Robust Exploration via Clustering-based Online Density Estimation

Abstract

Intrinsic motivation is a critical ingredient in reinforcement learning to enable progress when rewards are sparse. However, many existing approaches that measure the novelty of observations are brittle, or rely on restrictive assumptions about the environment which limit generality. We propose to decompose the exploration problem into two orthogonal sub-problems: (i) finding the right representation (metric) for exploration (ii) estimating densities in this representation space. To address (ii), we introduce Robust Exploration via Clustering-based Online Density Estimation (`RECODE`), a non-parametric method that estimates visitation counts for clusters of states that are similar according to the metric induced by any arbitrary representation learning technique. We adapt classical clustering algorithms to design a new type of memory that allows `RECODE` to keep track of the history of interactions over thousands of episodes, thus effectively tracking global visitation counts. This is in contrast to existing non-parametric approaches, that can only store the recent history, typically the current episode. The generality of `RECODE` allows us to easily address (i) by leveraging both off-the-shelf and novel representation learning techniques. In particular, we introduce a novel generalization of the action-prediction representation that leverages multi-step predictions and that we find to be better suited to a suite of challenging 3D-exploration tasks in `DM-HARD-8`. We show experimentally that our approach can work with a variety of RL agents, and obtain state-of-the-art performance on Atari and `DM-HARD-8`.

1 Introduction

Exploration mechanisms are a key component of reinforcement learning (RL, Sutton & Barto, 2018) agents, especially in sparse-reward tasks where long sequences of actions need to be executed before collecting a reward. The exploration problem has been studied theoretically (Kearns & Singh, 2002; Azar et al., 2017; Brafman & Tennenholtz, 2003; Auer et al., 2002; Agrawal & Goyal, 2012; Audibert et al., 2010; Jin et al., 2020) in the context of bandits (Lattimore & Szepesvári, 2020) and Markov Decision Processes (MDP, Puterman, 1990; Jaksch et al., 2010). Among those theoretical works, one simple and theoretically-sound approach to perform exploration efficiently in MDPs is to use a decreasing function of the visitation counts as an exploration bonus (Strehl & Littman, 2008; Azar et al., 2017). However, this approach is intractable with large or continuous state spaces, as generalization between states becomes essential. Several experimental works have tried to come up with ways to estimate visitation counts/densities in complex environments where counting is not trivial. Two partially successful approaches have emerged to empirically estimate visitation counts/densities in deep RL: (i) the parametric approach that uses neural networks and (ii) the non-parametric approach that uses a slot-based memory to store representations of visited states, where the representation learning method serves to induce a more meaningful metric[1] between states.

Parametric methods either explicitly estimate the visitation counts using density models (Bellemare et al., 2016; Ostrovski et al., 2017) or implicitly estimate the counts using e.g., Random Network Distillation (`RND`, Burda et al., 2019; Badia et al., 2020b). Non-parametric methods rely on a memory to store encountered state representations (Badia et al., 2020b) and representation learning to

---

[1]Usually this is a pseudometric on the space of observations, since $d(x, y) = 0$ for $x \neq y$ is permitted by typical network architectures, and may be desirable as a means to discard noisy or uncontrollable features

construct a metric that differentiates states meaningfully (Pathak et al., 2017). Parametric methods do not store individual states explicitly and as such their capacity is not directly bound by memory constraints; but they are less well suited to rapid adaptation on short timescales (e.g., within a single episode). To bring the best of both worlds into a single method, Never Give Up (`NGU`, Badia et al., 2020b) combines a short-term novelty signal based on an episodic memory and a long-term novelty via `RND`, into a single intrinsic reward. However, this approach also naturally inherits the disadvantages of `RND`; in particular, susceptibility to uncontrollable or noisy features (see Section 5). More details on related works are provided in App. B.

In this paper, we propose to decompose the exploration problem into two orthogonal sub-problems. First, (i) **Representation Learning** which is the task of learning an embedding function on observations or trajectories that encodes a meaningful notion of similarity. Second, (ii) **Density Estimation** which is the task of estimating smoothed visitation counts to derive a novelty-based exploration bonus. The first contribution of this paper is a general solution to (ii). We introduce Robust Exploration via Clustering-based Online Density Estimation (`RECODE`), a non-parametric method that estimates visitation counts for clusters of states that are similar according to the metric induced by any arbitrary representation. We leverage classical clustering algorithms to design a new type of memory that allows `RECODE` to keep track of histories of interactions spanning thousands of episodes. This is in contrast to existing non-parametric exploration methods, which store only the recent history and in practice usually only account for the current episode. The resulting exploration bonus is principled, simple, and matches state-of-the-art exploration results on Atari. In the presence of noise, we show that it strictly improves over state-of-the-art exploration bonuses such as `RND` or `NGU`. The generality of `RECODE` also allows us to easily leverage both off-the-shelf and novel representation learning techniques, leading to our second contribution. Specifically, we generalize the action-prediction representation learning method (Pathak et al., 2017), used in several state-of-the-art exploration agents, to a multi-step prediction setting that is better-suited to 3D and partially-observable domains. In particular, we show that it can yield significant performance gains in some hard 3D-exploration tasks included in the `DM-HARD-8` suite, and achieves a new state of the art in the single-task setting.

2 BACKGROUND AND NOTATION

In this section, we provide the necessary background and notation to understand our method (see Sec. 3). First, we present a general setting of interaction between an agent and its environment. Second, we define the terms embeddings, atoms and memory. Third, we present our notation for visitation counts. Finally, we show how we derive intrinsic rewards from visitations counts.

