Exploration for the Efficient Deployment of Reinforcement Learning Agents

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Abstract

1	Reinforcement learning (RL) provides a rich toolbox with which to learn sequential
2	decision making policies. Notably, the ability to learn solely from offline interaction
3	data has been a highly successful modality for training real-world policies without ever
4	interacting in the real world. However, a gap exists in this paradigm when the offline
5	dataset does not cover all the behaviors necessary to extract optimal policies. Naively,
6	one can pre-train a policy using offline RL and fine-tune it using online RL; this can
7	lead to catastrophe in safety critical settings, like healthcare and autonomous driving,
8	where deploying an unverified policy is irresponsible. Deployment efficient learning is
9	a potential solution, where the number of distinct data collection policies is relatively
10	low compared to the number of updates to the policy. We argue that safely improving
11	a dataset requires a deployment efficient algorithm with a carefully constructed data
12	collection policy. We introduce a framework with a stationary exploration policy that
13	aims to reduce out-of-distribution uncertainty while maintaining strong returns. We
14	establish theoretical guarantees of this exploration framework without finetuning and
15	demonstrate our methods on a small-scale toy environment and a large-scale supply
16	chain environment with real-world data.

17 **1** Introduction

Offline RL algorithms are popular in domains where online interactions can be costly or unsafe (Achiam & Amodei, 2019; Hu et al., 2024; Liu et al., 2023). To avoid potentially dangerous states, many offline algorithms (Kumar et al., 2020; Kostrikov et al., 2021) regularize the learned policy to take actions that stay within the distribution of interactions within the dataset. Naturally, the performance of policies trained with offline RL algorithms depends significantly on the coverage of this offline data. However, this restriction can be mitigated by performing some online exploration to improve the dataset's coverage.

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26 Offline-to-online RL algorithms seek to overcome this limitation by refining offline trained policies via online interaction with the environment (Nair et al., 2020; Mark et al., 2024; Ball et al., 27 28 2023; Wang et al., 2023; Zhou et al., 2025). However, this approach falls short in the real world 29 due to cost and safety considerations of online exploration. Real-world applications like health 30 care or autonomous driving (Gottesman et al., 2019; Kiran et al., 2021) have little tolerance for 31 error and typically require policies to be verified and tested before deployment. For this reason, 32 updating the policy parameters online, as most offline-to-online methods do, cannot be permitted in 33 the real world as every update to the policy parameters must be thoroughly tested and verified. As 34 testing and verification can be time consuming and expensive, it makes sense to use the number 35 of policy deployments as a suitable measure of efficiency. Specifically, the concept of deployment 36 *efficiency*, which is defined as the ratio of the number of unique policies deployed during training 37 to the number of samples collected, is most relevant for many real-world systems (Matsushima 38 et al., 2020). On-policy RL methods are at one extreme of the deployment efficiency spectrum, 39 requiring one deployment per update. Purely offline methods are at the other end, only utilizing one

40 deployment in total. In real-world settings, the only feasible way to improve an offline-trained policy

41 is to explore in a manner that is neither costly in terms of deployment efficiency nor leads to losses

42 due to poor selection of actions.

43 A high-profile and socio-economically relevant setting in which deployment efficiency is crucial is 44 that of supply chain management (Madeka et al., 2022), where an agent must place inventory orders 45 to vendors to stock a company's warehouses. In this domain, state-of-the-art RL agents (Andaz et al., 46 2023) are trained offline using historical data collected from a traditional linear programming-based behavior policy. However, to improve the offline policy, it is necessary to collect quality online 47 48 interactions through exploration in the real world, but each suboptimal action has severe financial 49 overheads. Since policies need to be verified and back-tested for safety and performance (Corsi 50 et al., 2024; Matsushima et al., 2020; Madeka et al., 2022; Amir et al., 2021) before deployment, it is 51 difficult to justify continuous online finetuning. Instead, we propose to use a stationary exploratory policy to collect high quality samples that can be used to re-train the policies offline on the augmented 52 53 dataset. This stationary exploration policy should satisfy two desiderata: (a) it should be *safe*, 54 meaning that it should not deviate too far from the well-tested policy, and (b) its exploration should 55 be *targeted*, meaning that it should carefully collect data that are close to the known safe regions, 56 while still meaningfully augmenting the dataset for high-quality offline policy improvements for 57 future deployments.

Our contributions can be summarized as: (1) establishing a framework for exploring through online interactions without fine-tuning the policy online, (2) developing a principled exploration strategy from the offline dataset that can collect informative samples through online interactions, and (3) empirically analyzing the samples collected using our exploration strategy on a discrete navigation environment and a real-world supply chain application (Madeka et al., 2022; Andaz et al., 2023).

63 2 Preliminaries

64 We consider problems that can be modelled as Markov Decision Processes (MDPs) (Puterman, 1990), which are defined as $\mathcal{M} = \langle \mathcal{S}, \mathcal{A}, P, r, \gamma, \rho_0 \rangle$ where \mathcal{S} is the state space, \mathcal{A} is the action 65 space, $P : S \times A \mapsto S$ is the transition probability function, $\gamma \in [0, 1)$ is the discount factor, 66 ρ_0 is the initial state distribution and $r: S \times A \longrightarrow \mathbb{R}$ is the reward function. A policy π_{θ} : 67 $\mathcal{S} \mapsto \mathcal{A}$ represents the probability of taking an action a from state s. The policy induces a 68 trajectory distribution $p^{\pi}(\tau) = \rho_0 \prod_{t=1}^{\infty} \pi(a_t|s_t) P(s_{t+1}|s_t, a_t)$ and a corresponding state-visitation distribution $d^{\pi}(s) = (1 - \gamma) \sum_{t=0}^{\infty} \gamma^t p^{\pi}(s_t = s)$. The expected return is defined as $J(\pi_{\theta}, \mathcal{M}) = \mathbb{E}_{\tau \sim p^{\pi}(\tau)}[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t)]$. The goal of the agent is to find the optimal policy π^* that maximizes 69 70 71 the expected return, i.e., $\pi^* = \arg \max_{\pi} J(\pi, \mathcal{M})$. 72

Offline RL algorithms try to regularize the policy to avoid taking actions out of dataset support. The regularization can be in the form of pessimism in Q-value for out-of-distribution actions (Kumar et al., 2020; Shimizu et al., 2024) or pessimism in the reward function based on uncertainties in the model predictions (Yu et al., 2020; Kidambi et al., 2021). In some sense, it can be assumed that the general objective for offline RL algorithms are,

$$\max_{\pi} \quad J(\pi, \mathcal{M})$$

$$s.t. \quad D(p^{\pi}(s, a) || \hat{p}(s, a)) \le \epsilon,$$

$$(1)$$

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where *D* is written as a divergence, but can more generally be any measure of the difference between distributions, $p^{\pi}(s, a)$ is a measure of the true likelihood of state-actions under the policy, and $\hat{p}(s, a)$ is a measure of the likelihood of the state-action in the dataset (Nachum et al., 2019).

