IMPROVING POLICY GRADIENT BY EXPLORING UNDER-APPRECIATED REWARDS

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ABSTRACT

This paper presents a novel form of policy gradient for model-free reinforcement learning (RL) with improved exploration properties. Current policy-based methods use entropy regularization to encourage undirected exploration of the reward landscape, which is ineffective in high dimensional spaces with sparse rewards. We propose a more directed exploration strategy that promotes exploration of *under-appreciated reward* regions. An action sequence is considered under-appreciated if its log-probability under the current policy under-estimates its resulting reward. The proposed exploration strategy is easy to implement, requiring small modifications to an implementation of the REINFORCE algorithm. We evaluate the approach on a set of algorithmic tasks that have long challenged RL methods. Our approach reduces hyper-parameter sensitivity and demonstrates significant improvements over baseline methods. Our algorithm successfully solves a benchmark multi-digit addition task and generalizes to long sequences. This is, to our knowledge, the first time that a pure RL method has solved addition using only reward feedback.

1 INTRODUCTION

Humans can reason about symbolic objects and solve algorithmic problems. After learning to count and then manipulate numbers via simple arithmetic, people eventually learn to invent new algorithms and even reason about their correctness and efficiency. The ability to invent new algorithms is fundamental to artificial intelligence (AI). Although symbolic reasoning has a long history in AI (Russell et al., 2003), only recently have statistical machine learning and neural network approaches begun to make headway in automated algorithm discovery (Reed & de Freitas, 2016; Kaiser & Sutskever, 2016; Neelakantan et al., 2016) heading to cross an important milestone on the path to AI. Nevertheless, most of the recent successes depend on the use of strong supervision to learn a mapping from a set of training inputs to outputs by maximizing a conditional log-likelihood, very much like neural machine translation systems (Sutskever et al., 2014; Bahdanau et al., 2015). Such a dependence on strong supervision is a significant limitation that does not match the ability of people to invent new algorithmic procedures based solely on trial and error.

By contrast, *reinforcement learning (RL)* methods (Sutton & Barto, 1998) hold the promise of searching over discrete objects such as symbolic representations of algorithms by considering much weaker feedback in the form of a simple verifier that tests the correctness of a program execution on a given problem instance. Despite the recent excitement around the use of RL to tackle Atari games (Mnih et al., 2015) and Go (Silver et al., 2016), standard RL methods are not yet able to consistently and reliably solve algorithmic tasks in all but the simplest cases (Zaremba & Sutskever, 2014). A key property of algorithmic problems that makes them challenging for RL is *reward sparsity*, *i.e.,* a policy usually has to get a long action sequence exactly right to obtain a non-zero reward.

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We believe one of the key limitations of the current RL methods, preventing them from making much progress in the sparse reward settings, is the use of *undirected exploration* strategies (Thrun, 1992), such as ϵ-greedy and entropy regularization (Williams & Peng, 1991). For long action sequences with delayed sparse reward, it is hopeless to explore the space uniformly and blindly. Instead, we propose a formulation to encourage exploration of action sequences that are *under-appreciated* by the current policy. We consider an action sequence to be under-appreciated if the model's log-probability assigned to an action sequence under-estimates the resulting reward from the action sequence. Exploring under-appreciated states and actions encourages the policy to have a better calibration between its log-probabilities and observed reward values, even for action sequences with negligible rewards. This effectively increases exploration around neglected action sequences.

We term our proposed technique *under-appreciated reward exploration (UREX)*. We show that the objective given by UREX is a combination of a mode seeking objective (standard REINFORCE) and a mean seeking term, which provides a good trade-off between exploitation and exploration. We apply the method to recurrent neural network (RNN)-based RL agents tackling algorithmic tasks such as sequence reversal, multi-digit addition, and binary search. The experiments demonstrate that UREX significantly outperforms baseline RL methods, such as entropy regularized REINFORCE and one-step Q-learning, especially on the seemingly more difficult tasks, such as multi-digit addition. Moreover, UREX is shown to be more robust to changes of hyper-parameters, which makes hyper-parameter tuning less tedious in practice. To our knowledge, the addition task has not been solved by any pure reinforcement learning approach. We observe that some of the policies learned by UREX can successfully generalize to long sequences; *e.g.,* in 2 out of 5 random restarts, the policy learned by UREX for the addition task correctly generalizes to addition of numbers with 2000 digits with no mistakes, even though training sequences are at most 33 digits long.