Interaction Process between an Agent and its Environment. We consider a discrete-time interaction process (McCallum, 1995; Hutter, 2004; Hutter et al., 2009; Daswani et al., 2013) between an agent and its environment where, at each time step $t \in \mathbb{N}$, the agent receives an observation $o_t \in \mathcal{O}$ and generates an action $a_t \in \mathcal{A}$. We consider an environment with stochastic dynamics $p : \mathcal{H} \times \mathcal{A} \to \Delta_{\mathcal{O}}{}^2$ that maps a history of past observations-actions and a current action to a probability distribution over future observations. More precisely, the space of past observations-actions is $\mathcal{H} = \bigcup_{t \in \mathbb{N}} \mathcal{H}_t$ where $\mathcal{H}_0 = \mathcal{O}$ and $\forall t \in \mathbb{N}^*, \mathcal{H}_{t+1} = \mathcal{H}_t \times \mathcal{A} \times \mathcal{O}$. We consider policies $\pi : \mathcal{H} \to \Delta_{\mathcal{A}}$ that maps a history of past observations-actions to a probability distribution over actions. Finally, an extrinsic reward function $r_e : \mathcal{H} \times \mathcal{A} \to \mathbb{R}$ maps a history to a scalar feedback.

Embeddings, Atoms and Memory. An embedder is a parameterized function $f_\theta : \mathcal{H} \to \mathcal{E}$ where $\mathcal{E}$ is an embedding space. Typically, the embedding space is the vector space $\mathbb{R}^N$ where $N \in \mathbb{N}^*$ is the embedding size. Therefore, for a given time step $t \in \mathbb{N}$, an embedder is a function f_θ that associates to any history $h_t \in \mathcal{H}_t$ a vector $e_t = f_\theta(h_t)$ called an embedding. There are several ways to train an embedder f_θ such as using an auto-encoding loss of the observation o_t (Burda et al., 2018), using an inverse dynamics loss (Pathak et al., 2017) or using a multi-step prediction-error loss at the latent level (Guo et al., 2020; 2022). Those techniques are referred as representation learning methods. An atom $f \in \mathcal{E}$ is a vector in the embedding space that is contained in a memory $M = \{f_i \in \mathcal{E}\}_{i=1}^{|M|}$ which is a finite slot-based container, where $|M| \in \mathbb{N}^*$ is the memory size. The

---

[2]We write $\Delta_{\mathcal{Y}}$ the set of probability distributions over a set $\mathcal{Y}$.

memory M is updated at each time step t by a non-parametric function of the memory M and the embedding e_t. In the simplest case, the memory is filled in a first-in first-out (FIFO) manner along the interactions (Badia et al., 2020b;a) and atoms are simply the embeddings themselves. However, more complex mechanisms than FIFO can be considered to fill/update a memory. For instance given a memory M and an embedding e_t, the embedding e_t can be inserted in the memory if and only if it is different from the other atoms in the memory and the memory is not at capacity. The update rule that defines the atoms in the memory is a key component of our method.

Visitation Counts. Let $M = \{f_l \in \mathcal{E}\}_{l=1}^{|M|}$ be a slot memory containing atoms. The vanilla visitation count, $N_\delta(M, e)$, for a given embedding $e \in \mathcal{E}$ with respect to the memory M is:

$$N_\delta(M, e) = \sum_{l=1}^{|M|} \delta(f_l, e), \text{ where } \delta(f, e) : (e, f) \in \mathcal{E}^2 = \begin{cases} 1, & \text{if } e = f \\ 0, & \text{otherwise,} \end{cases} \tag{1}$$

When the embedding space is complex and too large, the vanilla visitation count becomes uninformative because each embedding is potentially different from all the atoms. To overcome this problem, soft-visitation counts are computed. The soft-visitation count, $N_\mathcal{K}(M, e)$, for a given state e with respect to the memory M is $N_\mathcal{K}(M, e) = \sum_{l=1}^{|M|} \mathcal{K}(f_l, e)$, where $\mathcal{K} \in \mathbb{R}_+^{\mathcal{E}^2}$ is a definite positive kernel. Different choices of kernel can be made such as a Gaussian kernel $\mathcal{K}(f, e) = \exp(-\|e - f\|_2^2)$ or an inverse kernel $\mathcal{K}(f, e) = \frac{1}{1+\|e-f\|_2^2}$ where $\|.\|_2$ is the Euclidean distance in the embedding space $\mathcal{E}$. Finally, we can compute a weighted soft visitation count $N_\mathcal{K}(M, e, \{w_l\}_{l=1}^{|M|}) = \sum_{l=1}^{|M|} w_l \mathcal{K}(f_l, e)$, where the weights $w_l \in \mathbb{R}_+$ are positive real numbers. Note that the vanilla visitation count can be recovered from the more general weighted soft visitation count as a special case by setting the weights $w_l = 1$ and $\mathcal{K} = \delta$.

Intrinsic Rewards from Visitation Counts. It is pretty straightforward to define an intrinsic reward from visitation counts. Indeed, as the goal of an exploratory agent is to go to less-visited states, then an intrinsic reward can be any decreasing function of the visitation counts. In the literature, the inverse of the square root of the visitation counts is known to be theoretically sound (Azar et al., 2017). Therefore, for a given time t, the intrinsic reward associated to the transition (o_t, a_t, o_{t+1}), is defined as:

$$r_{t+1} = \left(\sqrt{N_\mathcal{K}(M, e_{t+1}, \{w_l\}_{l=1}^{|M|})} + c\right)^{-1}, \tag{2}$$

where a small constant $c \in \mathbb{R}_+$ increases stability, $e_{t+1} = f_\theta(h_{t+1})$ and $h_{t+1} = \{o_0, a_0, \cdots, o_{t+1}\}$.