82 3 Method

The success of exploring in the real world hinges on two key considerations. First, the policy must targetedly collect data that that will augment the offline dataset in such a way that it improves future policy deployments. Second, the exploration conducted online must be "safe", meaning that it should carefully stay close to the support of the offline data. In this section, we present the theoretical

formulation of our efficient exploration framework, along with practical approximations. We obtain 87

88 the optimal exploratory policy by improving the performance of the policy extracted from running

89 offline RL algorithms on the historical dataset.

3.1 The Exploratory Policy 90

First, we construct the exploratory policy given a dataset $\mathcal{D} = \{(s_i, a_i, s'_i, r_i)\}_{i=1}^N$; this is done using 91 a distribution matching objective against a target distribution. First, we formalize the sub-optimality 92 93 of a policy obtained using an offline dataset. We define $u(s,a) \approx \log p((s,a) \notin D)$ to provide a 94 measure of the likelihood of (s, a) not being in the dataset. Using u(s, a) we can formally define the 95 uncertain set (Kidambi et al., 2021):

96 **Definition 3.1.** Let $\mathcal{U}_{\mathcal{D}}$ be the set of state-action pairs (s, a) that are not contained in the dataset D.

97 Let u(s, a) represent the likelihood of $(s, a) \notin \mathcal{D}$. Define $\mathcal{U}_{\mathcal{D}} = \{(s, a) | u(s, a) > \alpha\} \approx \{(s, a) \in \mathcal{U}_{\mathcal{D}} \}$ 98 $\mathcal{S} \times \mathcal{A}|(s, a, ., .) \notin \mathcal{D}\}$, where α is a scalar parameter.

If $(s, a) \in \mathcal{U}_{\mathcal{D}}$, $p^{\pi}(s, a)$ would be low and if the probability $\pi(a|s)$ is high, then $D(p^{\pi}(s, a)||\hat{p}(s, a))$ 99 would be high. In other words, creating this partition in the state space allows the creation of an 100 101 approximation of the given MDP \mathcal{M} where the expected return is a pessimistic estimate of the 102 objective in Equation (1). This pessimistic MDP will ensure that the trained policy will restrict the 103 policy from taking actions outside the support of the dataset (Kidambi et al., 2021).

Definition 3.2. Given an MDP $\mathcal{M} = \langle S, \mathcal{A}, P, r, \gamma, \rho_0 \rangle$, a dataset $\mathcal{D} = \{(s_i, a_i, s'_i, r_i)\}_{i=1}^N$, define a 104 pessimistic MDP $\mathcal{M}_{\mathcal{D}} = \langle \mathcal{S} \cup HALT, \mathcal{A}, P_p, r_p, \gamma, \rho_0 \rangle$ where, 105

106
$$P_p(s'|s,a) = \begin{cases} \delta(s' = HALT), & (s,a) \in \mathcal{U}_{\mathcal{D}} \\ P(s'|s,a), & \text{otherwise} \end{cases} \quad r_p(s,a) = \begin{cases} -R_{max}, & (s,a) \in \mathcal{U}_{\mathcal{D}} \\ r(s,a), & \text{otherwise} \end{cases}$$

107 Additionally, we make the following assumption to derive the suboptimality gap in the offline data. This assumption is also made by most offline RL algorithms using Equation (1) as their objective. It 108 109 simply states that the offline RL algorithm produces the optimal policy for the pessimistic MDP $\mathcal{M}_{\mathcal{D}}$. Assumption 3.3. Let π_D^* be the best policy obtained from a dataset \mathcal{D} , essentially by optimizing 110 the objective in Equation (1). We assume that π_D^* maximizes the expected return in \mathcal{M}_D i.e. 111 $J(\pi_D^*, \mathcal{M}_D) \ge J(\pi, \mathcal{M}_D) \quad \forall \quad \pi.$ 112

Let $d^{\pi}(\mathcal{X})$ be the visitation of set \mathcal{X} following policy π and using the true dynamics P. We can now 113 bound the true returns of the best policy obtained using the offline RL objective eq. (1) with the return 114 115 of the optimal policy on MDP \mathcal{M} or in other words define the suboptimality gap in the offline dataset. **Theorem 3.4.** Let \mathcal{M} be a given MDP and \mathcal{D} be the offline dataset. Let $\pi^* = \arg \max_{\pi} J(\pi, \mathcal{M})$ be 116

the true optimal policy on \mathcal{M} and $\pi_D^* = \arg \max_{\pi} Equation (1) \approx \arg \max_{\pi} J(\pi, \mathcal{M}_D)$ be the best offline RL policy on dataset \mathcal{D} . The following holds: $J(\pi^*, \mathcal{M}) - J(\pi_D^*, \mathcal{M}) \leq \frac{2R_{max}}{(1-\gamma)^2} d^{\pi^*}(\mathcal{U}_D)$. 117 118

119 A direct consequence of Theorem 3.4 is that if $d^{\pi^*}(\mathcal{U}_{\mathcal{D}}) = 0$, i.e. all transitions taken by the optimal 120 policy are in the dataset \mathcal{D} , the optimal return of the best offline policy and the true optimal policy 121 are the same. In other words, the best offline policy is in fact the true optimal policy. In general, if 122 we want to improve the dataset, we need to tighten the bound or minimize $d^{\pi^*}(\mathcal{U}_{\mathcal{D}})$. This means the 123 exploratory policy must aim to maximize this visitation.

