfactory exploratory behavior: GPT-4 with chain-of-thought reasoning and an externally summarized interaction history, presented as sufficient statistics; ii) All other configurations did not result in robust exploratory behavior, including those with chain-of-thought reasoning but

1. Introduction

In-context learning is an important emergent capability of Large Language Models (LLMs) that enables one to use a pre-trained LLM to solve a problem by specifying the problem description and relevant data entirely *in-context*, i.e., within the LLM prompt, with no updates to the LLM

making agents in complex settings.

unsummarized history. Although these findings can be interpreted positively, they suggest that external summarization—which may not be possible in more complex settings—is important for obtaining desirable behavior from LLM agents. We conclude that non-trivial algorithmic interventions, such as fine-tuning or dataset curation, may be required to empower LLM-based decision

Abstract

parameters [\(Brown et al.,](#page-8-0) [2020\)](#page-8-0). For example, one can prompt an LLM with numeric covariate vectors and scalar targets and subsequently obtain regression-style predictions from the model by including new covariate vectors in the prompt [\(Garg et al.,](#page-8-1) [2022\)](#page-8-1). Perhaps surprisingly, LLMs are not explicitly trained for this behavior; instead the underlying algorithms employed for in-context learning are extracted from the training corpus and *emerge* at scale.

Since its discovery in the GPT-3 model [\(Brown et al.,](#page-8-0) [2020\)](#page-8-0), in-context learning has been the subject of a growing body of research. These works include theoretical investigations into the underlying mechanisms (e.g., [Xie et al.,](#page-10-0) [2021;](#page-10-0) Akyürek et al., [2022\)](#page-8-2), empirical probes (e.g., [Garg et al.,](#page-8-1) [2022;](#page-8-1) [Kirsch et al.,](#page-9-0) [2022\)](#page-9-0), and works leveraging in-context learning in applications (e.g., [Xu et al.,](#page-10-1) [2022;](#page-10-1) [Som et al.,](#page-10-2) [2023;](#page-10-2) [Edwards et al.,](#page-8-3) [2023\)](#page-8-3). This literature predominantly studies in-context learning for prediction or supervised learning tasks, and while theoretical progress is in its infancy, our understanding of how to use *in-context supervised learning* (ICSL) in practice is rapidly taking shape.

Although supervised learning is an important capability, many applications demand the use of ML models for downstream *decision making*. Thus, *in-context reinforcement learning* (ICRL) and sequential decision making is a natural next frontier. LLMs are already being used as decision making agents in applications ranging from experimental design in the natural sciences [\(Lee et al.,](#page-9-1) [2023b\)](#page-9-1) to game playing [\(Shinn et al.,](#page-9-2) [2023;](#page-9-2) [Wang et al.,](#page-10-3) [2023\)](#page-10-3), but our understanding—theoretically and operationally—of ICRL is far less developed than for ICSL. To date, we lack a systematic understanding as to whether LLMs can be considered general-purpose decision making agents.

Decision making agents must possess three core capabilities: *generalization* (required for supervised learning), *exploration* (making decisions that may be suboptimal in the short term for the sake of gathering more information) and *planning* (to account for long-term consequences of decisions). In this paper, we focus on exploration, the capability to deliberately gather information in order to evaluate alternatives and reduce uncertainty. A recent series of papers [\(Laskin](#page-9-3) [et al.,](#page-9-3) [2022;](#page-9-3) [Lee et al.,](#page-9-4) [2023a;](#page-9-4) [Raparthy et al.,](#page-9-5) [2023\)](#page-9-5) demonstrates in-context reinforcement learning behavior (including exploration) in transformer models when they are *ex-*

Can large language models explore in-context?

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⁰⁵² 053 054 Preliminary work. Under review by the 1st In-context Learning Workshop at the International Conference on Machine Learning (ICML). Do not distribute.

055 056 057 058 059 060 061 *plicitly trained* to produce this behavior using data from reinforcement learning agents or expert demonstrations on related tasks. Such training tends to be laborious, expensive, and possibly task-specific. In particular, these findings do not shed light into whether exploratory behavior manifests in general-purpose LLMs obtained via standard training methods, which suggests the following basic question:

Do contemporary LLMs exhibit the capability to explore in-context?

066 067 068 069 070 071 072 073 074 075 076 077 078 079 080 081 Contributions. We investigate this question by deploying LLMs as agents in simple synthetic reinforcement learning problems, namely *multi-armed bandits (MABs)* [\(Slivkins,](#page-10-4) [2019;](#page-10-4) Lattimore & Szepesvári, [2020\)](#page-9-6), specifying the environment description and interaction history entirely within the LLM prompt. Multi-armed bandits are a classical and well-studied type of RL problem that isolates the tradeoff between exploration and *exploitation*, i.e., making the best decision given the available data. They are also a fundamental building block toward general sequential decision making; the ability to solve MABs is a prerequisite for more challenging reinforcement learning tasks. Their simplicity, centrality to RL, and focus on exploration versus exploitation make MABs a natural choice for systematically studying the in-context exploration abilities of LLMs.

082 083 084 085 086 087 088 089 090 091 092 093 094 095 096 097 We evaluate the in-context exploration behavior of GPT-3.5 [\(Brown et al.,](#page-8-0) [2020\)](#page-8-0), GPT-4 [\(OpenAI,](#page-9-7) [2023\)](#page-9-7), and LLAMA2 [\(Touvron et al.,](#page-10-5) [2023\)](#page-10-5) in MAB environments, using a variety of prompt designs. In our experiments, we find that only a single configuration (i.e., a prompt design and LLM pair) results in satisfactory exploratory behavior. All other configurations exhibit exploration failures, failing to converge to the best decision (*arm*) with significant probability. We find that typically this happens due to *suffix failures*, where the LLM fails to select the best arm even once after some initial rounds (i.e., in some "time suffix"). This scenario is reflected in [Figure 1\(](#page-2-0)a): in particular, GPT-4 with our basic prompt design experiences a suffix failure in $> 60\%$ of the replicates. An alternative failure mode we identify is where the LLM behaves "uniformly", selecting all arms nearequally often and failing to narrow down to the better ones.

098 099 100 101 102 103 104 105 106 107 108 109 The single configuration thato succeeds in our experiments involves a combination of GPT-4 and an "enhanced" prompt that (a) provides a suggestive hint to explore, (b) externally summarizes the history of interaction into per-arm averages, and (c) asks the LLM to use zero-shot chain-of-thought reasoning [\(Wei et al.,](#page-10-6) [2022;](#page-10-6) [Kojima et al.,](#page-9-8) [2022\)](#page-9-8). This configuration is visualized in [Figure 1\(](#page-2-0)b). One can interpret this finding positively: state-of-the-art LLMs *do* possess the capability to robustly explore, provided that the prompt is carefully designed to elicit this behavior. On the other hand, we find that the same configuration without external

summarization fails, which leads to a negative interpretation: LLMs may fail to explore in more complex environments, where externally summarizing the history is a non-trivial algorithm design problem.^{[1](#page-1-0)}

We conclude that while the current generation of LLMs can perhaps explore in simple RL environments with appropriate prompt engineering, training interventions—in the spirit of [Lee et al.](#page-9-4) [\(2023a\)](#page-9-4); [Raparthy et al.](#page-9-5) [\(2023\)](#page-9-5)—may be required to endow LLMs with more sophisticated exploration capabilities required for more complex settings.

Methodology. An underlying technical challenge in assessing LLM capabilities and limitations is that one must search a combinatorially large space of prompt designs while obtaining statistically meaningful results, all while meeting the financial and computational constraints associated with LLMs. Assessing in-context bandit learning is even more challenging because (a) stochasticity in the environment demands a high degree of replication for statistical significance and (b) the sample complexity of learning/exploration demands that even a single experiment involve hundreds or thousands of LLM queries to obtain meaningful effect sizes (i.e., separation between successful and failing methods). To address these issues, our core technical contribution is to identify *surrogate statistics* as diagnostics for long-term exploration failure. The surrogate statistics we consider characterize long-term exploration failure, yet can be measured at moderate scale with few replicates and short learning horizons, even when the standard performance measure (namely, reward) is too noisy to be useful.

