QXPLORE: Q-LEARNING EXPLORATION BY MAXIMIZING TEMPORAL DIFFERENCE ERROR

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ABSTRACT

A major challenge in reinforcement learning is *exploration*, especially when reward landscapes are sparse. Several recent methods provide an intrinsic motivation to explore by directly encouraging agents to seek novel states. A potential disadvantage of pure state novelty-seeking behavior is that unknown states are treated equally regardless of their potential for future reward. In this paper, we propose an exploration objective using the temporal difference error experienced on extrinsic rewards as a secondary reward signal for exploration in deep reinforcement learning. Our objective yields novelty-seeking in the absence of extrinsic reward, while accelerating exploration of reward-relevant states in sparse (but nonzero) reward landscapes. This objective draws inspiration from dopaminergic pathways in the brain that influence animal behavior. We implement the objective with an adversarial Q-learning method in which Q and Q_x are the action-value functions for extrinsic and secondary rewards, respectively. Secondary reward is given by the absolute value of the TD-error of Q. Training is off-policy, based on a replay buffer containing a mix of trajectories sampled using Q and Q_x. We characterize performance on a set of continuous control benchmark tasks, and demonstrate comparable or faster convergence on all tasks when compared with other state-of-the-art exploration methods.

1 INTRODUCTION

Deep reinforcement learning (RL) has recently achieved impressive results across several challenging domains, such as playing games (Mnih et al., 2016; Silver et al., 2017; OpenAI, 2018; Baker et al., 2019) and controlling robots (OpenAI et al., 2018; Kalashnikov et al., 2018). In many of these tasks, a well-shaped reward function is critical to learning performant policies. On the other hand, deep RL still remains challenging for tasks where the reward function is sparse. In these settings, state-of-the-art RL methods often perform poorly and train very slowly, if at all, due to the low probability of observing improved rewards by following the current optimal policy or with a naive exploration policy such as ϵ-greedy sampling.

The challenge of learning from sparse rewards is typically framed as a problem of *exploration*, inspired by the notion that a successful RL agent must efficiently explore the state space of its environment in order to find improved sources of reward. One common exploration paradigm is to directly determine the novelty of states and to encourage the agent to visit states with the highest novelty. In small MDPs this can be achieved through counting how many times each state has been visited. This approach often performs poorly in high-dimensional or continuous state spaces, but recent work (Tang et al., 2017; Bellemare et al., 2016; Fu et al., 2017) using count-like statistics have shown success on benchmark tasks with complex state spaces. Another paradigm for exploration learns a dynamic model of the environment and computes a novelty measure proportional to the error of the model in predicting transitions in the environment. This exploration method relies on the core assumption that well-modeled regions of the state space are similar to previously visited states and thus are less interesting than other regions of state space. Predictions of the transition dynamics can be directly computed (Pathak et al., 2017; Stadie et al., 2015; Savinov et al., 2019; Burda et al., 2019a), or related to an information gain objective on the state space, as described in VIME (Houthooft et al., 2016) and EMI (Kim et al., 2018).

Several exploration methods have recently been proposed that capitalize on the function approximation properties of neural networks. Random network distillation (RND) trains a function to predict the output of a randomly-initialized neural network from an input state, and uses the approximation error as a reward bonus for a separately-trained RL agent (Burda et al., 2019b). Similarly, DORA (Fox et al., 2018) trains a network to predict zero on observed states and deviations from zero are used to indicate unexplored states.

An important shortcoming of existing exploration methods is that they only incorporate information about states and therefore assume all unobserved states are equally motivating, regardless of their viability for future reward. The viability of this assumption is highly task dependent: While games like Montezuma's Revenge or Super Mario Bros, where novelty correlates highly with success, can be attacked effectively by state novelty methods alone (Burda et al., 2019b; Pathak et al., 2017; Ecoffet et al., 2019; Kim et al., 2018), other tasks such as hide-and-seek or some Atari games where novelty and utility are less correlated tend to frustrate state novelty methods (Burda et al., 2019b; Baker et al., 2019; Burda et al., 2019a). Baker et al. (2019) explored using both RND and a simple state counting baseline to discover skills such as navigation and block-pushing in a hide-and-seek environment. However, the authors found that careful construction of the state representation used for novelty seeking was necessary to discover any such skills, as novelty in the full state space did not correspond to novelty in the intuitive sense (Baker et al., 2019).

In this paper we propose QXplore, a new exploration formulation that seeks novelty in the predicted reward landscape instead of novelty in the state space. QXplore exploits the inherent reward-space signal from the computation of temporal difference error (TD-error) in value-based RL, and explicitly promotes visiting states where the current understanding of reward dynamics is poor. Our formulation draws inspiration from biological models of dopamine pathways in the brain where levels of dopamine correlate with TD-error in learning trials (Niv et al., 2005). Dopamine-seeking behavior has previously been described in animals (Arias-Carrión & Pöppel, 2007) and serves as a biologically plausible exploration objective in contrast to simple state novelty. In the following sections, we describe QXplore and demonstrate its utility for efficient learning on a variety of complex benchmark environments with continuous controls and sparse rewards.

2 Preliminaries

We consider RL in the terminology of Sutton & Barto (1998), in which an agent seeks to maximize reward in a Markov Decision Process (MDP). An MDP consists of states $s \in \mathcal{S}$, actions $a \in \mathcal{A}$, a state transition function $S : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \to [0, 1]$ giving the probability of moving to state s_{t+1} after taking action a_t from state s_t for discrete timesteps $t \in 0, ..., T$. Rewards are sampled from reward function $r : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$. An RL agent has a policy $\pi(s_t, a_t) = p(a_t|s_t)$ that gives the probability of taking action a_t when in state s_t. The agent aims to learn a policy to maximize the expectation of the time-decayed sum of reward $R_\pi(s_0) = \sum_{t=0}^{T} \gamma^t r(s_t, a_t)$ where $a_t \sim \pi(s_t, a_t)$.