124 Formally, let $\mathcal{U}_{\mathcal{D}}^*$ be the set of state-action pairs visited by the optimal policy π^* which are in the set $\mathcal{U}_{\mathcal{D}}$. Mathematically, $p((s,a) \in \mathcal{U}_{\mathcal{D}}^*) = d^{\pi^*} \delta((s,a) \in \mathcal{U}_{\mathcal{D}})$. In practical situations, it is 125 difficult to obtain the set $\mathcal{U}_{\mathcal{D}}$. Rather, we will be using the measure u(s, a) to provide an estimate 126 of $(s, a) \in \mathcal{U}_{\mathcal{D}}$. We will approximate $\delta((s, a) \in \mathcal{U}_{\mathcal{D}})$ as $\frac{1}{Z(s)} \exp(u(s, a))$. The exploratory policy 127 128 must be the one that maximizes its visitation for the state-action pairs in $\mathcal{U}_{\mathcal{D}}^*$. Using $p((s, a) \in \mathcal{U}_{\mathcal{D}}^*)$ 129 as a target distribution, we can obtain the optimal policy minimizing an f-divergence between the 130 policy's visitation distribution and the target distribution as discussed in several previous works (Ma 131 et al., 2022; Agarwal et al., 2024). We use Forward KL because of its performance and exploration 132 properties. The optimization can be further simplified into a regularized RL objective.

$$\pi_{exp}^{*} = \underset{\pi}{\arg\min} D_{FKL}(d^{\pi}(s, a) || d^{*}(s, a) \exp(u(s, a)))$$

=
$$\underset{\pi}{\arg\max} \mathbb{E}_{d^{\pi}}[u(s, a)] - D_{KL}(d^{\pi}(s, a) || d^{*}(s, a)).$$
 (2)

133 Practically, we do not have access to π^* , preventing us from defining π^*_{exp} exactly. We will use a

biased estimate of π^* , which is the best offline policy, π_D^* . In general this isn't true, but if we restrict the marginal state visitation to be close to the dataset, i.e. ensuring $D(d^{\pi^*}(s)||d^{\pi_D^*}(s)) \le \epsilon$, we can further simplify this objective to,

$$\pi_{exp}^{*} = \arg\max_{\pi} \mathbb{E}_{d^{\pi}}[u(s,a)] - \beta D_{KL}(\pi || \pi_{D}^{*}).$$
(3)

137 Common offline RL algorithms (Kostrikov et al., 2021; Kumar et al., 2020) learn π_D^* that are highly 138 constrained to induce transitions that are found in *D*. For any given state, a policy trained using 139 AWR (Peng et al., 2019b) has negligible probability of taking an action that is not present in the 140 dataset, making out-of-distribution exploration difficult. We use fitted Q learning for some of our 141 experiments to avoid the regularizations that are common to recent offline RL methods.

Note that the KL constraint on visitations has been approximated to be on behavior or policy. This
approximation makes sense if the marginal state visitation is bounded to be close to the dataset.
Further, it has been shown in Mao et al. (2024) that semi-gradient updates for visitation regularized
offline RL is, in fact, performing the same updates as behavior regularized RL.

146 Since the policy π_{exp}^* needs to be obtained only from offline data, offline RL algorithms will overly

147 constrain π_{exp}^* to be within the dataset, which is not ideal for an exploratory policy. Hence, we

148 construct the exploratory policy to approximate the solution of Equation (3) directly using π_D^* , u(s, a)149 and the offline dataset \mathcal{D} .

150 3.2 Approximate Construction

151 Neither online interactions nor offline RL can be used to optimize Equation (3). We use the following 152 two sampling based approximations for π_{exp}^* :

153 **Single Step**: Equation (3) has a closed form solution as discussed in prior works (Peng et al., 2019a; 154 Rafailov et al., 2024). π_{exp}^* can be written in closed form as,

$$\pi_{exp}^*(a|s) \propto \pi_D^* \exp\left(\frac{1}{\beta}u(s,a)\right). \tag{4}$$

Equation (4) provides a single step exploratory policy. The partition function can be obtained for simple discrete action spaces but for general action spaces, sampling from this distribution can be complicated.

158 **Multi-Step**: Given the difficulty of sampling from a distribution such as Equation (4), we also 159 propose an alternative way to use the uncertainty metric u(s, a) for decision-making. Specifically, 160 we formulate the following online trajectory optimization problem with a learned dynamics model \hat{T} 161 and learned reward function \hat{r} ,

$$\pi_{exp}^{*}(a|s) = \arg\max_{a_{0}, \cdots, a_{H-1}} \mathbb{E}_{\hat{\pi}} \left[\sum_{t=0}^{H-1} \gamma^{t} \left(\hat{r}(s_{t}, a_{t}) + c \cdot u(s_{t}, a_{t}) \right) + \gamma^{H} V_{D}^{*}(s_{H}) \right], \quad (5)$$

162 such that

$$s_0 = s, \quad a_t \sim \hat{\pi}(\cdot | s_t), \quad s_{t+1} \sim \hat{T}(s_t, a_t)$$

163 where $c \in (0, 1]$ is a hyperparameter that trades off between exploration and exploitation. The *H*-step

164 rollouts are taken using $\hat{\pi}$ which a high-temperature version of the dataset policy:

$$\hat{\pi}(a|s) = \frac{e^{\pi_D(a|s)/T}}{\sum_{a'} e^{\pi_D^*(a'|s)/T}},$$

165 where $T \in \mathbb{R}^+$ is the temperature parameter of the softmax function. The argmax is over sequences

166 of actions, but we can use model predictive control (MPC) and only commit to the first action in the

167 sequence. This multi-step exploratory policy can be used to sample actions for arbitrary complex

168 action spaces.

169 3.3 Rolling out the Exploration Policy

Given that we have π_{exp}^* , we can simply execute it to collect samples. However, we want to stay close to our "safe" dataset. We had made an assumption that $D(d^{\pi_{exp}^*}(s)||d^{\pi_D^*}(s)) \le \epsilon$ which needs to maintained in the real world. Ideally we would want to start at each state in the offline dataset and run *k*-steps of exploration from there but resetting at a random state is not possible in the real world. We have the following choices,

175 **Reset**: The exploratory policy starts executing from the start-state defined by the initial state distri-176 bution. While this strategy is the most simple, the deviation from the "safe" policy grows as $O(T^2)$ 177 (Ross et al., 2010).