2. Experimental setup

Multi-armed bandits (MAB). We consider a basic multiarmed bandit variant, *stochastic Bernoulli bandits*. There are K possible actions (*arms*), indexed as $[K] :=$ $\{1, \ldots, K\}$. Each arm a is associated with mean reward $\mu_a \in [0, 1]$, which is unknown. An agent interacts with the environment for T time steps, where in each time step $t \in [T]$ the agent selects an arm $a_t \in [K]$ and receives a reward $r_t \in \{0, 1\}$ drawn independently from a Bernoulli distribution with mean μ_{a_t} . Thus, the MAB instance is determined by the mean rewards $\{\mu_a : a \in [K]\}$ and the time horizon T . The goal is to maximize the total reward, which roughly corresponds to identifying the *best arm*: an arm with the highest mean reward. A key feature of the MAB setup is that rewards for arms not chosen by the agent are not revealed, so exploration is necessary to identify the best arm.

¹ E.g., if there are many arms, or if we are considering contextual bandits with many contexts, then we may only play each arm (context-arm pair) a few times, so averaging reward separately for each—as we do in our experiments—does not provide much summarization. (See Appendix [B](#page-12-0) for further discussion.)

Can large language models explore in-context?

Figure 1. Representative experiments: Two prompt configurations for GPT-4 on a 5-armed bandit problem, demonstrating exploration failure (top) and success (bottom). The baselines are two standard bandit algorithms with performance guarantees, Upper Confidence Bound (UCB) and Thompson Sampling (TS), as well as the GREEDY algorithm, which always chooses an arm with the best average reward so far and is known to perform poorly. Visualizations are: (Left) histogram over replicates of the number of times the best arm is chosen, (Center) for each t, we plot the *suffix failure frequency*, the fraction of replicates for which the best arm is never chosen after time-step t , and (Right) cumulative time-averaged rewards, averaged over replicates.

135 136 137 138 (a) Top row. GPT-4 with our basic prompt design with zero temperature. The experiment runs for $T = 500$ rounds, and is replicated $N = 20$ times, varying environment randomness. This configuration exhibits highly bimodal behavior: a large ($> 60\%$) fraction of replicates choose the best arm only a handful of times and exhibit suffix failures, similar to GREEDY, and very unlike UCB and TS. This is suggestive of a long term failure to explore and, indeed, this configuration underperforms substantially in terms of reward.

139 140 141 142 (b) Bottom row. GPT-4 with a suggestive framing, summarized history, and chain-of-thought with zero temperature. The experiment runs for $T = 200$ rounds and is replicated $N = 40$ times. This configuration exhibits a unimodal distribution of plays of the best arm, very few suffix failures, and reward that is comparable to TS.

144 145 146 147 148 149 150 We focus on MAB instances where the best arm has mean reward $\mu^* = 0.5 + \Delta/2$ for a parameter $\Delta > 0$, while all other arms have mean reward $\mu = 0.5 - \Delta/2$ (so, $\Delta =$ $\mu^* - \mu$ is the *gap* between the best and the second-best arm). The main instance we consider has $K = 5$ arms and gap $\Delta = 0.2$. We call this the hard instance, as we also consider an easy instance with $K = 4$ and $\Delta = 0.5$ ^{[2](#page-2-1)}

152 153 154 155 156 157 158 159 160 Prompts. We employ LLMs to operate as decision making agents that interact with MAB instances by prompting them with a description of the MAB problem (including the time horizon T) and the history of interaction thus far. Our prompt design allows several independent choices. First is a "scenario", which provides a grounding for the decision making problem, positioning the LLM either a) as an agent choosing *buttons* to press, or b) as a recommendation engine displaying *advertisements* to users. Second, we specify a

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"framing" as either a) explicitly *suggestive* of the need to balance exploration and exploitation, or b) *neutral*. Third, the history can be presented as a) a *raw* list over rounds, or it can b) be *summarized* via number of plays and average rewards of each arm. Fourth, the requested final answer can be a) a single *arm*, or b) a *distribution* over arms. Finally, we either a) request the answer only, or b) also allow the LLM to provide a "chain-of-thought" (CoT) explanation. Altogether, these choices lead to $2^5 = 32$ prompt designs, illustrated in [Figure 2.](#page-3-0) More details about the prompt design, including examples, are provided in Appendix [D.](#page-15-0)

The most basic prompt design from the options above uses the buttons scenario, neutral framing, and raw history, and requests the LLM to return only an arm with no CoT. Each of the five possible modifications to this prompt can potentially help the LLM, and our experiments evaluate this. For example, both the advertising scenario and suggestive framing might help invoke the LLM's knowledge of bandit algorithms (as bandit algorithms are commonly used in

¹⁶¹ 162 163 ²A larger gap Δ makes it easier to distinguish arms, while smaller K means there are fewer alternatives to explore.

Figure 2. Prompt designs; see Figure [11](#page-15-1) for a more detailed view. A prompt is generated by traversing the graph from top to bottom.

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185 186 187 188 189 190 191 192 193 content recommendation). History summarization might help if the LLM cannot reliably summarize history itself (perhaps due to arithmetic errors^{[3](#page-3-1)}) and/or does not fully realize that it should. Returning a distribution might help if the LLM can identify a good distribution, but fails to correctly sample from it. Finally, chain-of-thought is known to help in a wide variety of LLM scenarios [\(Wei](#page-10-6) [et al.,](#page-10-6) [2022;](#page-10-6) [Malach,](#page-9-9) [2023\)](#page-9-9), even when used in a zero-shot manner [\(Kojima et al.,](#page-9-8) [2022\)](#page-9-8) as we do here.

194 195 196 197 198 199 200 201 202 203 204 205 206 Prompts are presented to each LLM using both system and user messages (exposed by all three LLM APIs). The system message presents information about the scenario and framing and prompts the LLM about whether to use CoT and whether (and how) to return a distribution. The user message presents the history and reminds the LLM about how to format its response. For GPT-4 only, we found that prompting the LLM to use CoT in the system prompt did not reliably elicit CoT outputs, so—for GPT-4 only—we also consider a *reinforced CoT* prompt design that additionally reminds the LLM to use CoT at the end of the user prompt. See Appendix [D](#page-15-0) for examples.

LLM configurations. We experiment with three LLMs: GPT-3.5, GPT-4, and LLAMA2. [4](#page-3-2) In addition to the prompt variations above, we also consider two choices for the temperature parameter, 0 and 1. A temperature of 0 forces the LLM to be deterministic and therefore isolates the "deliberate" exploration behavior of the LLM itself. A

temperature of 1 provides a source of external randomness in the LLM responses, which may or may not result in randomization among the arms. Allowing the LLM to return a distribution instead of a single arm also provides external randomness (as we sample from the returned distribution); to isolate sources of randomness, we do not consider temperature 1 with "return distribution" prompt designs.

We refer to the tuple (prompt design, temperature) as the *LLM configuration*. We identify each configuration with a 5-letter "code" $L_1L_2L_3L_4L_5$, with letters L_i denoting the choices:

- L_1 : 'B' or 'A' for, resp., buttons or advertisements scenario;
- L_2 : 'N' or 'S' for, resp., neutral or suggestive framing;
- L_3 : 'R' or 'S' for, resp., raw or summarized history;
- L_4 : 'C' or ' \tilde{C} ' or 'N' for, resp., chain-of-thought, reinforced CoT, or no CoT.
- L_5 : '0', '1' or 'D' for, resp., temperature and returning a distribution (with temperature 0).

We refer to "BNRN0" as the *basic* configuration going forward. Most of our experiments consider the "buttons" scenario, and we use the "advertisements" scenario primarily as a robustness check.

For GPT-3.5 and LLAMA2, we do not consider reinforced CoT as it is not required to reliably elicit CoT outputs; thus, we have 48 configurations total for these two LLMs. For GPT-4, we primarily used reinforced CoT, but did experiment with some standard CoT prompt designs; thus, there are 72 configurations total for GPT-4.

Baselines. For baselines, we consider two standard MAB algorithms, UCB [\(Auer et al.,](#page-8-6) [2002\)](#page-8-6) and Thompson Sampling (TS) [\(Thompson,](#page-10-7) [1933\)](#page-10-7), which are optimal in a certain theoretical sense and also reasonably effective in practice. We also consider the GREEDY algorithm, which does not explore and is known to fail.^{[5](#page-3-3)} While all three baselines have tunable parameters, we perform no parameter tuning (see Appendix [A.1](#page-11-0) for a detailed description of each algorithm with parameter settings). In addition to these baselines, some of our experiments include the the ϵ -GREEDY algorithm^{[6](#page-3-4)} with various choices of ϵ to quantitatively demonstrate tradeoffs between exploration and exploitation. We ran 1000 replicates

²¹⁴ 215 216 ${}^{3}E.g.,$ LLMs sometimes fail at basic arithmetic [\(Gao et al.,](#page-8-4) [2023;](#page-8-4) [Liu et al.,](#page-9-10) [2024\)](#page-9-10), though this is likely to improve in the near future via better training and/or integrating calculator-like tools.