2 Neural Networks for Learning Algorithms

Although research on using neural networks to learn algorithms has had a surge of recent interest, the problem of program induction from examples has a long history in many fields, including program induction, inductive logic programming (Lavrac & Dzeroski, 1994), relational learning (Kemp et al., 2007) and regular language learning (Angulin, 1987). Rather than presenting a comprehensive survey of program induction here, we focus on neural network approaches to algorithmic tasks and highlight the relative simplicity of our neural network architecture.

Most successful applications of neural networks to algorithmic tasks rely on strong supervision, where the inputs and target outputs are completely known *a priori*. Given a dataset of examples, one learns the network parameters by maximizing the conditional likelihood of the outputs via backpropagation (*e.g.,* Reed & de Freitas (2016); Kaiser & Sutskever (2016); Vinyals et al. (2015)). However, target outputs may not be available for novel tasks, for which no algorithm exists yet. A more desirable approach to inducing algorithms, followed in this paper, advocates using self-driven learning strategies that only receive reinforcement based on the outputs produced. Hence, just by having access to a verifier for an algorithmic problem, one can aim to learn an algorithm. For example, if one does not know how to sort an array, but can check the extent to which an array is sorted, then one can provide the reward signal necessary for learning sorting algorithms.

We formulate learning algorithms as an RL problem and make use of model-free policy gradient methods to optimize a set parameters associated with the algorithm. In this setting, the goal is to learn a policy π_θ that given an observed state $\mathbf{s}_t$ at step t, estimates a distribution over the next action $\mathbf{a}_t$, denoted $\pi_\theta(\mathbf{a}_t \mid \mathbf{s}_t)$. Actions represent the commands within the algorithm and states represent the joint state of the algorithm and the environment. Previous work in this area has focused on augmenting a neural network with additional structure and increased capabilities (Zaremba & Sutskever, 2015; Graves et al., 2016). In contrast, we utilize a simple architecture based on a standard recurrent neural network (RNN) with LSTM cells (Hochreiter & Schmidhuber, 1997) as depicted in Figure 1. At each episode, the environment is initialized with a latent state $\mathbf{h}$, unknown to the agent, which determines $\mathbf{s}_1$ and the subsequent state transition and reward functions. Once the agent observes $\mathbf{s}_1$ as the input to the RNN, the network outputs a distribution $\pi_\theta(\mathbf{a}_1 \mid \mathbf{s}_1)$, from which an action $\mathbf{a}_1$ is sampled. This action is applied to the environment, and the agent receives a new state observation $\mathbf{s}_2$. The state $\mathbf{s}_2$ and the previous action $\mathbf{a}_1$ are then fed into the RNN and the process repeats until the end of the episode. Upon termination, a reward signal is received.

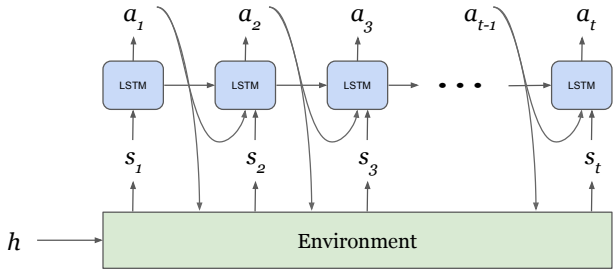

Figure 1: The agent's RNN architecture that represents a policy. The environment is initialized with a latent vector $\mathbf{h}$. At time step t, the environment produces a state $\mathbf{s}_t$, and the agent takes as input $\mathbf{s}_t$ and the previously sampled action $\mathbf{a}_{t-1}$ and produces a distribution over the next action $\pi_\theta(\mathbf{a}_t \mid \mathbf{s}_t)$. Then, we sample a new action $\mathbf{a}_t$ and apply it to the environment.

3 Learning a Policy by Maximizing Expected Reward

We start by discussing the most common form of policy gradient, REINFORCE (Williams, 1992), and its entropy regularized variant (Williams & Peng, 1991). REINFORCE has been applied to model-free policy-based learning with neural networks and algorithmic domains (Zaremba & Sutskever, 2015; Graves et al., 2016).