178 ϵ -exploration: This method mimics the epsilon greedy method. At any state, an exploratory action 179 is taken according to π_{exp}^* with probability ϵ and a greedy action is taken with probability $(1 - \epsilon)$. 180 Mathematically, this is synonymous to choosing a time step $t \sim Geom(\epsilon)$ to explore. This method 181 can lead to better exploration with the exploration happening closer to π_D^* . One might argue that the 182 time step could be chosen simply uniformly over the trajectory but the trajectory length is not often 183 known which makes a uniform sampling difficult.

184 We describe the connections between our framework and well-studied exploration methods in185 Appendix B.

186 4 Experiments

We present experiments that represent the exploration challenges of the real world; Namely, we use a stationary exploratory policy throughout each deployment and desire the exploratory policy perform similarly to the exploitation policy. Through these experiments we aim to demonstrate that careful consideration of uncertainty is critical when deploying stationary exploration policies. We use two domains: 1) a discrete navigation environment called *Nav-Chambers* for ablating design choices and 2) a large scale supply chain environment that is backtestable with real-world data (Andaz et al., 2023; Madeka et al., 2022) and has in fact been used to train real-world policies.

194 4.1 Discrete Navigation Environment: Nav-Chambers

Environment Description: We create a discrete navigation environment called Nav-Chambers. The environment has discrete state and action spaces. It acts as a playground to run ablations and compare the different design choices for the exploratory policies. Nav-Chambers consists of a discrete space divided into four chambers using walls with passages to move across each other. The agent needs to traverse these chambers to reach to the other end of the grid (see Appendix D.2 for details).

200 Baselines: There are two variants of our exploration: Single-Step (defined in Equation (4)) and 201 **Multi-Step** (defined in Equation (5)). These are compared against prototypical exploration method-202 ologies: *Naive-\epsilon*-greedy chooses an uniformly random action with probability ϵ and the greedy 203 action with probability $1 - \epsilon$. Weighted- ϵ -greedy chooses an action based on the uncertainty with 204 probability ϵ and the greedy action with probability $1 - \epsilon$. Bandit-Style Reward Bonus has no 205 explicit exploration action, but trains a Q-network with an uncertainty augmented reward target where $r' = r(s, a) + c \frac{1}{\sqrt{N_{(s,a)}}}$, where N(s, a) are tabular visitation counts, and $c \in [0, 1]$ is a fixed 206 207 hyperparameter.

Experiment Setup: We iterate between "explore" and "train" phases as would happen in the real world. The *explore* phase executes the exploratory policy in the environment to collect T



Figure 1: Comparison of our exploration policies (Single-Step and Multi-Step) against the baselines using **collect-returns** (left) and **eval-returns** (right). Each curve shows a mean of 5 seeds with a rolling average of window length 5 and the shaded region represents the 95% confidence interval.

trajectories and the *train* phase uses the combined buffer to train the policy for K steps using fitted Q-learning (Ernst et al., 2005; Riedmiller, 2005). We perform N such deployments. Our exploratory policy (both Single-Step and Multi-Step) and baselines are run as ϵ -exploration. We provide results for the reset setting in Appendix C.1. In these experiments, we show 100 deployments with 1000 environment and 1000 training steps, each.

As a measure of performance, we measure the mean return of the exploration policy and the greedy policy obtained from the offline RL algorithm and call these **eval-returns** and **collect-returns** respectively. **Collect-returns** is compared against the **eval-returns** to measure the deviation from the exploitation policy.

219 **Uncertainty Estimation:** Our exploration requires estimates of uncertainty of states with respect 220 to the dataset. To isolate the design of the exploration policy, we use the ground truth state-action 221 visitation to approximate uncertainty. Let $N_{(s,a)}$ denote the number of times the agent has taken 222 action *a* in state *s*. As in previous work (Strehl & Littman, 2008; Lobel et al., 2023), the square-root 223 inverse of the count $\frac{1}{\sqrt{N_{(s,a)}}}$ is used as a measure of uncertainty.

224 **Results:** Figure 1 shows the **collect-returns** (left) and **eval-returns** (right) of both of our exploratory policies compared against the baselines in the ϵ -exploration setting. The results in Figure 1a 225 226 demonstrate that our exploratory policies perform better when doing data collection than both variants of ϵ -greedy and all outperform the UCB baseline. We suspect the UCB baseline to perform 227 228 poorly because the reward targets are non-stationary and change significantly between deployments. 229 The performance of the exploitation policies, as shown in Figure 1b, is similar, which indicates 230 the similar quality of the samples collected during exploration. In short, our and the baseline 231 exploration methods collect similar data but our methods do so in a safer and more performant 232 manner. Additional discussion and results that focus on the performance difference across different 233 values of ϵ and annealed- ϵ -greedy can be found in Appendix E.1 and Appendix E.2, respectively.

234 4.2 Backtesting Exploration: Application to a Real-World Supply Chain

235 Next, we consider an application to an inventory control problem where a retailer needs to procure 236 inventory and balance the costs associated with over-stocking versus missing sales due to under-237 stocking. Andaz et al. (2023) considers how to learn dynamics models—specifically for inventory 238 arrivals from vendors-to construct a simulator for a large e-commerce retailer's supply chain. 239 Transitions in the simulator are modeled through dynamics models (Andaz et al., 2023) trained using 240 offline data. The dynamics models are only reliable on-policy (for the behavior policy) which affects 241 the performance of any policy trained on the simulator. To get a higher quality policy, exploration 242 is needed to improve the simulator. Policies can be trained using backpropagation through time 243 (Madeka et al., 2022) within this simulator and launched in the real-world supply chain pipeline.