3 RECODE

In this section, we introduce our Robust Exploration via Clustering-based Online Density Estimation (RECODE) approach that computes intrinsic rewards for exploration. At a high level, RECODE stores a fixed number of weighted atoms (typically $5 \cdot 10^4$ or $2 \cdot 10^5$ depending on the domain) that are interpreted in the following as cluster-centers, along with their counts. The update rule of our memory M for each new embedding $e \in \mathcal{E}$ and the computation of the intrinsic reward are detailed in Algorithm. 1. To each atom/cluster-center $f_l \in \mathcal{E}$, we associate a count $c_l \in \mathbb{N}$ (all initialized to 0) that are updated after each new embedding e is observed. The update rule has a close connection to the DP-means algorithm of Kulis & Jordan (2011), with two key differences:

- the counts of the cluster-centers are discounted at each step, allowing our approach to deal with the non-stationarity of the data due both to changes in the policy and the embedding function, effectively reducing the weight of stale cluster-centers in the memory,

- when creating a new cluster-center, we remove an underpopulated one, so as to keep the size of the memory constant.

A theoretical analysis is sketched in Appendix C. To help build some intuition about the quality of our density estimation, we illustrate on Figure 1 the result of Algorithm 1 on a toy example with a non-stationary embedding distribution. We find in particular that tuning the discount allows to

---

Algorithm 1: RECODE

Input : Embedding e, Memory $M = \{f_l\}_{l=1}^{|M|}$, cluster-center counts $\{c_l\}_{i=l}^{|M|}$, number of neighbors k, relative tolerance κ, squared distance estimate d_m^2, decay rate τ, discount γ, insertion probability η, kernel function $\mathcal{K}$, intrinsic reward constant c

Output: Updated memory $M = \{f_l\}_{l=1}^{|M|}$, updated cluster-center counts $\{c_l\}_{i=l}^{|M|}$, updated squared distance d_m^2, intrinsic reward r

1 Compute weighted smoothed visitation-count of e: $\mathcal{N}_\mathcal{K}(M, e, \{1 + c_l\}_{l=1}^{|M|}) = \sum_{l=1}^{|M|} (1 + c_l)\, \mathcal{K}(f_l, e)$

2 Compute intrinsic reward $r = \left(\sqrt{\mathcal{N}_\mathcal{K}(M, e, \{1 + c_l\}_{l=1}^{|M|})} + c \right)^{-1}$

3 Find nearest k cluster centers to the embedding e: $N_k(e)$

4 Update squared distance estimate: $d_m^2 \leftarrow (1 - \tau)\, d_m^2 + \frac{\tau}{k} \sum_{f \in N_k(e)} \|e - f\|_2^2$

5 Discount all cluster-center counts $c_l \leftarrow \gamma\, c_l \quad \forall l \in \{1, \cdots, |M|\}$

6 Find index of nearest cluster center $i = \arg\min_{l=1\cdots|M|} \|f_l - e\|_2$

7 Sample uniformly a real number in $[0, 1]$: $u \sim U[0, 1]$

8 **if** $\|f_i - e\|_2^2 > \kappa\, d_m^2$ and $u < \eta$ **then**

10   Sample index j of cluster center to remove with probability $P(j) \propto 1/c_j^2$ // Remove under-populated cluster

11   Find index of nearest cluster center to f_j: $n = \arg\min_{l=1\cdots|M|, l \neq j} \|f_l - f_j\|_2$

12   Redistribute the count of removed cluster center: $c_n \leftarrow c_j + c_n$

13   Insert e at index j with count 1: $f_j \leftarrow e$, $c_j \leftarrow 1$ // Create a new cluster

15 **else**

16   Update nearest cluster center $f_i \leftarrow \frac{c_i}{c_i+1} f_i + \frac{1}{c_i+1} e$

17   Update nearest cluster-center count $c_i \leftarrow c_i + 1$

18 **end**

Figure 1: Density estimation using RECODE on a toy example: for step $t = 0, \ldots, 100$, we sample a batch of 64 2D-embeddings uniformly from the square of side $1 + \sqrt{t}$. The support of the embedding distribution therefore expands over time to simulate a non-stationary distribution akin to the distribution of states visited by an RL agent over the course of exploration. We plot the clusters learned by RECODE with a size proportional to their count. We find that for a small enough discount, RECODE exhibits a short-term memory, accurately approximating the distribution of the final distribution. As we increase the discount, RECODE exhibits a longer-term memory, approximating the historical density of states, as can be seen by the concentration of probability mass in the bottom-left corner.

smoothly interpolate between short-term and long-term memory, a property that will prove crucial to achieve the strong experimental results of Section 5.