As mentioned above, we aim to learn a policy π_θ that given an observed state $\mathbf{s}_t$ at step t, estimates a distribution over the next action $\mathbf{a}_t$, denoted $\pi_\theta(\mathbf{a}_t \mid \mathbf{s}_t)$. The environment is initialized with a latent vector, $\mathbf{h}$, which determines the initial observed state $\mathbf{s}_1 = g(\mathbf{h})$, and the transition function $\mathbf{s}_{t+1} = f(\mathbf{s}_t, \mathbf{a}_t \mid \mathbf{h})$. Given a latent state $\mathbf{h}$, and $\mathbf{s}_{1:T} \equiv (\mathbf{s}_1, \ldots, \mathbf{s}_T)$, the model probability of an action sequence $\mathbf{a}_{1:T} \equiv (\mathbf{a}_1, \ldots, \mathbf{a}_T)$ is expressed as,

$$\pi_\theta(\mathbf{a}_{1:T} \mid \mathbf{h}) = \prod_{t=1}^{T} \pi_\theta(\mathbf{a}_t \mid \mathbf{s}_t) \;, \quad \text{where} \quad \mathbf{s}_1 = g(\mathbf{h}), \;\; \mathbf{s}_{t+1} = f(\mathbf{s}_t, \mathbf{a}_t \mid \mathbf{h}) \;\; \text{for} \;\; 1 \leq t < T \;.$$

The environment provides a reward at the end of the episode, denoted $r(\mathbf{a}_{1:T} \mid \mathbf{h})$. For ease of readability we drop the subscript from $\mathbf{a}_{1:T}$ and simply write $\pi_\theta(\mathbf{a} \mid \mathbf{h})$ and $r(\mathbf{a} \mid \mathbf{h})$.

The objective used to optimize the policy parameters, $\boldsymbol{\theta}$, consists of maximizing expected reward under actions drawn from the policy, plus an optional maximum entropy regularizer. Given a distribution over initial latent environment states $p(\mathbf{h})$, we express the regularized expected reward as,

$$\mathcal{O}_{\text{RL}}(\boldsymbol{\theta}; \tau) = \mathbb{E}_{\mathbf{h} \sim p(\mathbf{h})} \left\{ \sum_{\mathbf{a} \in \mathcal{A}} \pi_\theta(\mathbf{a} \mid \mathbf{h}) \Big[r(\mathbf{a} \mid \mathbf{h}) - \tau \log \pi_\theta(\mathbf{a} \mid \mathbf{h}) \Big] \right\} . \tag{1}$$

When π_θ is a non-linear function defined by a neural network, finding the global optimum of $\boldsymbol{\theta}$ is challenging, and one often resorts to gradient-based methods to find a local optimum of $\mathcal{O}_{\text{RL}}(\boldsymbol{\theta}; \tau)$. Given that $\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \pi_\theta(\mathbf{a}) = \pi_\theta(\mathbf{a}) \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \log \pi_\theta(\mathbf{a})$ for any $\mathbf{a}$ such that $\pi_\theta(\mathbf{a}) > 0$, one can verify that,

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \mathcal{O}_{\text{RL}}(\boldsymbol{\theta}; \tau \mid \mathbf{h}) = \sum_{\mathbf{a} \in \mathcal{A}} \pi_\theta(\mathbf{a} \mid \mathbf{h}) \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \log \pi_\theta(\mathbf{a} \mid \mathbf{h}) \Big[r(\mathbf{a} \mid \mathbf{h}) - \tau \log \pi_\theta(\mathbf{a} \mid \mathbf{h}) - \tau \Big] . \tag{2}$$

Because the space of possible actions $\mathcal{A}$ is large, enumerating over all of the actions to compute this gradient is infeasible. Williams (1992) proposed to compute the stochastic gradient of the expected reward by using Monte Carlo samples. Using Monte Carlo samples, one first draws N *i.i.d.* samples from the latent environment states $\{\mathbf{h}^{(n)}\}_{n=1}^{N}$, and then draws K *i.i.d.* samples $\{\mathbf{a}^{(k)}\}_{k=1}^{K}$ from $\pi_\theta(\mathbf{a} \mid \mathbf{h}^{(n)})$ to approximate the gradient of (1) by using (2) as,