A value function $V_\theta(s_t)$ with parameters θ is a function which computes $V_\theta(s_t) \approx R_\pi(s_t)$ for some policy π. Temporal Difference (TD) error δ_t measures the bootstrapped error between the value function at the current timestep and the next timestep as

$$\delta_t = V_\theta(s_t) - (r(s_t, a_t \sim \pi(s_t)) + \gamma V_\theta(s_{t+1})) \tag{1}$$

A Q-function is a value function of the form $Q(s_t, a_t)$, which computes $Q(s_t, a_t) = r(s_t, a_t) + \gamma \cdot \max_{a'} Q(s_{t+1}, a')$, the expected future reward assuming the optimal action is taken at each future timestep. An approximation to this optimal Q-function Q_θ with some parameters θ may be trained using a mean squared TD-error objective $L_{Q_\theta} = ||Q_\theta(s_t, a_t) - (r(s_t, a_t) + \gamma \cdot \max_{a'} Q'_{\theta'}(s_{t+1}, a'))||^2$ given some target Q-function $Q'_{\theta'}$, commonly a time-delayed version of Q_θ (Mnih et al., 2015). Extracting a policy π given Q_θ amounts to approximating $\text{argmax}_a Q_\theta(s_t, a)$. Many methods exist for approximating the argmax_a operation in both discrete and continuous action spaces (Lillicrap et al., 2015; Haarnoja et al., 2018). Following the convention of Mnih et al. (2016), we train Q_θ using an off-policy replay buffer of previously visited (s, a, r, s') tuples, which we sample uniformly.

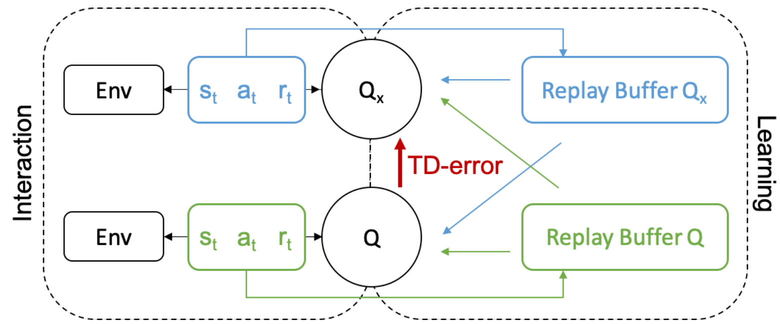


Figure 1: Method diagram for QXplore. We define two Q-functions which sample trajectories from their environment and store experiences in separate replay buffers. Q is a standard state-action value-function, whereas Q_x's reward function is the unsigned temporal difference error of the current Q on data sampled from both replay buffers. A policy defined by Q_x samples experiences that maximize the TD-error of Q, while a policy defined by Q samples experiences that maximize discounted reward from the environment.

3 QXPLORE: TD-ERROR AS ADVERSARIAL REWARD SIGNAL

3.1 METHOD OVERVIEW

We first provide an overview of the method - a visual representation is depicted in Figure 1. At a high level, QXplore is an exploration method that jointly trains two independent agents equipped with their own Q-functions and reward functions:

1. Q: A standard Q-function, that learns a value function on reward provided by the external environment.
2. Q_x: A Q-function that learns a value function directly on the TD-error of Q.

Together, Q, Q_x, and their policies form adversarial pairs, where the policy π_{Q_x} that samples Q_x is the adversary to Q and vice versa for π_Q. π_{Q_x} achieves reward when the agent ventures into states whose reward dynamics are foreign to Q (i.e. Q under/overestimates reward achieved). Separate replay buffers are maintained for each agent, but each agent receives samples from both buffers at train time. A similar adversarial sampling scheme was used to train an inverse dynamics model by Hong et al. (2018), but to our knowledge multiple adversarial sampling policies have not previously been used for exploration.

3.2 TD-ERROR OBJECTIVE

First we will describe our TD-error exploration objective. Schmidhuber et. al. first describe using reward misprediction and model prediction error for exploration (Schmidhuber, 1991; Thrun & Möller, 1991; 1992). However, the work was primarily concerned with model-building and system-identification in small MDPs, and used reward prediction error rather than TD-error. Later, Gehring & Precup (2013) used TD-error as a negative signal to constrain exploration to focus on states that are well understood by the value function to avoid common failure modes. Related to maximizing TD-error is maximizing the variance or KL-divergence of a posterior distribution over MDP's or Q-functions, which can be used as a measure of uncertainty (Osband & Van Roy, 2017; O'Donoghue et al., 2017; Chen et al., 2017). Posterior uncertainty over Q-functions can be used for information gain in the reward or Q-function space, as opposed to information gain in the state space as described by VIME among others (Houthooft et al., 2016), but to our knowledge posterior uncertainty methods have thus-far only been demonstrated in small MDP's or for local exploration as an alternative to dithering methods such as ϵ-greedy sampling.