Note that contrary to the usual episodic memory used in Badia et al. (2020b;a), the memory is never reset, and it is shared between all actors when using a distributed RL agent. We use the following kernel function defined for $(e, f) \in \mathcal{E}^2$ by:

$$\mathcal{K}(f, e) = \frac{\epsilon}{\epsilon + \frac{\|e - f\|_2^2}{d_m^2}} \, \mathbb{1}_{\left\{ \|e-f\|_2^2 < d_m^2 \right\}}, \tag{3}$$

where $\epsilon \in \mathbb{R}_+$, d_m^2 is an estimate of the squared distance between an embedding and its nearest neighbors in the memory (see Algorithm. 1)) and $\mathbb{1}_{\{.\}}$ is the indicator function. Compared to Badia et al. (2020b;a), our smoothed visitation-counts computes the normalized distances from a given embedding e to all its neighbors within a d_m^2-ball, instead of only the k-nearest neighbors. This change prevents some undesirable properties of the k-NN approach where inserting a cluster with

unit-count close to the embedding e might *reduce* its pseudo-count instead of increasing it if the k-th nearest neighbor of e had a large count.

We now detail how RECODE can be integrated in a typical distributed RL agent (Espeholt et al., 2018; Kapturowski et al., 2018) that comprises several processes that run in parallel and interact with each other. Classically, a Learner performs gradient steps to train a policy π_θ and an embedding (representation) function f_θ, forwarding the parameters θ to an Inference Worker. A collection of independent Actors query the inference worker for actions that they execute in the environment and send the resulting transitions to the Learner, optionally through a (prioritized) Replay (Mnih et al., 2015; Schaul et al., 2015). When using RECODE, the Actors additionally communicate with a shared Memory implementing Algorithm 1: at each step t, they query from the Inference Server an embedding $f_\theta(h_t)$ of their history and send it to the shared Memory which returns an intrinsic reward r_t that is then added to the extrinsic reward to train the policy in the Learner process. In practice, we normalize the intrinsic reward by a running estimate of its standard-deviation as in Burda et al. (2019). A diagram giving an overview of a distributed agent using RECODE is given in Fig. 10.

4   REPRESENTATION LEARNING METHODS

The Learner process uses the data sent by the actors to train the policy π_θ via an RL algorithm and to train the embedder f_θ via a representation learning loss. As noted in Section 2, the choice of the embedding function $f_\theta : \mathcal{H} \to \mathcal{E}$ induces a metric in the embedding space $\mathcal{E}$ allowing to compare histories. Many different representation learning techniques have been studied in the context of exploration in RL (Burda et al., 2018; Guo et al., 2020; 2022; 2021; Erraqabi et al., 2021). In the following, we focus on action prediction embeddings, introducing first the standard 1-step prediction formulation (Pathak et al., 2017; Badia et al., 2020b;a). Our embedding function f_θ is parameterized as a feed-forward neural network taking o_t, the observation at time t, as inputs. We further define a classifier g_ϕ that, given the embeddings of two consecutive observations $f_\theta(o_t), f_\theta(o_{t+1})$, outputs an estimate $p_{\theta,\phi}(a_t|o_t, o_{t+1}) = g_\phi\left(f_\theta(o_t), f_\theta(o_{t+1})\right)$ of the probability of taking an action given two consecutive observations (o_t, o_{t+1}). Both f_θ and g_ϕ are then jointly trained by minimizing an expectation of the following loss:

$$\min_{\theta,\phi} \mathcal{L}(\theta, \phi)(a_t) = -\ln(p_{\theta,\phi}(a_t|o_t, o_{t+1})), \tag{4}$$

where $\mathcal{L}(\theta, \phi)(a_t)$ is the negative log likelihood and a_t is the true action taken between o_t and o_{t+1}. These embeddings have been shown to be helpful in environment with many uncontrollable features in the observation (Badia et al., 2020b), such as the game of *Pitfall!* in Atari, where they might result in spurious sources of novelty even when the agent is standing still.

We note however that RECODE can be used with an arbitrary embedding function, e.g. one tailored for the domain of interest. One downside of the standard, 1-step action-prediction method is that the simplicity of the prediction task may only require highly localized and low-level features to be learned for its solution, which may not be informative of more geometrical or topological notions of environment structure, that partially-observable or 3D-exploration tasks might require. Other popular forms of representation learning such as Contrastive Predictive Coding (CPC, Oord et al. (2018)) or Predictions of Bootstrapped Latents (PBL, Guo et al. (2020)) utilize temporally-extended prediction tasks but do not enforce any notion of controllability. We now present a novel generalization of action-prediction embeddings that we show to yield strong results on DM-HARD-8 in section 5.

Perhaps the most straightforward generalization of 1-step action prediction is to predict sequences of actions between observations o_t and o_{t+k}, but in general there may be many such sequences which are possible, besides the one which is obtained by the behavior policy. This introduces an additional policy-dependent non-stationarity in the prediction task which could potentially hinder learning efficiency and stability. To counteract this problem we could instead provide as context the sequence $(o_t, a_t, a_{t+1} \ldots a_{t+k-2}, o_{t+k})$ for the prediction of a_{t+k-1}. However, in partially observed domains it is possible that these two observations alone are insufficient to accurately localize the agent's state, and therefore it may be beneficial to provide additional context before o_t or after o_{t+k}.

Concretely, we propose to apply a causally-masked transformer to sequences of observation and action embeddings, such that at each timestep t exactly one of o_t and a_t is provided. The transformer output is then projected down to the size of the embedding $f_\theta(o_t)$, and the difference between the

two is input into a final MLP classifier, g_ϕ. During training, we randomly sample $N = 4$ masks per trajectory to help reduce gradient variance. Note that we use $e_t = f_\theta(o_t)$, the transformer *inputs*, as the embeddings for RECODE in order to avoid leaking information about the agent's trajectory. As with 1-step action prediction, we train the representation using maximum likelihood. We refer to this approach as Coupled Action-State Masking (CASM) in the following. Figure 2 shows a diagram of the architecture.