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \mathcal{O}_{\text{RL}}(\boldsymbol{\theta}; \tau) \approx \frac{1}{NK} \sum_{n=1}^{N} \sum_{k=1}^{K} \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \log \pi_\theta(\mathbf{a}^{(k)} \mid \mathbf{h}^{(n)}) \Big[r(\mathbf{a}^{(k)} \mid \mathbf{h}^{(n)}) - \tau \log \pi_\theta(\mathbf{a}^{(k)} \mid \mathbf{h}^{(n)}) - \tau \Big] . \tag{3}$$

This reparametrization of the gradients is the key to the REINFORCE algorithm. To reduce the variance of (3), one uses rewards $\widehat{r}$ that are shifted by some offset values,

$$\widehat{r}(\mathbf{a}^{(k)} \mid \mathbf{h}) = r(\mathbf{a}^{(k)} \mid \mathbf{h}) - b(\mathbf{h}) \,, \tag{4}$$

where b is known as a *baseline* or sometimes called a *critic*. Note that subtracting any offset from the rewards in (1) simply results in shifting the objective $\mathcal{O}_{\mathrm{RL}}$ by a constant.

Unfortunately, directly maximizing expected reward (*i.e.,* when $\tau = 0$) is prone to getting trapped in a local optimum. To combat this tendency, Williams & Peng (1991) augmented the expected reward objective by including a maximum entropy regularizer ($\tau > 0$) to promote greater exploration. We will refer to this variant of REINFORCE as MENT (maximum entropy exploration).

4 Under-appreciated Reward Exploration (UREX)

To explain our novel form of policy gradient, we first note that the optimal policy π^*_τ, which globally maximizes $\mathcal{O}_{\mathrm{RL}}(\boldsymbol{\theta}; \tau \mid \mathbf{h})$ in (1) for any $\tau > 0$, can be expressed as,

$$\pi^*_\tau(\mathbf{a} \mid \mathbf{h}) = \frac{1}{Z(\mathbf{h})} \exp\left\{\frac{1}{\tau} r(\mathbf{a} \mid \mathbf{h})\right\} , \tag{5}$$

where $Z(\mathbf{h})$ is a normalization constant making π^*_τ a distribution over the space of action sequences $\mathcal{A}$. One can verify this by first acknowledging that,

$$\mathcal{O}_{\mathrm{RL}}(\boldsymbol{\theta}; \tau \mid \mathbf{h}) = -\tau \, D_{\mathrm{KL}}\left(\pi_\theta(\cdot \mid \mathbf{h}) \parallel \pi^*_\tau(\cdot \mid \mathbf{h})\right) \,. \tag{6}$$

Since $D_{\mathrm{KL}}\left(p \parallel q\right)$ is non-negative and zero iff $p = q$, then π^*_τ defined in (5) maximizes $\mathcal{O}_{\mathrm{RL}}$. That said, given a particular form of π_θ, finding θ that exactly characterizes π^*_τ may not be feasible.

The KL divergence $D_{\mathrm{KL}}\left(\pi_\theta \parallel \pi^*_\tau\right)$ is known to be mode seeking (Murphy, 2012, Section 21.2.2) even with entropy regularization ($\tau > 0$). Learning a policy by optimizing this direction of the KL is prone to falling into a local optimum resulting in a sub-optimal policy that omits some of the modes of π^*_τ. Although entropy regularization helps mitigate the issues as confirmed in our experiments, it is not an effective exploration strategy as it is undirected and requires a small regularization coefficient τ to avoid too much random exploration. Instead, we propose a directed exploration strategy that improves the mean seeking behavior of policy gradient in a principled way.