In contrast to these previous works, we directly treat TD-error as a reward signal and use a Q-function trained on this signal to induce an exploration policy, rather than as a supplementary objective or to compute a confidence bound. Crucially, when combined with neural network function approximators, this signal provides meaningful exploration information everywhere as discussed in Section 3.4. For

Algorithm 1 QXplore Algorithm

Input: MDP S, Q-function Q_θ with target $Q'_{\theta'}$, Q_x function $Q_{x,\phi}$ with target $Q'_{x,\phi'}$, replay buffers $\mathcal{Z}_Q$ and $\mathcal{Z}_{Q_x}$, batch size B and sampling ratios $\mathcal{R}_Q$ and $\mathcal{R}_{Q_x}$, CEM policies π_Q and π_{Q_x}, time decay parameter γ, soft target update rate τ, and environments E_Q, E_{Q_x}
while not converged **do**
  Reset E_Q, E_{Q_x}
  while E_Q and E_{Q_x} are not done **do**
    Sample environments
    $\mathcal{Z}_Q \leftarrow (s, a, r, s') \sim \pi_Q | E_Q$
    $\mathcal{Z}_{Q_x} \leftarrow (s, a, r, s') \sim \pi_{Q_x} | E_{Q_x}$
    Sample minibatches for Q_θ and $Q_{x,\phi}$
    $(s_Q, a_Q, r_Q, s'_Q) \leftarrow B * \mathcal{R}_Q$ samples from $\mathcal{Z}_Q$ and $B * (1 - \mathcal{R}_Q)$ samples from $\mathcal{Z}_{Q_x}$
    $(s_{Q_x}, a_{Q_x}, r_{Q_x}, s'_{Q_x}) \leftarrow B * \mathcal{R}_{Q_x}$ samples from $\mathcal{Z}_{Q_x}$ and $B * (1 - \mathcal{R}_{Q_x})$ samples from $\mathcal{Z}_Q$
    Train
    $r_{x,\theta} \leftarrow |Q_\theta(s_{Q_x}, a_{Q_x}) - (r_{Q_x} + \gamma Q'_{\theta'}(s'_{Q_x}, \pi_Q(s'_{Q_x})))|$
    $L_Q \leftarrow ||Q_\theta(s_Q, a_Q) - (r_Q + \gamma Q'_{\theta'}(s'_Q, \pi_Q(s'_Q)))||^2$
    $L_{Q_x} \leftarrow ||Q_{x,\phi}(s_{Q_x}, a_{Q_x}) - (r_{x,\theta} + \gamma Q'_{x,\phi'}(s'_{Q_x}, \pi_{Q_x}(s'_{Q_x})))||^2$
    Update $\theta \propto L_Q$
    Update $\phi \propto L_{Q_x}$
    $\theta' \leftarrow (1 - \tau)\theta' + \tau\theta$
    $\phi' \leftarrow (1 - \tau)\phi' + \tau\phi$
  end while
end while

a value function with parameters θ, and TD-error δ_t we define our exploration reward function as

$$r_{x,\theta}(s_t, a_t, s_{t+1}) = |\delta_t| = |Q_\theta(s_t, a_t) - (r_{\text{E}}(s_t, a_t) + \gamma \max_{a'} Q'_{\theta'}(s_{t+1}, a'))| \tag{2}$$

for some extrinsic reward function r_{E} and target Q-function Q'_θ. Notably, we use the absolute value of the temporal difference (rather than the squared error) used to compute updates for Q_θ to keep the magnitudes of r_{E} and r_x comparable and reduce the influence of outlier temporal differences on the gradients of Q_x, which we describe below.

Intuitively, a policy maximizing the expected sum of r_x will sample trajectories where Q_θ does not have an accurate estimate of the future rewards it will experience. This is useful for exploration because r_x will be large not only for state-action pairs producing unexpected reward, but for all state-action pairs leading to such states, providing a much denser exploration reward function. In addition, a policy maximizing TD error can be seen as an adversarial teacher for training Q_θ. Further, TD-error-based exploration with a dedicated exploration policy removes the exploitation-versus-exploration tradeoff that state-novelty methods must contend with, as maximizing TD-error will produce trajectories that provide information about the task for Q_θ to train on without impacting its ability to converge to an optimal Q-function.

3.3 Q_x: Learning a Q-function to maximize TD-error

Next, we will describe how we use the TD-error signal defined in Section 3.2 to define an exploration policy. r_x itself is a generic reward objective, which can be maximized by any RL algorithm. However, given its derivation from a bootstrapped Q-function, training a second Q-function to maximize r_x allows the entire algorithm to be trained off-policy with a replay buffer shared between Q_θ and the Q-function maximizing r_x, which we term Q_x. This approach is beneficial for exploration, as trajectories producing improved reward may be sampled only very rarely, and a shared replay buffer improves data efficiency for training both Q-functions.

We define a Q-function, $Q_{x,\phi}(s, a)$ with parameters ϕ, whose reward objective is r_x. We train $Q_{x,\phi}$ using the standard bootstrapped loss function

$$L_{Q_{x,\phi}} = ||Q_{x,\phi}(s_t, a_t) - (r_x(s_t, a_t, s_{t+1}) + \gamma \max_{a'} Q'_{x,\phi'}(s_{t+1}, a'))||^2 \tag{3}$$

The two Q-functions, Q_θ and Q_x, are trained off-policy in parallel, sharing replay data so that Q_θ can train on sources of reward discovered by Q_x and so that Q_x can better predict the TD-errors of

Q_θ. Since the two share data, π_{Q_x} acts as an adversarial teacher for Q_θ, sampling trajectories that produce high TD-error under Q_θ and thus provide novel information about the reward landscape. To avoid off-policy issues due to the different reward objectives, we sample a fixed ratio of experiences collected by each policy for each training batch. We use a nonparametric cross-entropy method policy inspired by Kalashnikov et al. (2018), previously described as more robust to hyperparameter variance (Simmons-Edler et al., 2019; Kalashnikov et al., 2018). We also experimented with a variant using DDPG-style parametric policies (Lillicrap et al., 2015) for both Q_θ and Q_x , but found preventing sampling collapse by Q_θ's policy difficult. Our full method is shown in Figure 1, and pseudocode in Algorithm 1.