Figure 2: Coupled Action-State Masking (CASM) architecture used for learning representations in partially observable environments. Note that masked inputs are shaded in pink.

5 EXPERIMENTS

In this section, we experimentally validate the generality of our approach by applying it to several domains with distinct properties. We first show that we can obtain state-of-the-art results on the hardest exploration games of the Atari domain, and even improve upon existing approaches when noise is added to the environment. We then turn to DM-HARD-8, a suite of partially-observable hard-exploration tasks, where we obtain results competitive with the recently proposed BYOL-Explore (Guo et al., 2022) agent. Unless otherwise noted, the agent we consider in this section is based on MEME (Kapturowski et al., 2022), a recent improvement over Agent57 (Badia et al., 2020a) that achieves much greater sample efficiency, and is the current state-of-the-art on Atari. Like its predecessors, MEME uses the NGU intrinsic reward, combining RND and Episodic Memory. We modify MEME by simply replacing the NGU reward by the simpler RECODE reward, and keep everything else fixed. We use a memory comprised of $5 \cdot 10^4$ atoms for our Atari experiments and $2 \cdot 10^5$ atoms for our DM-HARD-8 experiments. We find that the resulting agent runs at roughly the same speed as the original MEME agent. More hyperparameters values can be found in App A.

5.1 ATARI

The Atari Learning Environment (ALE, Bellemare et al., 2013) is one of the most used RL benchmarks for deep RL. It comprises 57 Atari games which are 2-D, fully-observable and (fairly) deterministic environments. In addition, they have a very long optimization horizon (episodes can last more than 10000 steps), complex observations (preprocessed greyscale images which are 210×160 byte arrays) but a fairly simple discrete action space composed of 18 actions. Among the 57 Atari games, only few games are considered hard-exploration games (Bellemare et al., 2016) such as Montezuma's Revenge, Pitfall and Private Eye. For evaluation, we follow the classical 30 random no-ops evaluation regime (Mnih et al., 2015; Van Hasselt et al., 2016), and average performance over 3 seeds. This evaluation regime does not use sticky actions (Machado et al., 2018).

We compare our approach with MEME and its ablations on 8 of the hardest exploration games on Fig. 3. We find that RECODE matches the performance of MEME with a single, simpler intrinsic reward, achieving super-human performance on all 8 hard exploration games. Indeed, as shown in the ablations reported in Appendix D, MEME requires both RND and episodic memory to solve all 8 games: RND on its own cannot solve Pitfall! because of the many uncontrollable features of its observations, while Episodic Memory on its own cannot solve Montezuma's Revenge because it requires long-term memory. Because RECODE estimates the visitation counts over many episodes

Figure 3: Comparison of `RECODE` and `MEME` on 8 hard exploration games from the Atari domain.

Figure 4: Distribution of the age of the clusters learned by `RECODE` on Montezuma's Revenge in terms of actor steps. We set $\gamma = 0.999$ as in the experiments of Figure 3. We indicate in red the average length of an episode, showing that in this setting that achieves high scores, `RECODE`'s memory reaches back thousands of episodes.

using Action Prediction embeddings that discard uncontrollable dynamics, it is able to solve both games with a single intrinsic reward. We probe how far back the memory of `RECODE` goes in Montezuma's Revenge in Figure 4 and find that the distribution of the age of the clusters learned by `RECODE` exhibits a mode around $2 \cdot 10^6$ actor steps, which corresponds to hundreds of episodes, with a significant number of clusters ten times older than that. In Appendix D, we also compare our approach with a modification of `RND` built on top of Action Prediction embeddings, in an attempt to fix the aforementioned undesirable properties of `RND`. We find that this approach does not allow to solve some of the hardest games such as Montezuma's Revenge or Pitfall!. One possible explanation of this failure is the fact that a large `RND` error can be caused by either the observation of a new state, or a drift in the representation of an already observed one. The failure of `RND` to disentangle these two effects results in poor exploration.

5.2 NOISY MONTEZUMA'S REVENGE

Atari Games are known to be fairly deterministic which is not a property commonly encountered in real-world environments which have noisy observations due to imperfect sensors. As `RND` relies on predicting a random embedding of the pixel observation to determine whether a state is new or not, it cannot learn to discard noisy features, hindering its ability to detect meaningful novelty in the presence of noise. In this section, we show that `MEME` inherits the limitations of `RND`. To this end, we consider the game of Montezuma's Revenge, for which effective exploration requires long-term memory as shown by the ablations of Section 5.1. We challenge `RND` by concatenating the original grey-scale, 210×160 pixels frame with a noisy frame of the same shape, where each pixel is sampled uniformly at random from the range $[0, 255]$. This type of noise is commonly referred to as noisy TV (Pathak et al., 2017).

Figure 5: (Left) : Performance of `RECODE` compared to `MEME` on Noisy Montezuma. (Middle and Right:) A frame of Noisy Montezuma where the noise is concatenated to the original frame.

The results of our experiments on this environment are presented on Figure 5. Perhaps as expected, we find that the performance of `MEME` is strongly deteriorated, since it relies on `RND` to build its exploration bonus, and reduced to that of a pure RL baseline without exploration bonus (Kapturowski et al., 2018). `RECODE`, on the other hand, relies on action-prediction embeddings to estimate the visitation-counts. In this embedding space, states that only differ in the noisy, uncontrollable part of the observation tend to be aliased together, so that the effect of the noise on exploration vanishes. Indeed, the performance of `RECODE` on Montezuma's Revenge is unchanged when adding noise.