244 **Experiment Setup:** Let the simulator described in Madeka et al. (2022) be M. Andaz et al. (2023) 245 showed that this simulator is well-calibrated with the real world. We create a suboptimal simulator M246 by training the dynamics models on data collected in M using a behavior policy which does not cover 247 the entire state, action spaces. In our experiments, M acts as the proxy for the real world and M as the proxy for the simulator. The Supply Chain Environment is grounded in a dataset containing 5 years 248 249 of real-world supply chain data (e.g., inventory levels, demand, delivery status, etc.) for thousands of 250 products sold by a large e-commerce company. Further, to demonstrate the deployment efficiency 251 regime, we segment the data into three chronological splits: T_1 , T_2 , and T_3 representing three, one, and 252 one years of data, respectively. Let M_{T_i} be the simulator trained using the real-world data from time 253 segment T_i . M_{T_i} denotes the simulator trained using the data collected from MDP M_{T_i} for time period 254 T_i (Madeka et al. (2022) uses an approach where samples are replayed from historic data). Finally, 255 we train a deterministic policy in M using DirectBackprop (Madeka et al., 2022) and denote it as π_M^* . The complementary exploration policy, π^*_{exp} is constructed from π^*_M and the uncertainty measure 256



Figure 2: This figure shows a confusion matrix de-271 scribing the relative difference in performance of a 272 policy trained using data collected by the Single-273 step, Greedy, and Epsilon-greedy exploration meth-274 ods as well as the original policy (Base). Each box 275 represents the percentage difference of the row 276 method against the column method. Bold num-277 bers denote statistical significance and "ns" de-278 notes not statistically significant. One, two, and 279 three asterisks denote a *p*-value of < 0.05, < 0.01, 280 and < 0.001, respectively. 281

We perform single deployment experiments in three phases: explore (i.e. deployment), retrain, and evaluate. At the start of the experiments, we are given \hat{M}_{T_1} on which $\pi^*_{\hat{M}_{T_1}}$ is trained and π^*_{exp} constructed. Next, we deploy π^*_{exp} in M_{T_2} to collect data and subsequently train $\hat{M}_{T_{1,2}}$. Finally, $\pi^*_{\hat{M}_{T_{1,2}}}$ is trained and evaluated in M_{T_3} . Our experiments demonstrate the effectiveness of our uncertainty-seeking exploration policy.

We provide implementation details and experimental setup for the Supply Chain Environment in Appendix D.1 and uncertainty estimation in Appendix F.

Constructing π_{exp}^* : The Supply Chain Environment is high-dimensional and continuous, so it is infeasible to measure uncertainty using a countbased metric as is done in the Nav-Chambers environment. Instead, we model uncertainty by fitting an *N*-component Gaussian Mixture Model (GMM) to a dataset of state-action pairs, but only use a subset of the state features. We denote the resulting joint distribution as $p_{\mathcal{G}}(s_r, a)$, where $s_r = s|_{\mathcal{I}}$ is the restriction of *s* to a selected index set $\mathcal{I} \subseteq \{1, \ldots, \dim(s)\}$. To calculate an exploratory action while in state *s*, we

resample a component-reweighted version of $p_{\mathcal{G}}$ according to the likelihood of the current state and proposed action pair. Further details can be found in Algorithm 2.

Baselines: We compare our single-step exploration against two common-sense exploration frameworks: 1) greedy, which uses $\pi^*_{\hat{M}_{T_1}}$ to explore in $M_{T_{1,2}}$, as is done in Matsushima et al. (2020), and 2) epsilon-greedy, which takes uniformly random action with probability ϵ and otherwise use $\pi^*_{\hat{M}_{T_1}}$.

Results: Figure 2 shows a comparison of the return achieved by various policies evaluated in M_{T_3} in terms of their relative performance. The policies being compared are trained in three distinct versions of $\hat{M}_{1,2}$, each constructed from data collected in $M_{1,2}$ by the greedy, epsilon-greedy, and our single-step exploration policies. We also compare against a policy that was only trained in \hat{M}_1 (Base). Firstly, we confirm that exploration is necessary by seeing that the Base policy under-performs all other methods (left column). Further, we see that the our single-step exploration method outperforms the other three policies to a statistically significant degree (top row). Importantly, the greedy policy does not sufficiently cover the state space to learn the most robust policy in the next round of deployment.

296 5 Related Work

Offline to Online finetuning: Offline RL algorithms are essentially off-policy RL algorithms that add additional constraints to the algorithm to ensure that the policy always stays within the data support. A number of such algorithms explicitly constrain the value functions (Kumar et al., 2020; Yu et al., 2020; Kidambi et al., 2021) or use regularization to ensure that the policy stays within the data support (Wu et al., 2019; Nachum et al., 2019). In all cases, the performance of the policy is restricted by the dataset quality (Kidambi et al., 2021).

Online finetuning has been extensively used (Nair et al., 2020; Mark et al., 2024; Ball et al., 2023;
Wang et al., 2023) to mitigate the dataset bias. While the offline RL algorithms themselves can be
directly used for online finetuning like in Peng et al. (2019a); Nair et al. (2020); Kumar et al. (2020);
Kostrikov et al. (2021), they are overly pessimistic. A number of works have been introduced that
simply reduce the regularization for conservatism during online finetuning (Lee et al., 2021; Zhang
et al., 2023; Hong et al., 2023; Ball et al., 2023; Zheng et al., 2023). There have also been works that
have used offline datasets as a prior for online RL algorithms (Mark et al., 2024; Ball et al., 2023).

All these methods have one major assumption: there is no restriction on online finetuning. The focus of all these works is to produce good policy updates combining the online samples and offline dataset. As discussed in works like Matsushima et al. (2020), there is often costs associated before deploying any policy in the real world. Our work differs from all these offline-to-online methods in that it aims

to develop an exploration scheme suitable for applications where it is not possible to deploy arbitrary policies.

Exploration: Our method constructs an exploratory policy from batched experience to deploy in the real world. Here, we will discuss some commonly used methods for constructing exploratory policies. Epsilon greedy (Watkins, 1989; Auer et al., 2002) is a simple, yet highly effective method used to take exploratory actions with probability ϵ . The idea is to ensure that the policy has some entropy and chooses every action with a non-zero probability. Another way of increasing the entropy of the policy is through explicit entropy maximization as in the MaxEnt RL methods (Haarnoja et al., 2017; 2018).