3.4 State Novelty from Neural Network Function Approximation Error

A key question in using TD-error for exploration is: What happens when the reward landscape is flat? Theoretically, in the case that $\forall(s,a), r(s,a) = C$ for some constant $C \in \mathbb{R}$, an optimal Q-function which generalizes perfectly to unseen states will, in the infinite time horizon case, simply output $\forall(s,a), Q^\star(s,a) = \sum_{t=0}^{\infty} C\gamma^t$. This results in a TD-error of 0 everywhere and thus no exploration signal. However, using neural network function approximation, we find that perfect generalization to unseen states-action pairs does not occur, and in fact observe in Figure 2 that the distance of a new datapoint from the training data manifold correlates with the magnitude of the network output's deviation from $\sum_{t=1}^{\infty} C\gamma^t$ and thus with TD-error. As a result, in the case where the reward landscape is flat TD-error exploration converges to a form of state novelty exploration. This property of neural network function approximation has been used by several previous exploration methods to good effect, including RND (Burda et al., 2019b) and DORA (Fox et al., 2018). In particular, the exploration signal used by RND (extrapolation error from fitting the output of a random network) should be analogous to r_x (extrapolation error from fitting a constant value), meaning we should expect to perform comparably to RND in the worst case where no extrinsic reward exists.

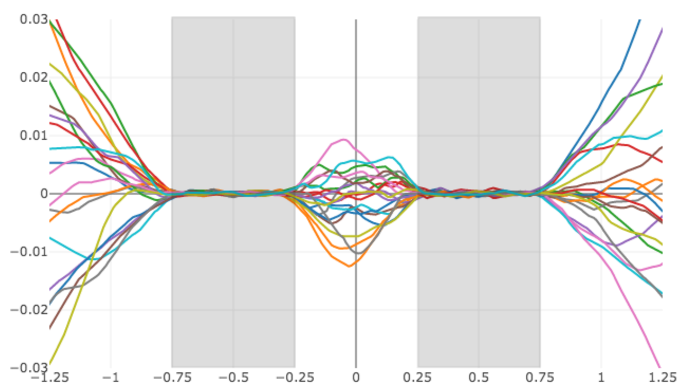


Figure 2: A neural network trained to predict a constant value does not interpolate or extrapolate well outside its training range, which can be exploited for exploration. Predictions of 3-layer MLPs of 256 hidden units per layer trained to imitate $f(x) = 0$ on $\mathbb{R} \to \mathbb{R}$ with training data sampled uniformly from the range $[-0.75, -0.25] \cup [0.25, 0.75]$. Each line is the final response curve of an independently trained network once its training error has converged (MSE $<$ 1e-7).

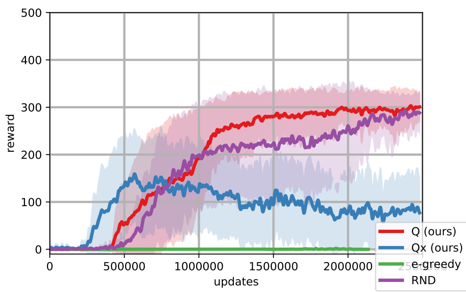
4 Experiments

We performed several experiments to demonstrate the effectiveness of Q_x on continuous control benchmark tasks. We first compare with a state of the art state novelty-based method, RND (Burda et al., 2019b), and with ϵ-greedy sampling as a simple baseline, in Figure 3. We then compare to results from several previous works on `SparseHalfCheetah`. Finally, we present two ablations to QXplore, as well as some analysis of its robustness in response to several hyperparameters. Implementation details and hyperparameters for QXplore, RND, and ϵ-greedy can be found in Appendix A.

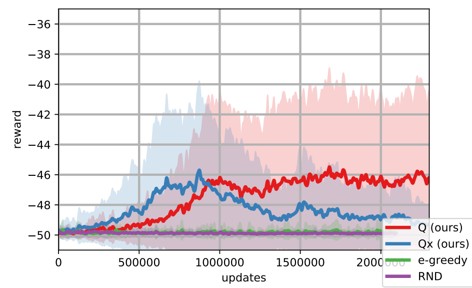
4.1 Experimental Setup

We benchmark on four continuous control tasks using the MuJoCo physics simulator that each require exploration due to sparse rewards. First, the `SparseHalfCheetah` task originally proposed by VIME (Houthooft et al., 2016). Next, we benchmark on three OpenAI gym tasks, `FetchPush`, `FetchSlide` and `FetchPickAndPlace`, originally developed for goal-directed exploration methods such as HER (Andrychowicz et al., 2017). We chose these tasks as they are challenging exploration problems that are relatively simple to control, but still involve large continuous state spaces and in the case of the `Fetch` tasks learning to generalize across random object/goal positions. More details on these environments can be found in Appendix F.

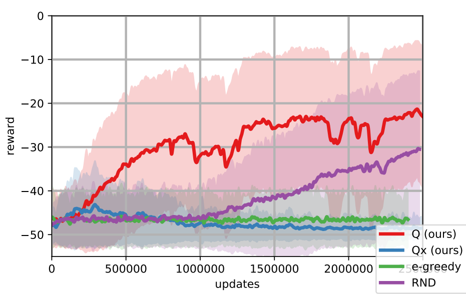
4.2 Exploration Benchmark Performance



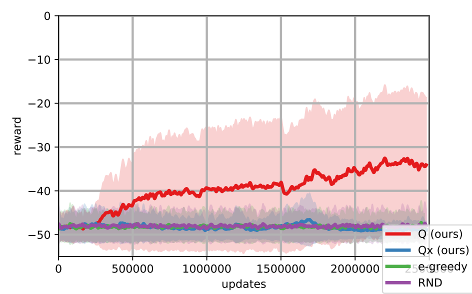
(a) SparseHalfCheetah-v1



(b) FetchSlide-v1



(c) FetchPush-v1



(d) FetchPickAndPlace-v1

Figure 3: Performance of QXplore compared with RND and ϵ-greedy sampling. QXplore outperforms RND and ϵ-greedy on continuous control tasks. QXplore performs better due to efficient exploration sampling by Q_x and the separation of the exploration and exploitation objectives.