5.3 `DM-HARD-8`

`DM-HARD-8` (Gulcehre et al., 2019) is a benchmark comprised of 8 hard exploration tasks, originally built to emphasize the difficulties encountered by an RL agent when learning from sparse rewards in a procedurally-generated 3-D world with partial observability, continuous control, and highly variable initial conditions. Each task requires the agent to interact with specific objects in its environment in order to reach a large apple that provides reward (see Figure 11 for an example). Being procedurally-generated, properties such as object shapes, colors, and positions are different every episode. A recently proposed approach called BYOL-Explore (Guo et al., 2022) was shown to be effective on this domain, while previous successes were only achieved through the use of human demonstrations (Gulcehre et al., 2019).

We first assess the effect of using the `RECODE` bonus over the `NGU` one by performing a drop-in replacement of the intrinsic reward in `MEME` as in Section 5. We consider the performance of the resulting agent in the single-task version of `DM-HARD-8` since `MEME` is not designed to work in the multi-task setting out-of-the-box. The results, presented on Fig. 6, show that our approach can solve 4 out of 8 games, largely improving over `MEME` or Episodic Memory in this direct comparison. Second, we turn to using the `CASM` approach introduced in Section 4 as our embedding. We find that the resulting agent attains state-of-the-art results on the `DM-HARD-8` benchmark, reliably solving 6 out of 8 games, and improving over the performance of BYOL-explore. Finally, to demonstrate the generality of our approach, we implemented `RECODE` with standard action-prediction embeddings in a VMPO-based agent similar to that used in Guo et al. (2022) and evaluate in the multi-task setting. The resulting agent reliably solves 4 games with zero additional tuning (App. F), matching the result obtained with Human Demonstrations in Gulcehre et al. (2019).

6 CONCLUSION AND DISCUSSION

We have introduced Robust Exploration via Clustering-based Online Density Estimation (`RECODE`), a principled yet simple exploration bonus for deep Reinforcement Learning (RL) agents that allows to perform robust exploration by computing visitation counts from a slot-based memory. Contrary to previous work, where the memory was short-term (i.e. only able to attend to the current episode due to memory limit), our memory is able to model a wide range of timescales determined by the

Figure 6: Performance of `RECODE` compared to `MEME` on the single-task version of `DM-HARD-8`.

Figure 7: Performance of `RECODE` using `CASM` embeddings compared to BYOL-Explore on the single-task version of `DM-HARD-8`. The BYOL-Explore results correspond to the final performance reported in Guo et al. (2022), after 10^9 environment frames, averaged over 3 seeds.

choice of discount. This is made possible by the use of an online clustering algorithm that is able to approximate the density of visited states and from which we derive a simple intrinsic reward.

We evaluate our exploration bonus on top of the recent `MEME` agent, which is a value-based agent making use of the `NGU` intrinsic reward, that achieves state-of-the-art results on the Atari domain. We show that we can replace the complex `NGU` intrinsic reward that combines `RND` and episodic memory with the simpler `RECODE` reward without loss of performance on the hardest exploration levels in Atari. Furthermore, we highlight some important failure modes of `NGU` in the presence of noise, and show that `RECODE`'s performance is unaffected. Similarly, we highlight the limitations of `NGU` in procedurally-generated 3D environments such as `DM-HARD-8`, and demonstrate the improvements brought by using `RECODE` as an intrinsic reward. Next we introduce a novel representation learning method better suited to 3D and partially observable domains, which provides a significant boost in performance on this task suite, enabling to achieve a new state-of-the-art on `DM-HARD-8` in the single-task setting.

Importantly we note that `RECODE` is agnostic to the choice of embeddings $f_\theta(h_t)$, and while `CASM` presents one compelling option to extend 1-step action prediction, we hypothesize that much progress could be made in challenging exploration problems by developing more sophisticated representations which can be used in conjunction with `RECODE`.

REFERENCES

Shipra Agrawal and Navin Goyal. Analysis of thompson sampling for the multi-armed bandit problem. In *Conference on learning theory*, pp. 39–1. JMLR Workshop and Conference Proceedings, 2012.

Jean-Yves Audibert, Sébastien Bubeck, and Rémi Munos. Best arm identification in multi-armed bandits. In *COLT*, pp. 41–53. Citeseer, 2010.

Peter Auer, Nicolo Cesa-Bianchi, and Paul Fischer. Finite-time analysis of the multiarmed bandit problem. *Machine learning*, 47(2):235–256, 2002.

Mohammad Gheshlaghi Azar, Ian Osband, and Rémi Munos. Minimax regret bounds for reinforcement learning. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pp. 263–272. JMLR. org, 2017.

Adrià Puigdomènech Badia, Bilal Piot, Steven Kapturowski, Pablo Sprechmann, Alex Vitvitskyi, Zhaohan Daniel Guo, and Charles Blundell. Agent57: Outperforming the atari human benchmark. In *International Conference on Machine Learning*, pp. 507–517. PMLR, 2020a.

Adrià Puigdomènech Badia, Pablo Sprechmann, Alex Vitvitskyi, Daniel Guo, Bilal Piot, Steven Kapturowski, Olivier Tieleman, Martin Arjovsky, Alexander Pritzel, Andrew Bolt, and Charles Blundell. Never give up: Learning directed exploration strategies. In *International Conference on Learning Representations*, 2020b.

André MS Barreto, Doina Precup, and Joelle Pineau. Practical kernel-based reinforcement learning. *The Journal of Machine Learning Research*, 17(1):2372–2441, 2016.