323 Selecting actions using an upper confidence estimator for the average return (Q-function in 324 case of RL algorithms) have been inspired from the UCB algorithm in multi-arm bandits (Auer 325 et al., 2002). Strehl & Littman (2008) proposed using an uncertainty bonus for the reward function 326 providing convergence guarantees. Algorithms have been proposed that extend the uncertainty 327 bonus in several ways: using pseudocounts (Bellemare et al., 2016; Lobel et al., 2023), model errors 328 (Burda et al., 2019) and using ensembles to estimate uncertainty (Kidambi et al., 2021). Distribution 329 matching approaches have also been proposed that aim to increase the entropy of the state-visitation 330 distribution (Lee et al., 2019; Agarwal et al., 2024). While our exploration method also draws from a 331 similar objective, these exploration strategies have been proposed in settings where the aim is to 332 explore all states, ultimately leading to a nearly zero uncertainty bonus for all states. Our method, on 333 the other hand, uses the uncertainty bonus to select a few states from the prior policy distribution.

334 6 Conclusion

335 In many real-world settings, policies cannot be continuously updated online; we proposed exploration 336 strategies for such domains. We adopted deployment efficiency as a relevant evaluation metric, and 337 showed how our algorithms lead to high return and deployment efficiency. We constructed two 338 exploration policies (single-step and multi-step) by combining a model of the uncertainty of a dataset 339 along with the optimal policy that can be extracted from it. Along with theoretical bounds on the 340 sub-optimality of these policies, we provide extensive experiments in the Nav-Chambers environment 341 and a well-calibrated simulator of a real-world supply chain environment. Our proposed methods 342 balance safety with exploration and show that it is possible to maintain performance while exploring 343 in the deployment efficient regime.

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474 Appendix

475 A Offline RL and Pessimism

476 Offline RL refers to the class of RL algorithms that train on a fixed dataset. Due to the inherent 477 overestimation biases (Hasselt, 2010) in RL algorithms, naively trained policies have a tendency to 478 steer out of the dataset towards the highly-biased value estimates. As a result, regularizations are added to the ensure pessimism in the value functions. These regularizations can be behavior based 479 480 (Kumar et al., 2019; Wu et al., 2019), value based (Kumar et al., 2020), visitation based (Sikchi et al., 481 2023) or reward based (Kidambi et al., 2021; Yu et al., 2020). Recent works have shown several 482 interconnections among these (Sikchi et al., 2023; Mao et al., 2024). We consider the following 483 constraint optimization as offline RL optimization problem:

$$\max_{\pi} J(\pi, \mathcal{M})$$
s.t. $D(p^{\pi}(s, a)||\hat{p}(s, a)) \le \epsilon,$
(6)

Equation 6 has been studied through common offline RL and imitation learning algorithms (Nachum et al., 2019; Sikchi et al., 2023). We approximate the optimization problem using a pessimistic MDP (as defined in Kidambi et al. (2021)). The pessimistic MDP ensures that $D(p^{\pi}(s, a)||\hat{p}(s, a)) \leq \epsilon$ is always satisfied as any transition outside the dataset is heavily penalized.

488 A.1 Proof of Theorem 3.4

We will be introducing some definitions and lemmas in order to prove Theorem 3.4. We begin by defining hitting time,

Definition A.1. (*Hitting time*) Given an MDP \mathcal{M} , starting state distribution ρ_0 , state-action pair (*s*, *a*) and a policy π , the hitting time $T^{\pi}_{(s,a)}$ is defined as the random variable denoting the first time action *a* is taken at state *s* by π on \mathcal{M} , and is equal to ∞ if *a* is never taken by π from state *s*. For a set of state-action pairs $S \subseteq S \times A$, we define $T^{\pi}_{S} \stackrel{\text{def}}{=} \min_{(s,a) \in S} T^{\pi}_{(s,a)}$. In other words, it is the time it takes to arrive at state *s*.

496 Using the definition, we can introduce the following Lemma that bounds the returns obtained in the 497 pessimistic MDP $\mathcal{M}_{\mathcal{D}}$ using the returns in the true MDP \mathcal{M} .

498 **Lemma A.2.** Let \mathcal{M} be a given MDP. The following is true for any offline dataset \mathcal{D} .

$$J(\pi, \mathcal{M}) - \frac{2R_{max}}{1 - \gamma} \mathbb{E}[\gamma^{T_{\mathcal{U}_{\mathcal{D}}}^{\pi}}] \le J(\pi, \mathcal{M}_{\mathcal{D}}) \le J(\pi, \mathcal{M})$$

$$\tag{7}$$

499

500 *Proof.* A more extensive theorem and corresponding proof exists in Kidambi et al. (2021). The 501 definition of pessimistic-MDP in the two works is slightly different leading to different bounds.

502 The rollout of any policy π on the pessimistic MDP $\mathcal{M}_{\mathcal{D}}$ would be the same as that of the true MDP 503 \mathcal{M} as long as an unknown state ($s \in \mathcal{U}_{\mathcal{D}}$) is encountered. At that point, the return of the policy on 504 the pessimistic MDP will be $\frac{-R_{max}}{1-\gamma}$. The maximum return of the policy for that rollout segment can 505 be $\frac{R_{max}}{1-\gamma}$. Hence,

$$J(\pi, \mathcal{M}) - \frac{2R_{max}}{1 - \gamma} \mathbb{E}[\gamma^{T_{\mathcal{U}_{\mathcal{D}}}^{\pi}}] \le J(\pi, \mathcal{M}_{\mathcal{D}})$$
(8)

Since $\mathcal{M}_{\mathcal{D}}$ is a pessimistic MDP for the corresponding MDP \mathcal{M} with each state in $\mathcal{M}_{\mathcal{D}}$ having rewards less than or equal to \mathcal{M} , for any policy, the return of will be higher in \mathcal{M} compared to $\mathcal{M}_{\mathcal{D}}$ i.e. $J(\pi, \mathcal{M}_{\mathcal{D}}) \leq J(\pi, \mathcal{M})$.