Episodes until mean reward of	**QXplore**	**VIME**	**EX2**	**EMI**	**SimHash**
50	**2000**	10000*	4740*	2580*	x*
100	**3000**	x*	6180*	4520*	x*
200	**4000**	x*	x*	8440*	x*
300	**7900**	x*	x*	x*	x*

Table 1: Number of episodes required to reach mean reward milestones on `SparseHalfCheetah` for several methods. QXplore outperforms previously published methods. Results marked with "*" are previously published numbers from VIME (Houthooft et al., 2016), EMI (Kim et al., 2018), or Tang et al. (2017). Results marked with "x" indicate that the mean reward was not achieved. Note that as QXplore performs rollouts for both Q and Q_x in parallel QXplore is less sample-efficient relative to single-policy methods.

We show the performance of each method on each task in Figure 3. QXplore outperforms RND modestly on the `SparseHalfCheetah` task, but performs much better comparatively on the `Fetch` tasks- only on `FetchPush`, the easiest task, did RND find non-random reward. We theorize that this improved performance on the `Fetch` tasks is because QXplore's TD-error exploration drives the agent to discover the conditional relationship between the changing goal position and the reward function, whereas RND and other state novelty methods are goal-agnostic since the goal is static for the entire episode. While QXplore is not a goal-directed RL method, the fact that this relationship is discovered through TD-error exploration is encouraging as to its broader applicability.

A separate comparison to several other prominent exploration methods is in Table 1. These methods are built on top of TRPO (Schulman et al., 2015), so a comparison in terms of training iterations as in Figure 3 would not be informative due to TRPO's variable update rule. We instead compare number of episodes of interaction required to reach a given level of reward, though QXplore was not intended to be performant with respect to this metric. Also, as noted in Section 4.3, it is possible to train a viable Q function completely off-policy, and thus a version of QXplore that is optimized for reduced environment interactions without significant loss of performance should be a simple extension. While some decrease in episode efficiency is expected due to differing baseline methods (TRPO (Schulman et al., 2015) versus Q-Learning), compared to published results for EMI (Kim et al., 2018), EX2 (Fu et al., 2017), VIME (Houthooft et al., 2016), and SimHash (Tang et al., 2017) on the `SparseHalfCheetah` task, QXplore reaches every reward milestone faster, and achieves a peak reward (300) not achieved by any previous method.

4.3 Robustness

As RL tasks are highly heterogeneous, and good parameterization/performance can be hard to obtain in practice for many methods (Henderson et al., 2018), we performed sweeps over several hyperparameters and introduce several ablations of QXplore on `SparseHalfCheetah` to demonstrate the method's robustness and validate aspects of the algorithm.

Parameter Sweeps We swept over the learning rates of Q and Q_x, as well as the ratio of self-collected versus other-collected data used to train each function. The results suggest that while the performance of Q is somewhat sensitive to learning rate, keeping learning rates for Q and Q_x the same works well. The results also show that performance is surprisingly invariant to the on/off-policy data ratio, including when Q is trained entirely off-policy on data collected by Q_x, suggesting that the data collected by Q_x is sufficient to train a policy to maximize reward without any on-policy rollouts. Results are shown in Figures 5 and 6 in Appendix B.

Weight Initialization Also, since neural network generalization is key to QXplore, we tested several different network weight initialization schemes, including some that were deliberately poor priors. We found that while the performance of Q is sensitive to initialization scheme, Q_x robustly finds reward in all cases. See Figure 7 in Appendix C.

The 'Noisy TV' Problem One challenge that state novelty exploration methods must overcome is that unpredictable observations (such as from a TV displaying static) act as maxima in the exploration reward function. One advantage to TD-error driven exploration is that it is not sensitive to unpredictable observations as they do not affect the underlying reward function. To demonstrate this, we tested QXplore with a variant of the `SparseHalfCheetah` task with noisy observations. We observe that QXplore performs as normal in this case. Detailed results and a description of the task can be found in Appendix D.

4.4 Ablations

There are two features of QXplore that distinguish it from prior work in exploration: the use of an adversarial pair of policies that share experiences, and the use of TD-Error to drive exploration. We conduct ablations that assess the impact that each of these two features has on the method. Results for both can be found in Figure 9 of Appendix E.

Single-Policy QXplore First, we test a single-policy version of QXplore by replacing $Q_\theta(s,a)$ with a value function $V_\theta(s)$ trained via bootstrap and computing $r_{x,\theta}(s_t,a_t,s_{t+1}) = |V_\theta(s_t) - (r_{\mathrm{E}}(s_t,a_t) + \gamma V'_{\theta'}(s_{t+1}))|$. This variant uses only a single sample policy, Q_x, which is trained via bootstrapped off-policy Q-learning using one-step reward targets $r_1 = (r_x(s_t,a_t,s_{t+1}) + \alpha r_{\mathrm{E}}(s_t,a_t)$ to maximize a combination of intrinsic and extrinsic rewards, controlled by the hyperparameter α. We find that this variant is sensitive to α, as it must trade off between exploration and exploitation, with the range of optimal values varying greatly between tasks. We evaluate the performance of this ablation using

$\alpha = 0.1$, observing that while the policy is able to find reward quickly and converge faster, the need to satisfy both objectives results in a lower converged reward than the original QXplore method.