We start by considering the alternate mean seeking direction of the KL divergence, $D_{\mathrm{KL}}\left(\pi^*_\tau \parallel \pi_\theta\right)$. Norouzi et al. (2016) considered this direction of the KL to directly learn a policy by optimizing

$$\mathcal{O}_{\mathrm{RML}}(\boldsymbol{\theta}; \tau) = \mathbb{E}_{\mathbf{h} \sim p(\mathbf{h})}\left\{\tau \sum_{\mathbf{a} \in \mathcal{A}} \pi^*_\tau(\mathbf{a} \mid \mathbf{h}) \log \pi_\theta(\mathbf{a} \mid \mathbf{h})\right\} , \tag{7}$$

for structured prediction. This objective has the same optimal solution π^*_τ as $\mathcal{O}_{\mathrm{RL}}$ since,

$$\mathcal{O}_{\mathrm{RML}}(\boldsymbol{\theta}; \tau \mid \mathbf{h}) = -\tau \, D_{\mathrm{KL}}\left(\pi^*_\tau(\cdot \mid \mathbf{h}) \parallel \pi_\theta(\cdot \mid \mathbf{h})\right) + \text{const} \,. \tag{8}$$

Norouzi et al. (2016) argue that in some structured prediction problems when one can draw samples from π^*_τ, optimizing (7) is more effective than (1), since no sampling from a non-stationary policy π_θ is required. If π_θ is a log-linear model of a set of features, $\mathcal{O}_{\mathrm{RML}}$ is convex in $\boldsymbol{\theta}$ whereas $\mathcal{O}_{\mathrm{RL}}$ is not, even in the log-linear case. Unfortunately, in scenarios that the reward landscape is unknown or computing the normalization constant $Z(\mathbf{h})$ is intractable, sampling from π^*_τ is not straightforward.

In the RL problems, the reward landscape is completely unknown, hence sampling from π^*_τ is intractable. This paper proposes to approximate the expectation with respect to π^*_τ in (7) by using *self-normalized importance sampling* (Owen, 2013), where the proposal distribution is π_θ and the reference distribution is π^*_τ. For importance sampling, one draws K *i.i.d.* samples $\{\mathbf{a}^{(k)}\}_{k=1}^K$ from $\pi_\theta(\mathbf{a} \mid \mathbf{h})$ and computes a set of normalized importance weights to approximate $\mathcal{O}_{\mathrm{RML}}(\boldsymbol{\theta}; \tau \mid \mathbf{h})$ as,

$$\mathcal{O}_{\mathrm{RML}}(\boldsymbol{\theta}; \tau \mid \mathbf{h}) \approx \tau \sum_{k=1}^{K} \frac{w_\tau(\mathbf{a}^{(k)} \mid \mathbf{h})}{\sum_{m=1}^K w_\tau(\mathbf{a}^{(m)} \mid \mathbf{h})} \log \pi_\theta(\mathbf{a}^{(k)} \mid \mathbf{h}) \,, \tag{9}$$

where $w_\tau(\mathbf{a}^{(k)} \mid \mathbf{h}) \propto \pi^*_\tau / \pi_\theta$ denotes an importance weight defined by,

$$w_\tau(\mathbf{a}^{(k)} \mid \mathbf{h}) = \exp\left\{\frac{1}{\tau} r(\mathbf{a}^{(k)} \mid \mathbf{h}) - \log \pi_\theta(\mathbf{a}^{(k)} \mid \mathbf{h})\right\} . \tag{10}$$

One can view these importance weights as evaluating the discrepancy between scaled rewards r/τ and the policy's log-probabilities $\log \pi_\theta$. Among the K samples, a sample that is least appreciated by the model, *i.e.,* has the largest $r/\tau - \log \pi_\theta$, receives the largest positive feedback in (9).

In practice, we have found that just using the importance sampling RML objective in (9) does not always yield promising solutions. Particularly, at the beginning of training, when π_θ is still far away from π^*_τ, the variance of importance weights is too large, and the self-normalized importance sampling procedure results in poor approximations. To stabilize early phases of training and ensure that the model distribution π_θ achieves large expected reward scores, we combine the expected reward and RML objectives to benefit from the best of their mode and mean seeking behaviors. Accordingly, we propose the following objective that we call *under-appreciated reward exploration (UREX)*,

$$\mathcal{O}_{\mathrm{UREX}}(\boldsymbol{\theta}; \tau) = \mathbb{E}_{\mathbf{h}\sim p(\mathbf{h})}\left\{ \sum_{\mathbf{a}\in\mathcal{A}} \Big[\pi_\theta(\mathbf{a} \mid \mathbf{h})\, r(\mathbf{a} \mid \mathbf{h}) + \tau\, \pi^*_\tau(\mathbf{a} \mid \mathbf{h}) \log \pi_\theta(\mathbf{a} \mid \mathbf{h})\Big] \right\}, \tag{11}$$