- 509 With this bound, we can compare the returns obtained by policies trained on the pessimistic MDP
- 510 with the corresponding returns in true MDP. To simplify this comparison, we use the following
- Lemma relates hitting times to visitation distributions. 511

Lemma A.3. (*Kidambi et al.*, 2021) (*Hitting time and visitation distributions*) For any set $\mathcal{X} \subseteq \mathcal{S} \times \mathcal{A}$, 512 and any policy π , we have $\mathbb{E}[\gamma^{T_{\mathcal{X}}^{\pi}}] \leq \frac{1}{1-\gamma} d^{\pi}(\mathcal{X}).$ 513

- 514 Now, we have all the components required to prove Theorem 3.4.
- **Theorem 3.4.** Let \mathcal{M} be a given MDP and \mathcal{D} be the offline dataset. Let $\pi^* = \arg \max_{\pi} J(\pi, \mathcal{M})$ be 515
- 516 the true optimal policy on \mathcal{M} and $\pi_D^* = \arg \max_{\pi} Equation$ (1) $\approx \arg \max_{\pi} J(\pi, \mathcal{M}_D)$ be the best
- offline *RL* policy on dataset \mathcal{D} . The following holds: $J(\pi^*, \mathcal{M}) J(\pi_D^*, \mathcal{M}) \leq \frac{2R_{max}}{(1-\gamma)^2} d^{\pi^*}(\mathcal{U}_{\mathcal{D}}).$ 517
- 518 *Proof.* From Lemma A.2,

519
$$J(\pi, \mathcal{M}) - \frac{2R_{\max}}{1 - \gamma} \mathbb{E}[\gamma^{T_{\mathcal{U}_{\mathcal{D}}}^{\pi}}] \le J(\pi, \mathcal{M}_{\mathcal{D}}) \le J(\pi, \mathcal{M})$$
$$J(\pi^*, \mathcal{M}) - J(\pi^*, \mathcal{M}_{\mathcal{D}}) \le \frac{2R_{\max}}{1 - \gamma} \mathbb{E}[\gamma^{T_{\mathcal{U}_{\mathcal{D}}}^{\pi^*}}]$$

0 D

520 From Lemma A.3, we replace the upper bound

$$J(\pi^*, \mathcal{M}) - J(\pi^*, \mathcal{M}_{\mathcal{D}}) \leq \frac{2R_{\max}}{(1-\gamma)^2} d^{\pi}(\mathcal{U}_{\mathcal{D}})$$
521 By definition, we know that $J(\pi^*, \mathcal{M}_{\mathcal{D}}) \leq J(\pi^*_{\mathcal{D}}, \mathcal{M}_{\mathcal{D}}) \leq J(\pi^*_{\mathcal{D}}, \mathcal{M})$. Thus we substitute
$$J(\pi^*, \mathcal{M}) - J(\pi^*_{\mathcal{D}}, \mathcal{M}) \leq \frac{2R_{\max}}{(1-\gamma)^2} d^{\pi}(\mathcal{U}_{\mathcal{D}})$$
522

 $\mathcal{D} \mathcal{R}$

B **Connections to Commonly Used Exploration** 523

524 As discussed above, defining u(s, a) is a major design decision that needs to be taken and there is no optimal way to define uncertainty. We can show that different heuristic definitions of u(s, a) and π_D^* 525 can draw connections to commonly used exploration techniques. 526

527 ϵ -greedy: Suppose u(s, a) is not learned but defined using a crude heuristic: For any state s, with 528 probability $1 - \epsilon$, the action is not uncertain i.e. $\exp \frac{1}{\beta}u(s, a) = 1$ and with probability ϵ , the action is uncertain with inversely depending on π_D^* i.e. $\exp \left[\frac{1}{\beta}u(s,a) = \frac{c}{\pi_D^*(a|s)}\right]$. Then, the corresponding exploration turns out to be ϵ -greedy. What does the uncertainty mean here? The value $\frac{c}{\pi_D^*(a|s)}$ means 529 530 531 that the uncertainty is lower for policy actions which makes some sense as the actions taken by the 532 policy are already known and present in the dataset.

533 **Bandit-style UCB**: Bandit-style UCB produces a policy that takes action according to Q(s, a) + 534 u(s, a) where u(s, a) is of a specific function depending on the frequency of actions. UCB is very efficient exploration method as it provides a logarithmic regret bound in bandits. If π_D^* is assumed to 535 be a softmax of the offline Q function i.e. $\pi_D^* \propto \exp Q(s, a)$, the exploration policy π_{exp}^* becomes a 536 soft version of the Bandit-style UCB. It must be noted though, for most offline RL algorithms, π_D^* is 537 538 not $\propto \exp Q(s, a)$ (Kostrikov et al., 2021; Sikchi et al., 2023).

539 Uncertainty aware reward bonus: A common way of exploring in RL is to use uncertainty based 540 reward bonus. This method is inspired from UCB and is formalized better in Strehl & Littman 541 (2008). Here the Q function are trained to be optimistic by adding u(s, a) to the reward function. Mathematically, $Q^{\pi}(s, a) = \mathbb{E}_{\pi}[\sum_{t} \gamma^{t}(r(s_{t}, a_{t}) + c \cdot u(s_{t}, a_{t}))]$. These algorithms are online 542 algorithms converging to optimal Q functions as $u(s, a) \rightarrow 0$. 543

544 C Additional Results

545 C.1 Reset Starting State

546 Figure 3 contains the results for using the *reset* setting to explore on the Chamber Navigation environment.



Figure 3: Comparison of our exploration methods against baselines while taking exploration steps beginning at each environmental reset.

547

548 **D** Experimental Setup

549 D.1 Supply Chain Environment

550 We use the supply chain environment described in detail in (Madeka et al., 2022; Andaz et al., 551 2023). Here the RL agent makes decisions about buying items from vendors. The agent takes in a 552 state x and its history of length H to predict the next action. The state consists of several features 553 including demand, inventory, cost, time of year, etc. The authors of Madeka et al. (2022) introduced 554 an algorithm to solve this domain and use real-world data by assuming the environmental setup to be 555 an Exogenous-MDP. A simulator is created with the learned dynamics models for the endogenous components and the exogenous components are sampled from the real-world data. Because of the 556 557 exogenous assumption, this simulator allows for back-testing of the policies and is calibrated with 558 the real world. An RL agent is trained in the simulator using the DirectBackprop algorithm (Madeka 559 et al., 2022).

560 While our method is designed for real-world exploration, it is infeasible to test in the real world due 561 to time-constraints (each step in the simulator represents one week). To overcome this, we partition 562 our data into three segments, T_1, T_2 , and T_3 that represent train, explore and test periods, respectively. 563 Further, we construct a reduced fidelity versions of the data by clamping some of the extreme (but 564 highly rewarding) features; this allows us to generate simulators that mimics low data coverage.