1-Step Reward Prediction Second, we run an ablation where we replaced $Q_\theta(s, a)$ in the calculation of TD-error with a function that simply predicts the current $r(s_t, a_t)$, shown in Figure 9. Using reward error instead of a value function in Q_x still produces the same state novelty fallback behavior in the absence of reward; however, it provides only limited reward-based exploration utility and does not allow us to use Q_θ as an optimal Q-function once trained. We tested this variant with other parameters held the same, and observe that it fails to find reward. Reward prediction error is not sufficient to allow strong exploration behavior.

4.5 Qualitative Behavioral Analysis

Qualitatively, on `SparseHalfCheetah` we observe interesting behavior from Q_x late in training. After initially converging to obtain reward consistently, Q_x appears to get "bored" and will try to move closer to the reward threshold, stopping short or jumping back and forth across it during an episode, which results in reduced reward but higher TD-error. This behavior is distinctive of TD-error seeking over state novelty seeking, as such states are not novel compared to moving past the threshold but do result in higher TD-error. Such behavior from Q_x motivates Q to explore the state space around the reward boundary. Example sequences of such behaviors are shown in Figure 4.

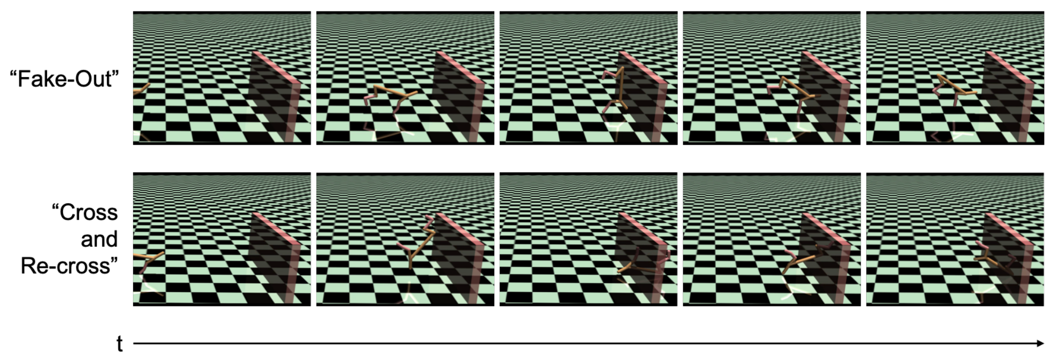


Figure 4: Example trajectories showing Q_x's behavior late in training that is distinctive of TD-error maximization. The corresponding Q network reliably achieves reward at this point. In "fake-out", Q_x approaches the reward threshold and suddenly stops itself. In "cross and re-cross", Q_x crosses the reward threshold going forward and then goes backwards through the threshold.

5 Discussion and Conclusions

Here, we have described a new biologically-inspired method for using TD-error to explore in reinforcement learning. We instantiate a reward function using TD-error, and show that when combined with neural network approximation, it is sufficient to discover solutions to challenging exploration tasks in fewer training iterations than recent state novelty-based exploration methods. TD-error has different advantages and disadvantages for exploration compared to state prediction, and we hope that our results can spur further work on diverse exploration signals in RL.

It is also worth noting that there may be additional benefits provided by Q_x for Q learning in non-exploration contexts. Maximizing TD-error can be seen as a form of hard example mining, and for complex tasks could result in better generalization behavior.

We emphasize that we have only described one possible approach for TD-error driven learning in this work. Our instantiation makes several assumptions, such as the use of off-policy Q-learning, two sampling policies, and unsigned TD-error which is positive for both under-prediction and over-prediction of future rewards. While these assumptions improve the performance of QXplore, more work remains to be done on the topic, including how best to trade off between TD-error exploration and extrinsic reward maximization, on-policy TD-error, and further developing the connections between TD-error and biological concepts of curiosity, boredom, and exploration, which may lead to new and improved exploration methods.

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Table 2: Parameters used for benchmark runs.

DEFAULT PARAMETERS	
CEM	
ITERATIONS	4
NUMBER OF SAMPLES	64
TOP K	6
ALL NETWORKS	
NEURONS PER LAYER	256
NUMBER OF LAYERS	3
NON-LINEARITIES	RELU
OPTIMIZER	ADAM
ADAM MOMENTUM TERMS	$\beta_1 = 0.9, \beta_2 = 0.99$
TRAINING	
Q LEARNING RATE	0.001
BATCH SIZE	128
TIME DECAY γ	0.99
TARGET Q-FUNCTION UPDATE τ	0.005
TARGET UPDATE FREQUENCY	2
TD3 POLICY NOISE	0.2
TD3 NOISE CLIP	0.5
TRAINING STEPS PER ENV TIMESTEP	1
QXPLORE-SPECIFIC	
Q_x LEARNING RATE	0.001
Q BATCH DATA RATIO	0.75
Q_x BATCH DATA RATIO	0.75
RND-SPECIFIC	
PREDICTOR NETWORK LEARNING RATE	0.001
ϵ-GREEDY-SPECIFIC	
ϵ	0.1

APPENDIX A: IMPLEMENTATION DETAILS AND HYPERPARAMETERS

We describe here the details of our implementation and training parameters. We held these factors constant and used a shared codebase for QXplore, RND, and ϵ-greedy to enable a fair comparison. We used an off-policy Q-learning method based off of TD3 (Fujimoto et al., 2018) and CGP (Simmons-Edler et al., 2019) with twin Q-functions and a cross-entropy method policy for better hyperparameter robustness. Each network (Q_θ, $Q_{x,\phi}$, RND's random and predictor networks) consisted of a 3-layer MLP of 256 neurons per hidden layer, with ReLU non-linearities. We used a batch size of 128 and learning rate of 0.001, and for QXplore sampled training batches for Q and Q_x of 75% self-collected data and 25% data collected by the other Q-function's policy as described in Algorithm 1.