which is the sum of the expected reward and RML objectives. In our preliminary experiments, we considered a composite objective of $\mathcal{O}_{\mathrm{RL}} + \mathcal{O}_{\mathrm{RML}}$, but we found that removing the entropy term is beneficial. Hence, the $\mathcal{O}_{\mathrm{UREX}}$ objective does not include entropy regularization. Accordingly, the optimum policy for $\mathcal{O}_{\mathrm{UREX}}$ is no longer π^*_τ, as it was for $\mathcal{O}_{\mathrm{RL}}$ and $\mathcal{O}_{\mathrm{RML}}$. Appendix A derives the optimal policy for $\mathcal{O}_{\mathrm{UREX}}$ as a function of the optimal policy for $\mathcal{O}_{\mathrm{RL}}$. We find that the optimal policy of UREX is more sharply concentrated on the high reward regions of the action space, which may be an advantage for UREX, but we leave more analysis of this behavior to future work.

To compute the gradient of $\mathcal{O}_{\mathrm{UREX}}(\boldsymbol{\theta}; \tau)$, we use the self-normalized importance sampling estimate outlined in (9). We assume that the importance weights are constant and contribute no gradient to $\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\mathcal{O}_{\mathrm{UREX}}(\boldsymbol{\theta}; \tau)$. To approximate the gradient, one draws N *i.i.d.* samples from the latent environment states $\{\mathbf{h}^{(n)}\}_{n=1}^N$, and then draws K *i.i.d.* samples $\{\mathbf{a}^{(k)}\}_{k=1}^K$ from $\pi_\theta(\mathbf{a} \,|\, \mathbf{h}^{(n)})$ to obtain

$$\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}}\mathcal{O}_{\mathrm{UREX}}(\boldsymbol{\theta}; \tau) \approx \frac{1}{N}\sum_{n=1}^{N}\sum_{k=1}^{K} \frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \log \pi_\theta(\mathbf{a}^{(k)} \,|\, \mathbf{h}^{(n)}) \left[\frac{1}{K}\widehat{r}(\mathbf{a}^{(k)} \mid \mathbf{h}^{(n)}) + \tau \frac{w_\tau(\mathbf{a}^{(k)} \,|\, \mathbf{h}^{(n)})}{\sum_{m=1}^K w_\tau(\mathbf{a}^{(m)} \,|\, \mathbf{h}^{(n)})}\right]. \tag{12}$$

As with REINFORCE, the rewards are shifted by an offset $b(\mathbf{h})$. In this gradient, the model log-probability of a sample action sequence $\mathbf{a}^{(k)}$ is reinforced if the corresponding reward is large, or the corresponding importance weights are large, meaning that the action sequence is under-appreciated. The normalized importance weights are computed using a softmax operator $\mathrm{softmax}(r/\tau - \log \pi_\theta)$.

5 Related Work on Exploration in Reinforcement Learning

The most common exploration strategy considered in value-based RL is ϵ-greedy Q-learning, where at each step the agent either takes the best action according to its current value approximation or with probability ϵ takes an action sampled uniformly at random. Like entropy regularization, such an approach applies undirected exploration, but it has achieved recent success in game playing environments (Mnih et al., 2013; Van Hasselt et al., 2016; Mnih et al., 2016).

Prominent approaches to improving exploration beyond ϵ-greedy in value-based or model-based RL have focused on reducing uncertainty by prioritizing exploration toward states and actions where the agent knows the least. This basic intuition underlies work on counter and recency methods (Thrun, 1992), exploration methods based on uncertainty estimates of values (Kaelbling, 1993; Tokic, 2010), methods that prioritize learning environment dynamics (Kearns & Singh, 2002; Stadie et al., 2015), and methods that provide an intrinsic motivation or curiosity bonus for exploring unknown states (Schmidhuber, 2006; Bellemare et al., 2016). We relate the concepts of value and policy in RL and propose an exploration strategy based on the discrepancy between the two.

In contrast to value-based methods, exploration for policy-based RL methods is often a by-product of the optimization algorithm itself. Since algorithms like REINFORCE and Thompson sampling choose actions according to a stochastic policy, sub-optimal actions are chosen with some non-zero probability. The Q-learning algorithm may also be modified to sample an action from the softmax of the Q values rather than the argmax (Sutton & Barto, 1998).