⁴ Specifically: GPT-3.5-TURBO-0613 (released 06/13/2023), GPT-4-0613 (released 06/13/2023), and LLAMA2-13B-CHAT quantized to 4-bits [\(Dettmers & Zettlemoyer,](#page-8-5) [2023\)](#page-8-5).

⁵In each round, GREEDY chooses an arm with the largest average reward so far. The algorithm is initialized with one sample of each arm. It *fails* in that with constant probability, it never chooses the best arm after initialization.

 6 e-GREEDY is a standard MAB algorithm which in each round chooses an arm uniformly at random with a given probability ϵ , and exploits (i.e., mimics GREEDY) otherwise.

220 221 for each baseline and each MAB instance (with rewards realized independently across the replicates).

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223 224 225 226 227 228 229 230 231 Scale of the experiments. Our main set of experiments has time horizon $T = 100$. To account for randomness in rewards (and possibly in the LLM, via temperature) we ran $N \in \{10, 20\}$ replicates for each LLM configuration and each bandit instance, with rewards generated independently across the replicates. As a robustness check, we ran a single experiment on GPT-4 with the basic configuration for $T =$ 500 rounds (with $N = 20$), and obtained consistent/stronger conclusions, depicted in [Figure 1\(](#page-2-0)a).

232 233 234 235 236 237 238 239 240 241 242 243 244 245 246 In more detail, for GPT-3.5 we used $N = 20$ replicates across all 48 prompt configurations, resulting in $\approx 200K$ queries in total. GPT-4 was an order of magnitude more expensive, considerably slower on throughput, and subject to unpredictable throttling. As such, we only used $N = 10$ replicates across 10 representative prompt configurations.[7](#page-4-0) For additional robustness checks, we ran four GPT-4 configurations with $T = 200$, two for $N = 20$ replicates and two for $N = 40$ replicates. In total, this resulted in $\approx 50K$ queries issued to GPT-4. LLAMA2 was essentially free from our perspective (since it was locally hosted), but its performance was consistently sub-par; we limited our experiments to the hard MAB instance, 32 configurations, and $N = 10$ replicates.

247 248 249 250 251 252 253 254 255 256 257 258 259 260 261 262 263 264 265 266 We emphasize that bandit experiments with LLMs are quite costly in terms of money and time. They take $N \cdot T$ LLM queries for each LLM configuration and each MAB instance being tested. Both N and T must be relatively large to obtain statistically meaningful results: N governs the significance level and must be large to overcome randomness in reward realizations, while T governs the effect size and must be large so that good algorithms have enough time to identify the optimal arm. Both issues are more pronounced in harder MAB instances (many arms K and/or small gap Δ), but exploration failures also tend to be less frequent in (very) easy MAB instances.^{[8](#page-4-1)} Further, we need to cover the space of possible prompt designs, which is essentially infinitely large, to ensure that our findings do not overfit to one particular design. Thus, ideally we would take N , T , the number of MAB instances, and the number of prompts to be rather large, but doing so is not practically feasible.^{[9](#page-4-2)} Instead, we use moderately small gap $\Delta = 0.2$, moderately large choices for $N \in \{10, 20\}$ and $T = 100$,

Figure 3. Scatter plot summarizing all experiments with $T = 100$. We plot suffix failures (expressed via SuffFailFreq $(T/2)$) vs. uniform-like failures (expressed via $K \cdot$ MinFrac (T)). Each LLM/configuration pair maps to a dot on this plane (some dots may overlap). The GPT-4 configuration labeled with a star is BSSC0, which is the only configuration that succeeds. We also plot ϵ -GREEDY, tracing out the different tradeoffs obtained for different values of ϵ .

and the prompt design space as described above.

As we will see below, these choices (specifically, $N \in$ $\{10, 20\}$ and $T = 100$ and $\Delta = 0.2$) do not provide enough statistical power to distinguish between successful and unsuccessful methods based solely on accumulated rewards. In lieu of further increasing the scale of the experiments, which is not practically feasible, we rely on *surrogate statistics* which can be detected at our moderate scale, and which are highly suggestive of long-term/persistent exploration failures. Our robustness checks with larger T and N , as well as qualitative findings that we report below provide supporting evidence for this methodology.

3. Experimental results

In this section, we present our experimental findings, beginning with a summary in Section [3.1.](#page-4-3) In Section [3.2](#page-5-0) we investigate failing LLM configurations in detail, and in Section [3.3](#page-6-0) we focus on the single successful LLM configuration our experiments identified. Finally, in Section [3.4](#page-7-0) we attempt to diagnose the underlying causes for exploration failures.

3.1. Overview

We find that all but one of the LLM configurations we consider exhibit exploration failures, not converging to the best arm with significant probability. This happens either due to *suffix failures*, where the LLM never selects the best arm after a small number of initial rounds, or (in a smaller num-

⁷Precisely, $N = 10$ for the buttons scenario, and $N = 3$ for the robustness check with the advertisements scenario.

²⁶⁸ 269 270 ⁸ For example, GREEDY always succeeds when the gap is $\Delta =$ 1, i.e., there is no noise, and trivially succeeds with probability at least $(1 + \Delta)^2/4$ when the initial samples evaluate to 1 for the good arm and 0 for the bad arm.

⁹Raw-history prompts and chain-of-thought outputs are particularly expensive, as LLM APIs bill per token.

275 276 277 278 279 280 ber of configurations) due to *uniform-like failures*, where the LLM selects all arms at an approximately uniform rate, failing to eliminate poorly performing arms. The only one exception is GPT-4 with the BSSC0 configuration, i.e., with the buttons scenario, suggestive framing, summarized history, reinforced CoT, and temperature 0.

281 282 283 284 285 286 287 288 289 290 291 292 293 294 295 296 297 298 299 300 We summarize our key findings in [Figure 3](#page-4-4) and [Figure 5.](#page-13-0) [Figure 3](#page-4-4) summarizes the main set of experiments (which we recall consider the hard MAB instance), visualizing each LLM configuration with a single point on a scatter plot where the axes correspond to two *surrogate statistics*, SuffFailFreq and MinFrac, which represent the strength of the two failure modes (SuffFailFreq measures suffix failures, and $K \cdot$ MinFrac measures uniform-like failures); these statistics are described in detail in the sequel. [Figure](#page-13-0) [5](#page-13-0) displays SuffFailFreq, MinFrac, GreedyFrac (which measures how similar a method is to GREEDY), and additional summary statistics for each of the GPT-4 configurations in the main set of experiments. These statistics reveal that all of the LLM configurations, except for GPT-4-BSSC0 (the blue star in [Figure 3\)](#page-4-4), behave fundamentally differently from the baseline algorithms UCB and TS, and we find that these differences result in a large, persistent drop in performance. Conversely, we find that GPT-4-BSSC0 successfully explores and (as a result) converges to the best arm.

301 302 3.2. Identifying failures

303 304 305 306 307 308 309 310 311 312 313 314 315 We now give a precise overview of the exploration failures illustrated in [Figure 3](#page-4-4) and [Figure 5,](#page-13-0) and provide additional results and figures that illustrate failure in greater detail. We focus on GPT-4, as we find that GPT-3.5 and LLAMA2 perform worse (and often *much* worse) in all experiments; detailed results for GPT-3.5 and LLAMA2 are included in Appendix [E](#page-18-0) for completeness. We begin with detailed background on the surrogate statistics, SuffFailFreq and MinFrac, used to quantify failures in Figures [3](#page-4-4) and [5](#page-13-0) and beyond, providing evidence that exploration failure—as quantified by these statistics—results in a persistent drop in performance.

316 317 318 319 320 321 322 323 324 325 326 327 328 329 Suffix failures. Most of the LLM configurations we consider exhibit highly *bimodal* behavior, whereby a large fraction of the replicates choose the best arm very rarely, and a few replicates converge to the best arm extremely quickly. Consistent with this bimodal behavior, we observe a large incidence of *suffix failures*, where the best arm is not selected even once after a small number initial of rounds (i.e., in some "time suffix"). Suffix failures are suggestive of a long-term failure to explore which cannot be improved by running the algorithm for longer, because, without playing the optimal arm, one cannot acquire information to learn that it is indeed optimal. Such behaviors are qualitatively similar to those of GREEDY and qualitatively very different

from those of UCB and Thompson Sampling.