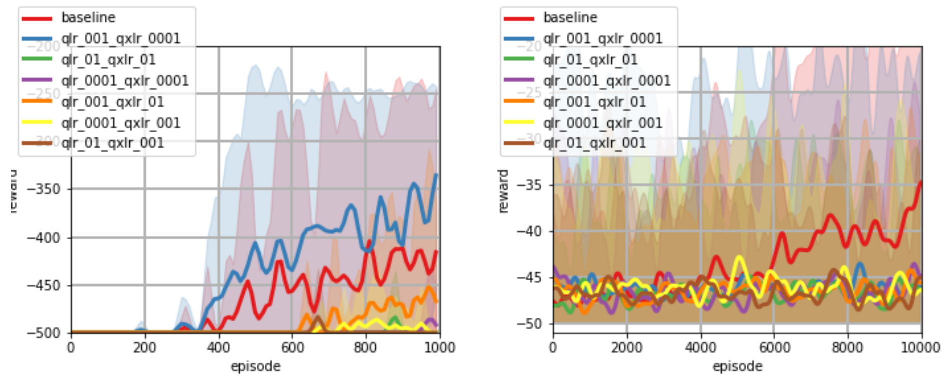
We present the parameters we used for the benchmark tasks in Table 2.

APPENDIX B: PARAMETER SWEEPS

We performed two sets of parameter sweeps for QXplore: varying the learning rates of Q and Q_x, and varying the ratios of data sampled by each Q-function's policy used in training batches for each method. For learning rate, we tested combinations (QLR, QxLR) (0.01, 0.01), (0.01, 0.001), (0.001, 0.01), (0.001, 0.001), (0.001, 0.0001), (0.0001, 0.001), (0.0001, 0.0001).

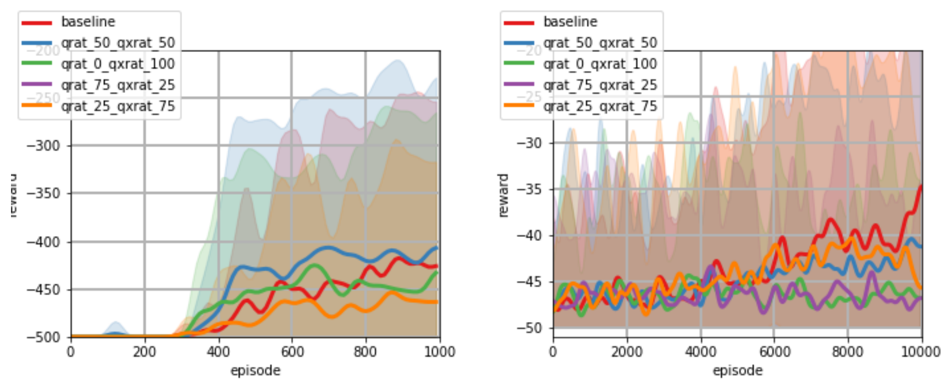
For batch data ratios, we tested combinations (specified as self-fraction for Q, then self-fraction for Q_x) of (0, 1), (0.25, 0.75), (0.5, 0.5), (0.75, 0.25).

Results for these sweeps can be seen in Figures 5 and 6. QXplore is sensitive to learning rate, but relatively robust to the training data mix, to the point of Q training strictly off-policy with only modest performance loss.



(a) SparseHalfCheetah (b) FetchPush-v1

Figure 5: Learning rate sweeps for Q and Q_x



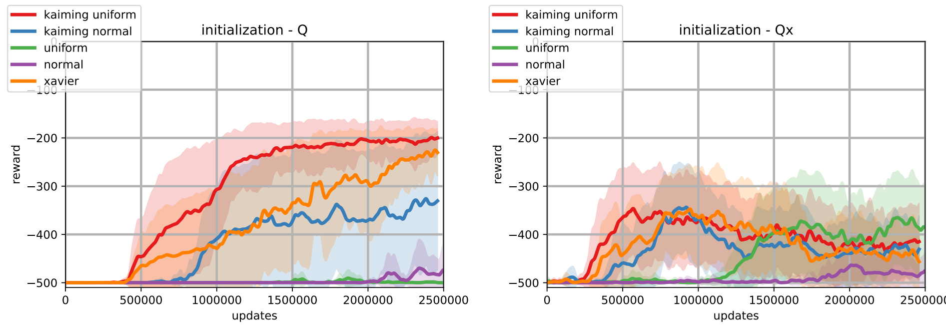
(a) SparseHalfCheetah (b) FetchPush-v1

Figure 6: Sample ratio sweeps for Q and Q_x

APPENDIX C: WEIGHT INITIALIZATION

As we use neural net function approximation error as a state novelty baseline for early exploration, the behavior of Q_x may be sensitive to weight initialization. To test this, in addition to the Pytorch default initialization method "Kaiming-Uniform," (He et al., 2015) which we used for all runs outside this section, we also tested initializing both Q and Q_x with "Kaiming-Normal" and "Xavier-Uniform," (Glorot & Bengio, 2010) two other standard initialization methods. We further tested two naive distributions that produced very high magnitude initial outputs, "Normal," sampling weight values from $\mathbf{N}(0, 1)$ and "Uniform," sampling values from $\mathbf{U}(-1, 1)$. These configurations were not expected to perform well, but do test the ability of Q_x to explore given a poor initialization. In all cases other than "Kaiming-Uniform" we set the bias of each neuron to 0. The results of this test for `SparseHalfCheetah` are shown in Figure 7.