Marc Bellemare, Joel Veness, and Erik Talvitie. Skip context tree switching. In *International conference on machine learning*, pp. 1458–1466. PMLR, 2014.

Marc Bellemare, Sriram Srinivasan, Georg Ostrovski, Tom Schaul, David Saxton, and Remi Munos. Unifying count-based exploration and intrinsic motivation. In *Advances in neural information processing systems*, pp. 1471–1479, 2016.

Marc G Bellemare, Yavar Naddaf, Joel Veness, and Michael Bowling. The arcade learning environment: An evaluation platform for general agents. *Journal of Artificial Intelligence Research*, 47: 253–279, 2013.

Ronen Brafman and Moshe Tennenholtz. R-max – a general polynomial time algorithm for near-optimal reinforcement learning. *Journal of Machine Learning Research*, 3:213–231, 2003.

Yuri Burda, Harri Edwards, Deepak Pathak, Amos Storkey, Trevor Darrell, and Alexei A Efros. Large-scale study of curiosity-driven learning. *arXiv preprint arXiv:1808.04355*, 2018.

Yuri Burda, Harrison Edwards, Amos Storkey, and Oleg Klimov. Exploration by random network distillation. In *Seventh International Conference on Learning Representations*, pp. 1–17, 2019.

Mayank Daswani, Peter Sunehag, and Marcus Hutter. Q-learning for history-based reinforcement learning. In *Asian Conference on Machine Learning*, pp. 213–228. PMLR, 2013.

Omar Darwiche Domingues, Pierre Menard, Matteo Pirotta, Emilie Kaufmann, and Michal Valko. Kernel-based reinforcement learning: A finite-time analysis. In *Proceedings of the 38th International Conference on Machine Learning*, volume 139 of *Proceedings of Machine Learning Research*, pp. 2783–2792. PMLR, 2021a.

Omar Darwiche Domingues, Corentin Tallec, Rémi Munos, and Michal Valko. Density-based bonuses on learned representations for reward-free exploration in deep reinforcement learning. In *ICML 2021 Workshop*, 2021b.

Akram Erraqabi, Mingde Zhao, Marlos C Machado, Yoshua Bengio, Sainbayar Sukhbaatar, Ludovic Denoyer, and Alessandro Lazaric. Exploration-driven representation learning in reinforcement learning. In *ICML 2021 Workshop on Unsupervised Reinforcement Learning*, 2021.

Lasse Espeholt, Hubert Soyer, Remi Munos, Karen Simonyan, Vlad Mnih, Tom Ward, Yotam Doron, Vlad Firoiu, Tim Harley, Iain Dunning, et al. Impala: Scalable distributed deep-rl with importance weighted actor-learner architectures. In *International conference on machine learning*, pp. 1407–1416. PMLR, 2018.

Caglar Gulcehre, Tom Le Paine, Bobak Shahriari, Misha Denil, Matt Hoffman, Hubert Soyer, Richard Tanburn, Steven Kapturowski, Neil Rabinowitz, Duncan Williams, et al. Making efficient use of demonstrations to solve hard exploration problems. In *International conference on learning representations*, 2019.

Zhaohan Daniel Guo, Bernardo Avila Pires, Bilal Piot, Jean-Bastien Grill, Florent Altché, Rémi Munos, and Mohammad Gheshlaghi Azar. Bootstrap latent-predictive representations for multi-task reinforcement learning. In *International Conference on Machine Learning*, pp. 3875–3886. PMLR, 2020.

Zhaohan Daniel Guo, Mohammad Gheshlagi Azar, Alaa Saade, Shantanu Thakoor, Bilal Piot, Bernardo Avila Pires, Michal Valko, Thomas Mesnard, Tor Lattimore, and Rémi Munos. Geometric entropic exploration. *arXiv preprint arXiv:2101.02055*, 2021.

Zhaohan Daniel Guo, Shantanu Thakoor, Miruna Pîslar, Bernardo Avila Pires, Florent Altché, Corentin Tallec, Alaa Saade, Daniele Calandriello, Jean-Bastien Grill, Yunhao Tang, et al. Byol-explore: Exploration by bootstrapped prediction. *arXiv preprint arXiv:2206.08332*, 2022.

Elad Hazan, Sham Kakade, Karan Singh, and Abby Van Soest. Provably efficient maximum entropy exploration. In *International Conference on Machine Learning*, pp. 2681–2691, 2019.

Marcus Hutter. *Universal artificial intelligence: Sequential decisions based on algorithmic probability*. Springer Science & Business Media, 2004.

Marcus Hutter et al. *Feature reinforcement learning: Part I. unstructured MDPs*. De Gruyter Open, 2009.

Thomas Jaksch, Ronald Ortner, and Peter Auer. Near-optimal regret bounds for reinforcement learning. *Journal of Machine Learning Research*, 11(Apr):1563–1600, 2010.

Chi Jin, Akshay Krishnamurthy, Max Simchowitz, and Tiancheng Yu. Reward-free exploration for reinforcement learning. In *International Conference on Machine Learning*, pp. 4870–4879. PMLR, 2020.

Steven Kapturowski, Georg Ostrovski, John Quan, Remi Munos, and Will Dabney. Recurrent experience replay in distributed reinforcement learning. In *International conference on learning representations*, 2018.

Steven Kapturowski, Víctor Campos, Ray Jiang, Nemanja Rakićević, Hado van Hasselt, Charles Blundell, and Adrià Puigdomènech Badia. Human-level atari 200x faster. *arXiv preprint arXiv:2209.07550*, 2022.