Our surrogate statistic for measuring suffix failures is defined as follows: For an experiment replicate R and round t, let SuffFail (t, R) be a binary variable that is 1 if the best arm is never chosen in rounds $[t, T]$. Then let SuffFailFreq $(t) := \text{mean}(\{\text{SuffFail}(t, R) :$ replicates R). Suffix failures manifest in most of our experiments at $T = 100$. In the scatter plot in [Figure](#page-4-4) [3,](#page-4-4) the X-axis plots SuffFailFreq $(T/2)$ for each LLM configuration, and we find that all but five configurations have SuffFailFreq $(T/2)$ > 15%. Recalling the definition of suffix failures, this means that $> 15\%$ of the time, these configurations do not pull the best arm *even once* in the last half of the rounds.

A more detailed view of suffix failures and bimodal behavior can be obtained by focusing on individual LLM configurations. We visualize this for the basic configuration (GPT-4-BNRN0) in [Figure 1](#page-2-0) (top) for $T = 500$, and in [Fig](#page-13-1)[ure 6](#page-13-1) for GPT-4 (BNRN0 and BNRN1) at $T = 100$. In these detailed views, the middle panels plot SuffFailFreq (t) at each time t for the given LLM configurations, as well as UCB, TS, and GREEDY. We find that these LLM configurations have much higher suffix failure rates than both UCB and TS. Bimodal behavior is visualized in the left panel of each plot, where for each configuration, a large fraction of replicates rarely pulls the best arm, while the remaining fraction almost always pulls the best arm. Because of this bimodal behavior (particularly because a constant fraction of replicates by chance almost always pull the best arm), suffix failures are not fully reflected in the total reward plots in the right panels of [Figure 6,](#page-13-1) since the time horizon $T = 100$ is not large enough. However, as mentioned, suffix failures are suggestive of an irrecoverable failure to explore which leads to stark differences in reward for larger T . This is precisely what we find at $T = 500$ in [Figure 1,](#page-2-0) which suggests that suffix failures indeed lead to poor long-term performance.

Uniform-like failures. Returning to the left panel of [Figure](#page-4-4) [3,](#page-4-4) we see that three GPT-4 configurations avoid suffix failures. Two of these configurations exhibit a different type of failure, where the LLM selects arms in roughly equal proportions for the entirety of the T rounds and fails to exploit the acquired information to focus on the better arms. We call this a *uniform-like failure*.

Our surrogate statistic for measuring such failures is defined as follows: For a particular experiment replicate R and round t, let $f_a(t, R)$ be the fraction of rounds in which a given arm a is chosen, MinFrac $(t, R) :=$ $\min_a f_a(t, R)$, and MinFrac $(t) := \text{mean}(\{\text{MinFrac}(t, R):$ replicates R}). Since MinFrac $(t) \leq 1/K$, $\forall t \in [T]$, we always plot $K \cdot \text{MinFrac}(t)$, so as to rescale the range to [0, 1]. Larger MinFrac (t) corresponds to a more uniform selection

330 331 332 333 of arms at time t. When an LLM's MinFrac (t) does not decrease over time and stays substantively larger than that of the baselines (especially as t approaches the time horizon T), we take it as an indication of a uniform-like failure.

334 335 336 337 338 339 340 341 342 343 344 345 346 347 348 349 350 351 352 353 The Y-axis of [Figure 3](#page-4-4) records $K \cdot MinFrac(T)$ for each configuration, where we see that of the three GPT-4 configurations that avoid suffix failures, two configurations have very high MinFrac (T) relative to UCB and TS (the third configuration is GPT-4-BSS \widetilde{C} 0, which is successful). These two configurations are GPT-4-BNRND and GPT-4-BSSCD, both of which use the *distributional* output format. We provide a more detailed view of GPT-4-BNRND (as well as GPT-4-BNSND, which also exhibits uniform-like failures, but only differs from GPT-4-BNRND in the use of summarized history) in [Figure 7,](#page-13-2) which considers a longer horizon and more replicates ($T = 200$ and $N = 20$). The middle panel reveals that $K \cdot$ MinFrac(t) does not decrease over time for these LLM configurations, while it does for the baselines. This behavior results in no suffix failures, but leads to much lower reward than the baselines. In particular, we obtain a clear separation in total reward, showing that uniform-like failures indeed result in poor long-term performance.

354 355 356 357 358 359 360 361 Generality of the failures. To summarize, [Figure 3](#page-4-4) shows that all LLM configurations except GPT-4-BSSC0 exhibit either a suffix failure or a uniform failure for the hard MAB instance and the buttons scenario. Scatter plots for the other three experiments (i.e., the advertisements scenario and/or the easy MAB instance) are qualitatively similar and are deferred to Appendix [E.](#page-18-0)

362 363 364 365 366 367 368 369 The same data, but with attributions to specific LLM configurations, are presented for *all* GPT-4 configurations in [Figure 5;](#page-13-0) analogous tables for other LLMs and experimental settings are given in Appendix [E.](#page-18-0) As it is not instructive to present detailed plots such as [Figure 6](#page-13-1) for every LLM configuration, [Figure 5](#page-13-0) summarizes the performance of each configuration with just a few statistics. We include:

• SuffFailFreq $(T/2)$ and MinFrac (T) , defined above.

- MedianReward: the rescaled median (over replicates) of the time-averaged total reward.^{[10](#page-6-1)}
- GreedyFrac: the fraction of *greedy rounds*, averaged over the replicates. A greedy round is one in which an arm with a largest average reward is selected. This is one way to quantify the extent to which a configuration behaves like GREEDY.

We now summarize further findings from the scatter plots (Figures [3](#page-4-4) and [12\)](#page-18-1) and the summary tables (Figures [13](#page-19-0) to [19\)](#page-25-0). First, GPT-4 performs much better than GPT-3.5, and LLAMA2 performs much worse (in particular, the suffix failure frequency for LLAMA2 ranges from that of GREEDY to much larger). Second, we observe that all LLMs are sensitive to small changes in the prompt design. However, the different modifications we consider appear to interact with each other, and it is difficult to identify which individual modifications improve performance and which degrade it.

3.3. Investigating successes

On the hard MAB instance, the only configuration in our experiments that avoids both suffix failures and uniform-like failures is GPT-4 with the BSSC0 prompt design. As can be seen from [Figure 5,](#page-13-0) at $T = 100$, this configuration has no suffix failures, the $K \cdot$ MinFrac value is only slightly larger than TS, and the reward is comparable to TS. These statistics suggest that this configuration succeeds, and in this section we present further evidence supporting this claim.

To do so, we run GPT-4-BSS \widetilde{C} 0 on the hard MAB instance with $T = 200$ and $N = 40$ to obtain more statistically meaningful results. We also consider GPT-4-BSRC0, which swaps summarized history for raw history, as an ablation. [Figure 8](#page-14-0) provides a summary of the results from this experiment, while [Figure 1\(](#page-2-0)b) provides a detailed view of the BSSC0 configuration. The figures reveal that BSSC0 continues to avoid suffix failures and performs relatively well in terms of reward for larger T . On the other hand, we see that BSRC0 exhibits a non-trivial fraction of suffix failures, demonstrating that this ablation results in fundamentally different behavior.

We also provide two additional visualizations that provide some qualitative evidence toward the success of BSSC0, as well as the failure of other configurations. These are presented in [Figure 9](#page-14-1) and [Figure 10.](#page-14-2) In [Figure 9](#page-14-1) we visualize the arm chosen at each time step for various replicates of several different methods (LLMs and baselines). Specifically, [Figure 9](#page-14-1) shows four replicates for the basic configuration (BNRN0) and the two configurations with reinforced CoT (BSRC0 and BSSC0), as well as one replicate of each of the baseline algorithms. We see that the basic configuration BNRN0 tends to commit to a single arm for several rounds, a behavior that is similar to that of GREEDY and very different from both UCB and TS. BSRC0 also commits for long periods, but to a lesser extent than the basic configuration. In contrast, BSSC0 switches arms much more frequently, and qualitatively appears much more similar to TS.