"Kaiming-Normal" and "Xavier-Uniform" both showed modest decrease in overall performance, but both Q and Q_x were able to converge on reward. "Normal" and "Uniform" however both more-or-less prevented Q from converging on reward, though there is some sign that "Normal" is recovering. The performance of Q_x however is much more mild- only "Normal" and to a lesser extent "Uniform" caused significant issues with discovering and converging on reward. This suggests that Q_x is not particulary dependent on careful weight initialization to explore with function approximation error.



(a) Initialization of Q

(b) Initialization of Q_x

Figure 7: Several alternate initialization schemes for Q and Q_x. While Q is negatively impacted, Q_x is relatively robust to poor initializations such as "Normal" and "Uniform."

Appendix D: The 'Noisy TV' Problem

The 'Noisy TV' problem is a classic issue with some state-novelty exploration methods in which states with unpredictable observations serve as maxima in the novelty reward space. QXplore's TD-error objective is not fundamentally vulnerable to the problem, but to demonstrate that our function approximation early in training is also no subject to it, we trained QXplore on a variant of the `SparseHalfCheetah` task where we add a random normally-distributed value to the observation vector of the agent. The variance of this noise value increases proportionately to the movement of the cheetah in the negative direction (away from the reward threshold). An agent vulnerable to the noisy tv problem will be enticed to explore in the negative direction rather than forward, as this maximizes the novelty/unpredictability of the observations.

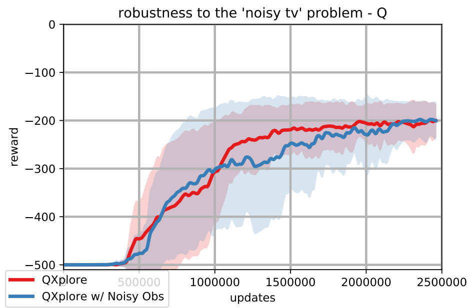
We show the results of training QXplore on this environment in Figure 8 for both Q and Q_x, as well as the mean position of the cheetah along the movement dimension during Q_x's training rollouts. As expected, the performance of neither Q nor Q_x is meaningfully altered relative to the baseline, and Q_x is not biased to explore backwards to a greater degree than it typically does early in training.

Appendix E: Ablations

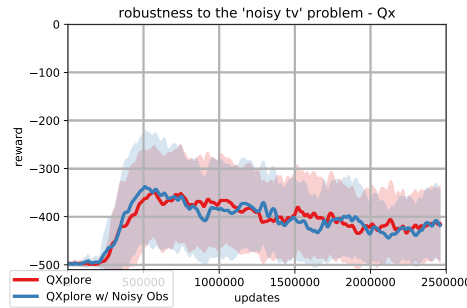
To demonstrate the necessity of the major components of QXplore, we performed two ablations, shown in Figure 9 and discussed in the main paper in Section 4.4.

Appendix F: Environment Details

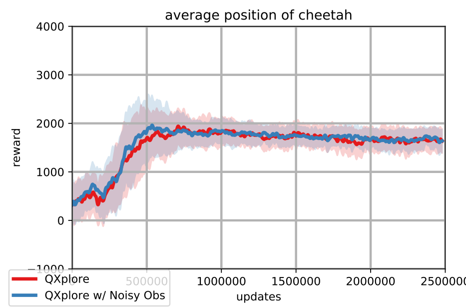
We use the `SparseHalfCheetah` environment proposed by Houthooft et al. (2016) in which a simulated cheetah receives a reward of 0 if it is at least 5 units forward from the initial position and otherwise receives a reward of -1. We also use the OpenAI gym tasks, `FetchPush`, `FetchSlide`, and `FetchPickAndPlace`, which were originally developed for benchmarking HER Andrychowicz et al. (2017). The objective in these environments is to move a block to a target position, with a reward function returning -1 if the block is not at the target and 0 if it is at the target. For consistency between benchmarks, we structured the reward function of the `SparseHalfCheetah` task to match the `Fetch` tasks, such that the baseline reward level is -1 while a successful state provides 0 reward, but report reward values on a 0 to 500 scale for direct comparison with previous work. We trained each method with 5 random seeds for 5,000 episodes on `SparseHalfCheetah` and 50,000 episodes on `Fetch` tasks. Time to convergence on these tasks for any exploration method is highly variable, and as such we visualize the mean and standard deviation of the runs in our results.



(a) Noisy observation effects on Q



(b) Noisy observation effects on Q_x



(c) Noisy observation effects on absolute position

Figure 8: QXplore trained on a 'noisy tv' variant of `SparseHalfCheetah` where one element of the observation vector is normally distributed random value whose variance increases if the cheetah moves in the negative direction. The performance of QXplore is not impacted in any way by this noise, and it trains as normal.

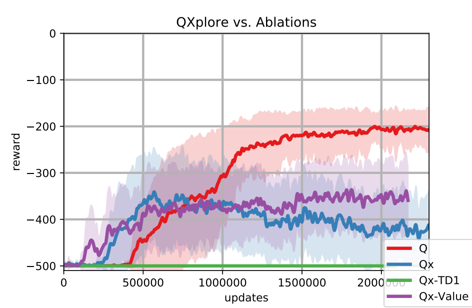


Figure 9: Plot showing the performance of two ablations, 1-Step Reward Prediction and Single-Policy QXplore, compared to the original QXplore method. In the 1-Step ablation, Q_x is trained to predict a combination of extrinsic reward and reward prediction error, and fails to make progress. In the Single-Policy ablation, the policy converges faster, but to a worse policy than vanilla QXplore due to the need to balance TD-error and extrinsic reward maximization.