Asynchronous training has also been reported to have an exploration effect on both value- and policy-based methods. Mnih et al. (2016) report that asynchronous training can stabilize training

by reducing the bias experienced by a single trainer. By using multiple separate trainers, an agent is less likely to become trapped at a policy found to be locally optimal only due to local conditions. In the same spirit, Osband et al. (2016) use multiple Q value approximators and sample only one to act for each episode as a way to implicitly incorporate exploration.

6 SIX ALGORITHMIC TASKS

We assess the effectiveness of the proposed approach on five algorithmic tasks from the OpenAI Gym (Brockman et al., 2016), as well as a new *binary search* problem. Each task is summarized below with further details available on the Gym website[1] or in their open-source code.[2] In each case, the environment has a hidden tape and a hidden sequence. The agent observes the sequence via a pointer to a single character, which can be moved by a set of *pointer control actions*.

1. **Copy**: The agent should emit a copy of the sequence. The pointer actions are move left and right.
2. **DuplicatedInput**: In the hidden tape, each character is repeated twice. The agent must deduplicate the sequence and emit every other character. The pointer actions are move left and right.
3. **RepeatCopy**: The agent should emit the hidden sequence once, then emit the sequence in the reverse order, then emit the original sequence again. The pointer actions are move left and right.
4. **Reverse**: The agent should emit the hidden sequence in the reverse order. As before, the pointer actions are move left and right.
5. **ReversedAddition**: The hidden tape is a $2 \times n$ grid of digits representing two numbers in base 3 in little-endian order. The agent must emit the sum of the two numbers, in little-endian order. The allowed pointer actions are move left, right, up, or down.

The OpenAI Gym provides an additional harder task called ReversedAddition3, which involves adding three numbers. We omit this task, since none of the methods make much progress on it.

For these tasks, during training, input sequences range from a length of 2 characters to 33. A reward of 1 is given for each correct emission. On an incorrect emission, a small penalty of -0.5 is incurred and the episode is terminated. The agent is also terminated and penalized with a reward of -1 if the episode exceeds a certain number of steps. Each of the Gym tasks has a *success threshold*, which determines the required average reward over 100 episodes for the agent to be considered successful.

We also conduct experiments on an additional algorithmic task described below:

6. **BinarySearch**: Given an integer n, the environment has a hidden array of n distinct numbers stored in ascending order. The environment also has a query number x unknown to the agent that is contained somewhere in the array. The goal of the agent is to find the query number in the array in a small number of actions. The environment has three integer registers initialized at $(n, 0, 0)$. At each step, the agent can interact with the environment via the four following actions:
   - $\mathrm{INC}(i)$: increment the value of the register i for $i \in \{1, 2, 3\}$.
   - $\mathrm{DIV}(i)$: divide the value of the register i by 2 for $i \in \{1, 2, 3\}$.
   - $\mathrm{AVG}(i)$: replace the value of the register i with the average of the two other registers.
   - $\mathrm{CMP}(i)$: compare the value of the register i with x and receive a signal indicating which value is greater. The agent succeeds when it calls CMP on an array cell holding the value x.

   The agent is terminated when the number of steps exceeds a maximum threshold of $2n+1$ steps and recieves a reward of 0. If the agent finds x at step t, it recieves a reward of $10(1-t/(2n+1))$.

We set the maximum number of steps to $2n+1$ to allow the agent to perform a full linear search. A policy performing full linear search achieves an average reward of 5, because x is chosen uniformly at random from the elements of the array. A policy employing binary search can find the number x in at most $2 \log_2 n + 1$ steps. If n is selected uniformly at random from the range $32 \leq n \leq 512$, binary search yields an optimal average reward above 9.55. We set the *success threshold* for this task to an average reward of 9.

[1] gym.openai.com

[2] github.com/openai/gym

Table 1: Each cell shows the percentage of 60 trials with different hyper-parameters (η, c) and random restarts that successfully solve an algorithmic task. UREX is more robust to hyper-parameter changes than MENT. We evaluate MENT with a few temperatures and UREX with $\tau = 0.1$.