In [Figure 10,](#page-14-2) we plot the fraction of rounds in $[0, t]$ where the optimal arm was pulled as a function of t for individual replicates. BSRC0 is visually similar to UCB, except that a non-trivial fraction of runs exhibit suffix failures (the

³⁸¹ 382 383 384 ¹⁰More precisely, let $\Phi(R)$ be the time-averaged total reward for a given replicate R. Then $\mathbb{E}\{\Phi(R)\}\)$ ranges in the interval $[1/2 - \Delta/2, 1/2 + \Delta/2]$. We rescale $\Phi(R)$, by translating and multiplying, so that $\mathbb{E}\{\Phi(R)\}\$ ranges in [0, 1].

385 386 387 388 389 390 curves that converge to 0 on the plot). Meanwhile, BSSC 0 is visually similar to TS, with almost all replicates slowly converging to 1. These visualizations, along with the summary statistics, suggest that BSSC0 behaves most similarly to TS, which further suggests it will successfully converge to the optimal arm given a long enough time horizon.

3.4. Root causes

Figure 4. Per-round decisions with some GPT-3.5 configurations. $T = 100$, histories of length $t = 30$, hard MAB instance.

Our experimental findings above shed light on how LLMbased decision making agents behave, but it is also worthwhile to understand *why* they behave the way they do (and particularly, why they fail). This question is rather challenging to answer decisively, but two natural hypotheses are that the configurations we consider (outside of GPT-4-BSSC0) are either a) too greedy, or b) too uniform-like. In this section, we describe how our experiments offer some insight into this hypotheses.

418 419 420 421 422 423 424 425 426 427 428 429 430 First, focusing on GPT-4, our experiments reveal qualitatively different behavior between the easy and hard instances [\(Figure 13\(](#page-19-0)a) and [Figure 13\(](#page-19-0)c)). Indeed, the easy instance appears to be *much* easier; most GPT-4 configurations avoid suffix failures and accrue large rewards on this instance, and the GreedyFrac statistic offers a potential explanation as to why. On the easy instance, most GPT-4 configurations have very high GreedyFrac values, so they behave similarly to GREEDY, which performs quite well (even though GREEDY provably fails with small constant probability and, empirically, has many suffix failures on this instance).^{[11](#page-7-1)} A plausible hypothesis from this is that GPT-4 performs quite well in low-noise settings, which is precisely when GREEDY also performs well.

431 432 433 A stronger hypothesis would be that most GPT-4 configurations (except perhaps those using reinforced CoT) behave

like GREEDY on *all* instances, but this hypothesis is invalidated by the GreedyFrac statistics for our experiments on the hard instance. On the hard instance, it seems that most GPT-4 configurations are doing something non-trivial (albeit flawed); their behavior is neither completely GREEDY-like nor like uniform-at-random.

Toward a more fine-grained understanding, we ran a collection of small-scale secondary experiments focusing on the *per-round decisions* of LLM-agents. The experiments focus on a single round t in a bandit problem. Each experiment considers a particular "data source" (a distribution of bandit histories), samples $N = 50$ bandit histories of length t from this distribution, and presents them to the agents (the LLMs and the baselines) and asks them to output an arm or distribution over arms. We track two statistics for each agent: GreedyFrac and LeastFrac, the fraction of replicates in which the agent chose, resp., an empirically best arm so far and a least-chosen arm so far. We vary the data source, i.e., the algorithm which generates the history. In particular, we consider histories generated by sampling uniformly at random (Unif) and by running our baselines UCB and TS for t rounds.

Results are summarized in [Figure 4.](#page-7-2) Unfortunately, we find that per-round performance of both the LLMs and the baselines is very sensitive to the particular data source. For example, the MinFrac statistic of UCB can vary from as high as 0.46 on histories generated uniformly at random to as low as 0.09 on histories generated by UCB itself. It seems plausible to conclude the BNSN0 is too greedy while BSRN0 is too uniform, but the statistics for the other two LLM configurations (BNRN0 and BNRC0)—both of which fail in our longitudinal experiments—fall within the reasonable range provided by the baselines. Thus, we find that it is challenging to assess whether LLM agents are too greedy or too uniform-like based on per-round decisions, even though these agents behave rather differently from the baselines in the longitudinal experiments.

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⁴³⁴ 435 436 437 438 439 11 Indeed, in [Figure 13\(](#page-19-0)c) we see that most GPT-4 configurations have very high GreedyFrac but no suffix failures. Apparently, even a very small amount of exploration suffices for easy instances (and makes a big difference, relative to GREEDY). However, this should not be construed as evidence for the more general and robust exploratory behavior necessary for harder bandit instances.

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605 A. Related work

606 607 608 609 610 611 This paper belongs to a recent body of work that aims to understand the capabilities of LLMs, i.e., what they can and cannot do well, and why. Capabilities that have received considerable attention, but are peripheral to the present paper, include general intelligence [\(Bubeck et al.,](#page-8-7) [2023\)](#page-8-7), causal [\(Kıcıman et al.,](#page-9-11) [2023;](#page-9-11) [Yiu et al.,](#page-10-8) [2023\)](#page-10-8) and mathematical reasoning [\(Cobbe](#page-8-8) [et al.,](#page-8-8) [2021;](#page-8-8) [Lu et al.,](#page-9-12) [2023\)](#page-9-12), planning [\(Valmeekam et al.,](#page-10-9) [2023;](#page-10-9) [Momennejad et al.,](#page-9-13) [2023;](#page-9-13) [Brooks et al.,](#page-8-9) [2023\)](#page-8-9), and compositionality [\(Yu et al.,](#page-10-10) [2023\)](#page-10-10).

612 613 614 615 616 617 618 619 620 621 622 623 624 625 In more detail, our work contributes to the broader literature on capabilities of in-context learning. Prior studies of in-context learning include theoretical [\(Xie et al.,](#page-10-0) [2021;](#page-10-0) Akyürek et al., [2022;](#page-8-2) [Zhang et al.,](#page-10-12) [2023b;](#page-10-11) [Abernethy et al.,](#page-7-3) [2023;](#page-7-3) Zhang et al., [2023a;](#page-10-12) [Han et al.,](#page-8-10) [2023a;](#page-8-10) [Cheng et al.,](#page-8-11) [2023;](#page-8-11) [Ahn et al.,](#page-7-4) [2023;](#page-7-4) [Wies et al.,](#page-10-13) [2023;](#page-10-13) [Fu et al.,](#page-8-12) [2023;](#page-8-12) [Wu et al.,](#page-10-14) [2023;](#page-10-14) [Huang et al.,](#page-9-14) [2023;](#page-9-14) [Hendel et al.,](#page-9-15) [2023;](#page-9-15) [Li et al.,](#page-9-16) [2023;](#page-9-16) [Von Oswald et al.,](#page-10-15) [2023;](#page-10-15) [Bai et al.,](#page-8-13) [2023;](#page-8-13) [Hahn & Goyal,](#page-8-14) [2023;](#page-8-14) [Jeon et al.,](#page-9-17) [2024\)](#page-9-17) and empirical [\(Garg et al.,](#page-8-1) [2022;](#page-9-0) [Kirsch et al.,](#page-9-0) 2022; [Ahuja et al.,](#page-8-15) [2023;](#page-9-19) [Han et al.,](#page-9-18) [2023b;](#page-9-18) Raventós et al., 2023; [Weber](#page-10-16) [et al.,](#page-10-16) [2023;](#page-9-20) [Bhattamishra et al.,](#page-8-16) 2023; [Guo et al.,](#page-8-17) 2023; [Shen et al.,](#page-9-20) 2023; Akyürek et al., [2024\)](#page-8-18) investigations, though as mentioned in the prequel, the vast majority of this work pertains to in-context supervised learning; in-context reinforcement learning has received far less attention. The small collection of empirical works that study in-context RL [\(Laskin et al.,](#page-9-3) [2022;](#page-9-3) [Lee et al.,](#page-9-4) [2023a;](#page-9-4) [Raparthy et al.,](#page-9-5) [2023;](#page-9-5) [Xu et al.,](#page-10-1) [2022\)](#page-10-1) focus on models trained from scratch using trajectory data collected from another agent (either an RL algorithm or an expert); theoretically, [Lee et al.](#page-9-4) [\(2023a\)](#page-9-4) and later [Lin et al.](#page-9-21) [\(2023\)](#page-9-21) justify this approach with a Bayesian meta-reinforcement learning perspective [\(Simchowitz et al.,](#page-10-17) [2021\)](#page-10-17), and show that pre-trained transformers can implement classical exploration strategies like Thompson sampling and upper confidence bounds (UCB). However, these works require interventions to the *pre-training* phase of the language model, and do not study whether existing LLMs exhibit exploration capabilities under standard training conditions.