565 D.2 Nav-Chamber Experiments

The Nav-Chambers is a gridworld-like environment where the action space is [Up, Down, Left, Right] and the reward is -1 everywhere except the goal, where it is +1. In the Nav-Chambers environment, we implement deployment efficient exploration using count-based uncertainty estimation and train extract a policy using fitted Q-iteration, as described in Algorithm 1. The results shown use 100 deployments, each with 1000 train steps and 1000 collect steps.



Figure 4: Obstacle map for the Nav-Chambers environment.

Algorithm 1 Deployment Efficient Exploration with Fitted Q-Iteration

1: Initialize dataset of interactions $\mathcal{D} \leftarrow \{\}$, initialize Q-function $Q_{\theta}(s, a)$ 2: for n = 1 to N do for k = 1 to K do 3: Sample s from environment or replay buffer 4: Sample action $a \sim \pi^{\text{exploration}}(a \mid s)$ 5: Execute a, observe r, s'6: Add transition to dataset: $\mathcal{D} \leftarrow \mathcal{D} \cup \{(s, a, r, s')\}$ 7: 8: end for Fit Q_{θ} to minimize Bellman loss on \mathcal{D} : 9: $\mathcal{L}(\theta) = \sum_{(s,a,r,s') \in \mathcal{D}} \left(Q_{\theta}(s,a) - \left[r + \gamma \max_{a'} Q_{\theta'}(s',a') \right] \right)^2$

10: Optionally update target network $\theta' \leftarrow \theta$

11: end for

12: **return** final Q-function Q_{θ}

571 Across the experiments, the exploration policy is deployed a total of 100 times, collecting 1000

572 transitions and training the policy for 1000 gradient steps. After each deployment, we use fitted

573 E Ablation

574 E.1 Epsilon

575 We ablate over different values of epsilon to demonstrate the importance of uncertainty across a 576 variety of exploration budgets. Figure 5 shows the **eval-returns** (bottom row) and **collect-returns** 577 (top row) of our method and various baselines across different epsilons. These results show the 578 ϵ -exploration setting. Finally, from left to right, the value of ϵ increases. We see relative performance 579 improvements on the **collect-returns** of our single- and multi-step methods as ϵ increases.





Figure 5: Comparison of our exploration policies (Single-Step and Multi-Step) against the baselines using **collect-returns** (top row) and **eval-returns** (bottom row). Each curve shows a mean of 5 seeds with a rolling average of window length 5 and the shaded region represents the 95% confidence interval. From left to right, each column represents a different value of epsilon (ϵ used for the ϵ -exploration across methods.)



Figure 6: Comparison of our exploration policies (Single-Step and Multi-Step) against the baselines using **collect-returns** (top row) and **eval-returns** (bottom row). Each curve shows a mean of 5 seeds with the shaded region as the 95% confidence interval. From left to right, each column represents a different value of epsilon (ϵ used for the ϵ -exploration across methods.

580 E.2 Annealed epsilon greedy experiment

581 One advantage of our single- and multi-step exploration methods is that they achieve high performance 582 when in the collection phase of the deployment without sacrificing data quality for the policy extraction 583 phase. We hypothesize that this advantage stems from the methods' ability to automatically converge 584 to the exploiting policy once enough exploration has occurred. To test this, we compare the single-step 585 exploration method to a linearly-decaying epsilon-greedy exploration. Define annealed epsilon-greedy 586 as:

$$\pi_{\text{Annealed }\epsilon-\text{greedy}}(a|s,t) = \begin{cases} \arg\max Q(s,a) & \text{with probability } (1-f(t)) \\ \mathcal{U}(\mathcal{A}) & \text{with probability } f(t) \end{cases}$$
(9)

where $f(t) \in [0, 1)$ is some scalar-valued function that takes as input a notion of time (usually how many steps of experience have been gained at that point) and outputs an exploration parameter ϵ . Typically, f(t) is a linearly decays from a value of ϵ_{start} to ϵ_{end} over a period of time. Figure 6 demonstrates potential decays over a training period of 100k steps.

591 F Uncertainty-aware Exploration Policy in Supply Chain Environment

592 Because the Supply Chain Environment has high dimensional state and action spaces, we approximate 593 uncertainty with a *N*-component Gaussian mixture model (GMM), and then construct an uncertainty-594 aware exploration policy by reweighting the model components at explore-time. The Gaussian

Algorithm 2 Uncertainty-aware Action Resampling

1: Given:

- Policy π_M
- Fitted GMM $p_{\mathcal{G}}(s_r, a)$
- Temperature parameter $\tau > 0$
- Input state s, with relevant feature subset $s_r = s|_{\mathcal{I}}$
- 2: Compute action: $a \leftarrow \pi_M(s)$
- 3: Evaluate state-action likelihood: $p_{\mathcal{G}}(s_r, \pi_M(s_r))$
- 4: Extract GMM component contributions: $\{w_i\}_{i=1}^K$
- 5: Compute reweighted components:

$w'_i \leftarrow \frac{\exp(w_i/\tau)}{\sum_{j=1}^K \exp(w_j/\tau)}$ for $i = 1, \dots, K$

- 6: Construct reweighted GMM $p'_{\mathcal{G}}$ using $\{w'_i\}$ 7: Sample new action: $a' \sim p'_{\mathcal{G}}(\cdot \mid s_r)$
- 595 mixture model p_G is learned to approximate the joint distribution of s_r and a present in the dataset, 596 where s_r is defined in Section 4.2. To take an uncertainty-maximizing action in the Supply Chain 597 Environment, the agent first calculates its deterministic nominal action $a = \pi(s)$. Next, calculate 598 the likelihood of the proposed state-action pair with respect to $p_{\mathcal{G}}$ and determine contributions w 599 of each of the N component Gaussians. Lastly, resample the action a from the conditional GMM 600 $p'_{G}(a|s_{r})$ but reweigh the components using a higher temperature distribution based on the component
- 601 contributions w where

$$w_i' = \frac{\exp(w_i/\tau)}{\sum_i \exp(w_i/\tau)}.$$
(10)

602 The procedure is outlined in detail in Algorithm 2.