Michael Kearns and Satinder Singh. Near-optimal reinforcement learning in polynomial time. *Machine learning*, 49(2-3):209–232, 2002.

Brian Kulis and Michael I Jordan. Revisiting k-means: New algorithms via bayesian nonparametrics. *arXiv preprint arXiv:1111.0352*, 2011.

Branislav Kveton and Georgios Theocharous. Kernel-based reinforcement learning on representative states. In *Twenty-Sixth AAAI Conference on Artificial Intelligence*, 2012.

Tor Lattimore and Csaba Szepesvári. *Bandit algorithms*. Cambridge University Press, 2020.

Lisa Lee, Benjamin Eysenbach, Emilio Parisotto, Eric Xing, Sergey Levine, and Ruslan Salakhutdinov. Efficient exploration via state marginal matching. *arXiv preprint arXiv:1906.05274*, 2019.

Hao Liu and Pieter Abbeel. Behavior from the void: Unsupervised active pre-training. *Advances in Neural Information Processing Systems*, 34:18459–18473, 2021.

Marlos C Machado, Marc G Bellemare, Erik Talvitie, Joel Veness, Matthew Hausknecht, and Michael Bowling. Revisiting the arcade learning environment: Evaluation protocols and open problems for general agents. *Journal of Artificial Intelligence Research*, 61:523–562, 2018.

R Andrew McCallum. Instance-based utile distinctions for reinforcement learning with hidden state. In *Machine Learning Proceedings 1995*, pp. 387–395. Elsevier, 1995.

Volodymyr Mnih, Koray Kavukcuoglu, David Silver, Andrei A Rusu, Joel Veness, Marc G Bellemare, Alex Graves, Martin Riedmiller, Andreas K Fidjeland, Georg Ostrovski, et al. Human-level control through deep reinforcement learning. *nature*, 518(7540):529–533, 2015.

Aaron van den Oord, Yazhe Li, and Oriol Vinyals. Representation learning with contrastive predictive coding. *arXiv preprint arXiv:1807.03748*, 2018.

Dirk Ormoneit and Śaunak Sen. Kernel-based reinforcement learning. *Machine Learning*, 2002.

Georg Ostrovski, Marc G Bellemare, Aäron van den Oord, and Rémi Munos. Count-based exploration with neural density models. In *Proceedings of the 34th International Conference on Machine Learning-Volume 70*, pp. 2721–2730. JMLR. org, 2017.

Emanuel Parzen. On estimation of a probability density function and mode. *The Annals of Mathematical Statistics*, 33, 1962. ISSN 0003-4851. doi: 10.1214/aoms/1177704472.

Deepak Pathak, Pulkit Agrawal, Alexei A Efros, and Trevor Darrell. Curiosity-driven exploration by self-supervised prediction. In *Proceedings of the IEEE Conference on Computer Vision and Pattern Recognition Workshops*, pp. 16–17, 2017.

Jason Pazis and Ronald Parr. Pac optimal exploration in continuous space markov decision processes. In *Twenty-Seventh AAAI Conference on Artificial Intelligence*, 2013.

Vitchyr H Pong, Murtaza Dalal, Steven Lin, Ashvin Nair, Shikhar Bahl, and Sergey Levine. Skewfit: State-covering self-supervised reinforcement learning. *arXiv preprint arXiv:1903.03698*, 2019.

Martin L Puterman. Markov decision processes. *Handbooks in operations research and management science*, 2:331–434, 1990.

Murray Rosenblatt. Remarks on some nonparametric estimates of a density function. *The Annals of Mathematical Statistics*, 27, 1956. ISSN 0003-4851. doi: 10.1214/aoms/1177728190.

Tom Schaul, John Quan, Ioannis Antonoglou, and David Silver. Prioritized experience replay. *CoRR*, abs/1511.05952, 2015.

Younggyo Seo, Lili Chen, Jinwoo Shin, Honglak Lee, Pieter Abbeel, and Kimin Lee. State entropy maximization with random encoders for efficient exploration. In *International Conference on Machine Learning*, pp. 9443–9454. PMLR, 2021.

Alexander L Strehl and Michael L Littman. An analysis of model-based interval estimation for markov decision processes. *Journal of Computer and System Sciences*, 74(8):1309–1331, 2008.

Richard S Sutton and Andrew G Barto. *Reinforcement learning: An introduction*. MIT press, 2018.

Haoran Tang, Rein Houthooft, Davis Foote, Adam Stooke, OpenAI Xi Chen, Yan Duan, John Schulman, Filip DeTurck, and Pieter Abbeel. #Exploration: A study of count-based exploration for deep reinforcement learning. In *Advances in Neural Information Processing Systems*, 2017. URL https://proceedings.neurips.cc/paper/2017/file/3a20f62a0af1aa152670bab3c602feed-Paper.pdf.

Ruo Yu Tao, Vincent François-Lavet, and Joelle Pineau. Novelty search in representational space for sample efficient exploration. *Advances in Neural Information Processing Systems*, 33:8114–8126, 2020.

Aaron Van den Oord, Nal Kalchbrenner, Lasse Espeholt, Oriol Vinyals, Alex Graves, et al. Conditional image generation with pixelcnn decoders. *Advances in neural information processing systems*, 29, 2016.

Hado Van Hasselt, Arthur Guez, and David Silver. Deep reinforcement learning with double q-learning. In *Proceedings of the AAAI conference on artificial intelligence*, volume 30, 2016.