626 627 628 629 630 In parallel, there is a rapidly growing line of work that applies LLMs to real-world decision-making applications. Beyond previously mentioned works [\(Shinn et al.,](#page-9-2) [2023;](#page-9-2) [Wang et al.,](#page-10-3) [2023;](#page-10-3) [Lee et al.,](#page-9-1) [2023b\)](#page-9-1), which consider applications to gaming, programming, and medicine, highlights include [Park et al.](#page-9-22) [\(2023\)](#page-9-22), who introduce generative agents which simulate human behavior in an open-world environment, [Ahn et al.](#page-8-19) [\(2022\)](#page-8-19); [Xu et al.](#page-10-18) [\(2023\)](#page-10-18), who develop LLM-enabled robots.

631 632 633 634 635 636 637 638 639 640 Concurrent work of [Wu et al.](#page-10-19) [\(2024\)](#page-10-19) studies LLM performance in a battery of tasks that aim to characterize "intelligent agents", with two-armed bandits as a specific task of interest. Their bandit experiments differ in several key respects: They consider a very easy MAB instance (with 2 arms and a gap $\Delta = 0.6$, which is much easier than both of our instances), focus on a single prompt design (similar to our basic prompt), and compare to human players rather than algorithmic benchmarks. These differences lead to very different experimental findings. In particular, they find that GPT-4 performs well on their simple MAB instance, converging very quickly to the best arm, while we find that GPT-4 with a similar prompt fails on a harder MAB instance. However, their finding is consistent with ours, as we also find that several configurations of GPT-4 do well on the easy MAB instance. As we discuss in Section [3.4,](#page-7-0) this instance is too simple to provide compelling evidence for principled exploratory behavior.

A.1. Further background on multi-armed bandits

642 643 644 Here, we provide additional background on the multi-armed bandit problem, and on the baseline algorithms used in this paper. Deeper discussion can be found in [Bubeck & Cesa-Bianchi](#page-8-20) [\(2012\)](#page-8-20); [Slivkins](#page-10-4) [\(2019\)](#page-10-4); Lattimore & Szepesvári [\(2020\)](#page-9-6).

645 646 647 648 649 650 The UCB algorithm [\(Auer et al.,](#page-8-6) [2002\)](#page-8-6) explores by assigning each arm a an *index*, defined as the average reward from the arm so far plus a *bonus* of the form $\sqrt{C/n_a}$, where $C = \Theta(\log T)$ and n_a is the number of samples from the arm so far. In each round, it chooses an arm with the largest index. The bonus implements the principle of *optimism under uncertainty*. We use a version of UCB that sets $C = 1$ (a heuristic), which has been observed to have a favorable empirical performance (e.g., [Slivkins et al.,](#page-10-20) [2013;](#page-10-20) [Ho et al.,](#page-9-23) [2016\)](#page-9-23).

651 652 653 654 655 656 657 658 Thompson Sampling [\(Thompson,](#page-10-7) [1933;](#page-10-7) [Russo et al.,](#page-9-24) [2018,](#page-9-24) for a survey) proceeds as if the arms' mean rewards were initially drawn from some Bayesian prior. In each round, it computes a Bayesian posterior given the history so far, draws a sample from the posterior, and chooses an arm with largest mean reward according to this sample (i.e., assuming the sample were the ground truth). In our setting, the prior is essentially a parameter to the algorithm. We choose the prior that draws the mean reward of each arm independently and uniformly at random from the $[0, 1]$ interval. This is one standard choice, achieving near-optimal regret bounds, as well as good empirical performance [\(Kaufmann et al.,](#page-9-25) [2012;](#page-9-25) [Agrawal & Goyal,](#page-7-5) [2012;](#page-7-5) [2017\)](#page-7-6). Each arm is updated independently as a Beta-Bernoulli conjugate prior. Further optimizing UCB and Thompson Sampling is non-essential to this paper, as they already perform quite well in our experiments.

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660 Provable guarantees for bandit algorithms are commonly expressed via *regret*: the difference in expected total reward of the

661 662 663 best arm and the algorithm. Both baselines achieve regret $O(\sqrt{KT \log T})$, which is nearly minimax optimal as a function of T and K. They also achieve a nearly instance-optimal regret rate, which scales as $O\{K/\Delta \log T\}$ for the instances we consider.

664 665 666 667 The ϵ -GREEDY algorithm (Footnote [6\)](#page-3-4) is fundamentally inefficient in that it does not adaptively steer its exploration toward better-performing arms. Accordingly, its regret rate scales as $T^{2/3}$ (for an optimal setting of $\epsilon \sim T^{-1/3}$). Fixing such ϵ , regret does not improve for easier instances.

668 669 670 671 The GREEDY algorithm (Footnote [5\)](#page-3-3) does not explore at all, which causes suffix failures. This is obvious when the algorithm is initialized with a single sample $(n = 1)$ of each arm: a suffix failure happens when the good arm returns 0, and one of the other arms returns 1. However, suffix failures are not an artifact of small n: they can happen for any n, with probability that scales as $\Omega(1/\sqrt{n})$ [\(Banihashem et al.,](#page-8-21) [2023\)](#page-8-21).

B. Discussion and open questions

Our investigation suggests that contemporary LLMs do not robustly engage in exploration required for very basic statistical reinforcement learning and decision making problems, at least without further intervention. In what follows, we identify several next steps to further evaluate this hypothesis and search for interventions to mitigate this behavior.

679 680 Basic interventions and the need for methodological advancements. In light of our negative results, the most obvious interventions one might consider include:

- 1. *Experiment with other prompts.* As with many other settings [\(Sclar et al.,](#page-9-26) [2023\)](#page-9-26), it is possible that small changes to our prompt template might improve performance. However, sensitivity to prompt design is already concerning.
- 2. *Experiment with few-shot prompting,* where the prompt contains examples of exploratory behavior, or use such examples to *fine-tune* the LLM.
- 3. *Train the LLM to use auxiliary tools,* such as a calculator for basic arithmetic or a "randomizer" to correctly sample from a distribution.

690 691 692 693 While these steps are quite natural, cost, access to models, and compute pose significant barriers to further study, particularly because of the need to employ long horizons T and many replicates N to obtain statistically meaningful results. To this end, we believe that further methodological and/or statistical advancements to enable cost-effective diagnosis and understanding of LLM-agent behavior (e.g., our surrogate statistics) are essential.

695 696 697 698 699 700 701 702 703 704 705 Implications for complex decision making problems. Our focus on simple multi-armed bandit problems provides a clean and controllable experimental setup to study the exploratory behavior of LLMs and potential algorithmic interventions. Exploration failures here suggest that similar failures will also occur in more complex RL and decision making settings. On the other hand, caution must be exercised in developing mitigations, as solutions that succeed for the MAB setting may not generalize to more complex settings. For example, while GPT-4 with summarized interaction history and reinforced CoT seems to successfully explore in our MAB setting, it is not clear how one should externally summarize the history in settings with complex, high-dimensional observations such as contextual bandits (see Footnote [1\)](#page-1-0). Indeed, even for linear contextual bandits, the approach may not be applicable without a substantial algorithmic intervention (such as, e.g., a linear regression computed externally and included in the prompt) and the many explicit modeling and algorithmic choices involved in such interventions. We believe a deeper investigation of algorithmic interventions is essential to understand the extent to which LLMs can operate as decision making agents.

C. Additional figures

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Can large language models explore in-context?

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717		TS.	UCB	Greedy	BNRNO	BNRN1	BNRND	BNRCO	BNSNO	BSRN0	BSSC0	BSSC1	BSSCD	BSSC ₀
718	MedianReward	0.47	0.55	0.40	0.63	0.70	0.33	0.35	0.60	0.45	0.68	0.28	0.37	0.47
719 720	SuffFailFreq(T/2)	0.01	0.02	0.48	0.50	0.40	0.00	0.50	0.60	0.70	0.30	0.20	0.00	0.00
721 722	K*MinFrac	0.28	0.18	0.05	0.03	0.04	0.41	0.09	0.07	0.05	0.09	0.19	0.49	0.33
723 724	GreedyFrac	0.62	0.76	1.00	0.52	0.46	0.45	0.78	0.99	0.59	0.93	0.88	0.49	0.69
725 726	Replicates	1000	1000	1000	10	10	10	10	10	10	10	10	10	10

Figure 5. GPT-4 for $T = 100$: a per-configuration summary table on the hard MAB instance. Only three GPT-4 configurations do not exhibit suffix failures; two of these (BNRND and BSSCD) exhibit uniform-like failures. The final configuration (BSSC0) succeeds.

Figure 6. Detailed view of bimodal behavior and suffix failures for GPT-4 with $T = 100$. Configurations visualized are the basic configuration (BNRN0) and the same configuration but with temperature 1 (BNRN1). Visualizations are the same as in [Figure 1.](#page-2-0)

Figure 7. Detailed view of uniform-like failures for GPT-4 (the BNRND and BNSND configurations) with $T = 200$. Visualizations are: (Left) suffix failure frequency, (Center) $K \cdot$ MinFrac(t) as a function of t and (Right) cumulative time-averaged rewards. These configurations exhibit uniform-like failures but not suffix failures, and uniform-like failures are detrimental to long-term rewards.

Can large language models explore in-context?

	TS	UCB	Greedy	BSRCO	BSSCO
MedianReward	0.59	0.70	0.60	0.65	0.54
SuffFailFreq(T/2)	0.00	0.02	0.47	0.12	0.03
K*MinFrac	0.23	0.12	0.03	0.11	0.29
GreedyFrac	0.66	0.81	1.00	0.75	0.68
Replicates	1000	1000	1000	40	40

Figure 8. Summary statistics of two GPT-4 configurations with reinforced CoT (BSRC0 and BSSC0) when run on the hard MAB instance with $T = 200$ for $N = 40$ replicates. BSRC0 exhibits suffix failures. BSSC0 exhibits neither suffix failures nor uniform-like failures and has reasonable reward, so we declare it to be successful.

Figure 9. Traces of the arm chosen at each time step for (a) 4 of the replicates of the basic configuration (GPT-4-BNRN0) (left four cells in top row), (b) 4 of the replicates of GPT-4-BSRC0 (left four cells of the middle row), (c) 4 of the replicates of GPT-4-BSSC0 (left four cells of the bottom row), as well as one replicate of GREEDY (red border), UCB (green border) and TS (orange border). For each of the $T = 100$ time steps (X-axis) we indicate which of the five arms was chosen (Y-axis). The best arm is the top row of each plot, highlighted with blue boxes.

Figure 10. Visualization of the per-replicate behavior of two GPT-4 configurations with reinforced-CoT and the baselines. For each algorithm, replicate and time step t, we plot the fraction of rounds in $[0, t]$ where the optimal arm was pulled.

D. Prompt designs

Figure 11. Prompt designs with text in the buttons scenario, expanding on [Figure 2.](#page-3-0)

880 D.1. Prompt examples

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Let us present three full examples of our prompts. We remove the blank lines for the sake of readability.

883 884 885 (a) Our basic prompt design (i.e., BNRN, as temperature is specified elsewhere): the buttons scenario with neutral framing and raw histories, asking the LLM to return an action without chain-of-thought reasoning.

887 888 889 890 891 [SYSTEM] You are in a room with 5 buttons labeled blue, green, red, yellow, purple. Each button is associated with a Bernoulli distribution with a fixed but unknown mean; the means for the buttons could be different. For each button, when you press it, you will get a reward that is sampled from the button's associated distribution. You have 10 time steps and, on each time step, you can choose any button and receive the reward. Your goal is to maximize the total reward over the 10 time steps.

- 892 893 894 895 896 At each time step, I will show you your past choices and rewards. Then you must make the next choice, which must be exactly one of blue, green, red, yellow, purple. You must provide your final answer immediately within the tags <Answer>COLOR</Answer> where COLOR is one of blue, green, red, yellow, purple and with no text explanation.
- 897 [USER] So far you have played 2 times with the following choices and rewards:
- 898 blue button, reward 1
- 899 900 green button, reward 0
	- Which button will you choose next? Remember, YOU MUST provide your final answer within the tags <Answer>COLOR</Answer> where COLOR is one of blue, green, red, yellow, purple.

904 905 906 (b) The adverts scenario with all the "advanced" modifications (i.e., ASSCD) : suggestive framing, summarized histories, asking the LLM to return a distribution over actions, and asking for a chain-of-thought reasoning.

908 909 910 911 912 [SYSTEM] You are recommendation engine that chooses advertisements to display to users when they visit your webpage. There are 5 advertisements you can choose from, named A, B, C, D, E. When a user visits the webpage you can choose an advertisement to display and you will observe whether the user clicks on the ad or not. You model this by assuming that each advertisement has a certain click rate and users click on advertisements with their corresponding rates.

913 914 915 You have a budget of 10 users to interact with and your goal is to maximize the total number of clicks during this process.

916 917 918 A good strategy to optimize for clicks in these situations requires balancing exploration and exploitation. You need to explore to try out all of the options and find those with high click rates, but you also have to exploit the information that you have to accumulate clicks.

- 919 When each user visits the webpage, I will show you a summary of the data you have collected so far.
- 920 921 922 Then you must choose which advertisement to display. You may output a distribution over the 5 choices formatted EXACTLY like "A:n1,B:n2,C:n3,D:n4,E:n5".
- 923 924 Let's think step by step to make sure we make a good choice. Then, you must provide your final answer within the tags <Answer>DIST</Answer> where DIST is the distribution in the format specified above.
- 925 926 [USER] So far you have interacted with 2 users. Here is a summary of the data you have collected:
- 927 Advertisement A was shown to 1 users with an estimated click rate of 1.00
- 928 Advertisement B was shown to 1 users with an estimated click rate of 0.00
- 929 Advertisement C has not been shown
- 930 Advertisement D has not been shown
- 931 Advertisement E has not been shown
- 932 933 934 Which advertisement will you choose next? Remember, YOU MUST provide your final answer within the tags <Answer>DIST</Answer> where DIST is formatted like "A:n1,B:n2,C:n3,D:n4,E:n5".

 (c) The successful configuration for GPT-4 (i.e., $BSS\tilde{C}$, as temperature is specified elsewhere), which uses the buttons scenario, suggestive framing, summarized histories, and reinforced chain-of-thought reasoning.

 [SYSTEM] You are a bandit algorithm in a room with 5 buttons labeled blue, green, red, yellow, purple. Each button is associated with a Bernoulli distribution with a fixed but unknown mean; the means for the buttons could be different. For each button, when you press it, you will get a reward that is sampled from the button's associated distribution. You have 10 time steps and, on each time step, you can choose any button and receive the reward. Your goal is to maximize the total reward over the 10 time steps.

 At each time step, I will show you a summary of your past choices and rewards. Then you must make the next choice, which must be exactly one of blue, green, red, yellow, purple. Let's think step by step to make sure we make a good choice. You must provide your final answer within the tags $\langle \text{Answer}\rangle \text{COLOR} \langle \text{Answer}\rangle$ where COLOR is one of blue, green, red, yellow, purple.

- [USER] So far you have played 2 times with your past choices and rewards summarized as follows:
- blue button: pressed 1 times with average reward 1.00
- green button: pressed 1 times with average reward 0.00
- red button: pressed 0 times
- yellow button: pressed 0 times
- purple button: pressed 0 times

 Which button will you choose next? Remember, YOU MUST provide your final answer within the tags <Answer>COLOR</Answer> where COLOR is one of blue, green, red, yellow, purple. Let's think step by step to make sure we make a good choice.

1022 1023 1024 1025 Figure 12. All scatter plots for the main experiments $(T = 100)$: suffix failures vs. uniform-like failures. Specifically: SuffFailFreq($T/2$) vs $K \cdot$ MinFrac(T). Each LLM/configuration pair maps to a dot on this plane. (However, some dots may be hidden by some others.) We also plot ϵ -GREEDY, tracing out the different tradeoffs obtained for different values of ϵ .

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1097 Figure 13. GPT-4 for $T = 100$: the per-configuration summary tables. The "fails" row indicates that all replicates completed successfully.

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Can large language models explore in-context?

1100 1101		MedianReward	SuffFailFreq(T/2)	K*MinFrac	GreedyFrac	Replicates
1102 1103	TS	0.47	0.01	0.28	0.62	1000
1104	UCB	0.55	0.02	0.18	0.76	1000
1105 1106	Greedy	0.40	0.48	0.05	1.00	1000
1107 1108	BNRNO	0.22	0.50	0.16	0.30	20
1109 1110	BNRN1	0.22	0.00	0.41	0.28	20
1111 1112	BNRND	0.12	0.55	0.07	0.40	20
1113	BNRC0	0.12	0.80	0.01	0.51	20
1114 1115	BNRC1	0.10	0.50	0.03	0.57	20
1116 1117	BNRCD	0.65	0.45	0.01	0.75	20
1118 1119	BNSN0	0.12	0.85	0.00	1.00	20
1120 1121	BNSN1	0.22	0.25	0.04	0.76	20
1122 1123	BNSND	0.20	0.20	0.52	0.38	20
1124 1125	BNSCO	0.12	0.85	0.00	0.95	20
1126	BNSC1	0.22	0.70	0.01	0.88	20
1127 1128	BNSCD	0.05	0.50	0.11	0.50	20
1129 1130	BSRN0	0.17	0.30	0.25	0.32	20
1131 1132	BSRN1	0.25	0.00	0.66	0.29	20
1133 1134	BSRND	0.42	0.25	0.12	0.33	20
1135 1136	BSRC0	0.10	0.65	0.03	0.44	20
1137	BSRC1	0.05	0.25	0.12	0.47	20
1138 1139	BSRCD	0.28	0.15	0.11	0.60	20
1140 1141	BSSN0	0.12	0.85	0.00	1.00	20
1142 1143	BSSN1	0.25	0.30	0.03	0.78	20
1144 1145	BSSND	0.25	0.15	0.45	0.42	20
1146 1147	BSSC0	0.17	0.85	0.00	1.00	20
1148	BSSC1	0.17	0.55	0.02	0.83	20
1149 1150	BSSCD	0.20	0.35	0.10	0.78	20

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Figure 14. GPT-3.5 for $T = 100$: the per-configuration summary table. The buttons scenario, hard MAB instance.

Can large language models explore in-context?

1155 1156		MedianReward	SuffFailFreq(T/2)	K*MinFrac	GreedyFrac	Replicates
1157 1158	TS	0.47	0.01	0.28	0.62	1000
1159	UCB	0.55	0.02	0.18	0.76	1000
1160 1161	Greedy	0.40	0.48	0.05	1.00	1000
1162 1163	ANRNO	0.22	0.65	0.03	0.48	20
1164 1165	ANRN1	0.22	0.50	0.05	0.33	20
1166 1167	ANRND	0.15	0.70	0.00	1.00	20
1168	ANRC0	0.15	0.85	0.00	0.98	20
1169 1170	ANRC1	0.20	0.50	0.00	0.80	20
1171 1172	ANRCD	0.15	0.70	0.00	1.00	20
1173 1174	ANSN0	0.12	0.85	0.00	1.00	20
1175 1176	ANSN1	0.12	0.20	0.04	0.93	20
1177 1178	ANSND	0.15	0.70	0.00	1.00	20
1179	ANSC0	0.17	0.80	0.00	1.00	20
1180 1181	ANSC1	0.12	0.55	0.01	0.93	20
1182 1183	ANSCD	0.15	0.70	0.00	1.00	20
1184 1185	ASRN0	0.25	0.70	0.03	0.48	20
1186 1187	ASRN1	0.05	0.42	0.06	0.28	20
1188 1189	ASRND	0.15	0.70	0.00	1.00	20
1190	ASRC0	0.37	0.40	0.06	0.64	20
1191 1192	ASRC1	0.30	0.25	0.11	0.65	20
1193 1194	ASRCD	0.15	0.70	0.00	1.00	20
1195 1196	ASSN0	0.15	0.85	0.00	1.00	20
1197 1198	ASSN1	0.25	0.42	0.05	0.92	20
1199 1200	ASSND	0.15	0.70	0.00	1.00	20
1201	ASSC0	0.12	0.80	0.01	0.99	20
1202 1203	ASSC1	0.30	0.15	0.14	0.83	20
1204 1205	ASSCD	0.15	0.70	0.00	1.00	20

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1208 Figure 15. GPT-3.5 for $T = 100$: the per-configuration summary table. The advertisements scenario, hard MAB instance.

Can large language models explore in-context?

1210 1211		MedianReward	SuffFailFreq(T/2)	K*MinFrac	GreedyFrac	Replicates
1212	TS	0.84	0.00	0.14	0.88	1000
1213 1214	UCB	0.88	0.00	0.09	0.94	1000
1215 1216	Greedy	0.92	0.19	0.04	1.00	1000
1217 1218	BNRNO	0.23	0.55	0.02	0.85	20
1219 1220	BNRN1	0.72	0.05	0.16	0.62	20
1221 1222	BNRND	0.14	0.25	0.17	0.46	20
1223	BNRC0	0.84	0.25	0.03	0.56	20
1224 1225	BNRC1	0.81	0.05	0.08	0.77	20
1226 1227	BNRCD	0.88	0.10	0.04	0.92	20
1228 1229	BNSNO	0.18	0.65	0.00	1.00	20
1230 1231	BNSN1	0.60	0.40	0.02	0.89	20
1232 1233	BNSND	0.26	0.10	0.54	0.52	20
1234 1235	BNSCO	0.18	0.65	0.00	1.00	20
1236	BNSC1	0.16	0.55	0.01	0.95	20
1237 1238	BNSCD	0.62	0.35	0.03	0.77	20
1239 1240	BSRN0	0.73	0.30	0.11	0.57	20
1241 1242	BSRN1	0.35	0.00	0.48	0.42	20
1243 1244	BSRND	0.21	0.25	0.09	0.43	20
1245 1246	BSRC0	0.87	0.05	0.06	0.72	20
1247	BSRC1	0.73	0.05	0.16	0.72	20
1248 1249	BSRCD	0.81	0.05	0.11	0.76	20
1250 1251	BSSN0	0.18	0.65	0.00	1.00	20
1252 1253	BSSN1	0.17	0.25	0.02	0.89	20
1254 1255	BSSND	0.26	0.30	0.39	0.60	20
1256 1257	BSSC0	0.19	0.60	0.00	0.99	20
1258	BSSC1	0.53	0.35	0.03	0.82	20
1259 1260	BSSCD	0.78	0.25	0.02	0.90	20

1261 1262

Figure 16. GPT-3.5 for $T = 100$: the per-configuration summary table. The buttons scenario, easy MAB instance.

Can large language models explore in-context?

1265 1266		MedianReward	SuffFailFreq(T/2)	K*MinFrac	GreedyFrac	Replicates
1267 1268	TS	0.84	0.00	0.14	0.88	1000
1269	UCB	0.88	0.00	0.09	0.94	1000
1270 1271	Greedy	0.92	0.19	0.04	1.00	1000
1272 1273	ANRNO	0.18	0.65	0.01	0.81	20
1274 1275	ANRN1	0.10	0.35	0.03	0.47	20
1276 1277	ANRND	0.10	0.55	0.00	1.00	20
1278	ANRC0	0.13	0.60	0.00	0.96	20
1279 1280	ANRC1	0.77	0.35	0.03	0.89	20
1281 1282	ANRCD	0.10	0.55	0.00	1.00	20
1283 1284	ANSN0	0.18	0.65	0.00	1.00	20
1285 1286	ANSN1	0.69	0.15	0.03	0.97	20
1287 1288	ANSND	0.10	0.55	0.00	1.00	20
1289	ANSC0	0.23	0.60	0.00	1.00	20
1290 1291	ANSC1	0.71	0.20	0.03	0.96	20
1292 1293	ANSCD	0.10	0.55	0.00	1.00	20
1294 1295	ASRN0	0.08	0.75	0.01	0.81	20
1296 1297	ASRN1	0.08	0.45	0.05	0.40	20
1298 1299	ASRND	0.10	0.55	0.00	1.00	20
1300	ASRC0	0.68	0.10	0.08	0.86	20
1301 1302	ASRC1	0.74	0.00	0.13	0.86	20
1303 1304	ASRCD	0.10	0.55	0.00	1.00	20
1305 1306	ASSN0	0.29	0.00	0.04	0.92	20
1307 1308	ASSN1	0.79	0.10	0.05	0.93	20
1309 1310	ASSND	0.10	0.55	0.00	1.00	20
1311	ASSC0	0.89	0.20	0.01	1.00	20
1312 1313	ASSC1	0.82	0.10	0.11	0.92	20
1314 1315	ASSCD	0.10	0.55	0.00	1.00	20

1316 1317

Figure 17. GPT-3.5 for $T = 100$: the per-configuration summary table. The adverts scenario, easy MAB instance.

Figure 18. LLAMA2 for $T = 100$: the per-configuration summary tables. The buttons scenario, hard MAB instance.

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 Figure 19. LLAMA2 for $T = 100$: the per-configuration summary tables. The advertisements scenario, hard MAB instance.