	REINFORCE / MENT				UREX
	$\tau = 0.0$	$\tau = 0.005$	$\tau = 0.01$	$\tau = 0.1$	$\tau = 0.1$
Copy	85.0	88.3	**90.0**	3.3	75.0
DuplicatedInput	68.3	73.3	73.3	0.0	**100.0**
RepeatCopy	0.0	0.0	11.6	0.0	**18.3**
Reverse	0.0	0.0	3.3	10.0	**16.6**
ReversedAddition	0.0	0.0	1.6	0.0	**30.0**
BinarySearch	0.0	0.0	1.6	0.0	**20.0**

7 EXPERIMENTS

We compare our policy gradient method using under-appreciated reward exploration (UREX) against two main RL baselines: (1) REINFORCE with entropy regularization termed MENT (Williams & Peng, 1991), where the value of τ determines the degree of regularization. When $\tau = 0$, standard REINFORCE is obtained. (2) one-step double Q-learning based on bootstrapping one step future rewards.

7.1 ROBUSTNESS TO HYPER-PARAMETERS

Hyper-parameter tuning is often tedious for RL algorithms. We found that the proposed UREX method significantly improves robustness to changes in hyper-parameters when compared to MENT. For our experiments, we perform a careful grid search over a set of hyper-parameters for both MENT and UREX. For any hyper-parameter setting, we run the MENT and UREX methods 5 times with different random restarts. We explore the following main hyper-parameters:

- The *learning rate* denoted η chosen from a set of 3 possible values $\eta \in \{0.1, 0.01, 0.001\}$.
- The maximum L2 norm of the gradients, beyond which the gradients are *clipped*. This parameter, denoted c, matters for training RNNs. The value of c is selected from $c \in \{1, 10, 40, 100\}$.
- The temperature parameter τ that controls the degree of exploration for both MENT and UREX. For MENT, we use $\tau \in \{0, 0.005, 0.01, 0.1\}$. For UREX, we only consider $\tau = 0.1$, which consistently performs well across the tasks.

In all of the experiments, both MENT and UREX are treated exactly the same. In fact, the change of implementation is just a few lines of code. Given a value of τ, for each task, we run 60 training jobs comprising 3 learning rates, 4 clipping values, and 5 random restarts. We run each algorithm for a maximum number of steps determined based on the difficulty of the task. The training jobs for Copy, DuplicatedInput, RepeatCopy, Reverse, ReversedAddition, and BinarySearch are run for $2K$, 500, $50K$, $5K$, $50K$, and $2K$ stochastic gradient steps, respectively. We find that running a trainer job longer does not result in a better performance. Our policy network comprises a single LSTM layer with 128 nodes. We use the Adam optimizer (Kingma & Ba, 2015) for the experiments.

Table 1 shows the percentage of 60 trials on different hyper-parameters (η, c) and random restarts which successfully solve each of the algorithmic tasks. It is clear that UREX is more robust than MENT to changes in hyper-parameters, even though we only report the results of UREX for a single temperature. See Appendix B for more detailed tables on hyper-parameter robustness.

7.2 RESULTS

Table 2 presents the number of successful attempts (out of 5 random restarts) and the expected reward values (averaged over 5 trials) for each RL algorithm given the best hyper-parameters. One-step Q-learning results are also included in the table. It is clear that UREX outperforms the baselines on these tasks. On the more difficult tasks, such as Reverse and ReverseAddition, UREX is able to consistently find an appropriate algorithm, but MENT and Q-learning fall behind. Importantly, for the BinarySearch task, which exhibits many local maxima and necessitates smart exploration, UREX is the only method that can solve it consistently. The Q-learning baseline solves some of the simple

Table 2: Results on several algorithmic tasks comparing Q-learning and policy gradient based on MENT and UREX. We find the best hyper-parameters for each method, and run each algorithm 5 times with random restarts. Number of successful attempts (out of 5) that achieve a reward threshold is reported. Expected reward computed over the last few iterations of training is also reported.

	Num. of successful attempts out of 5			Expected reward		
	Q-learning	MENT	UREX	Q-learning	MENT	UREX
Copy	5	5	5	31.2	31.2	31.2
DuplicatedInput	5	5	5	15.4	15.4	15.4
RepeatCopy	1	3	4	39.3	69.2	81.1
Reverse	0	2	4	4.4	21.9	27.2
ReversedAddition	0	1	5	1.1	8.7	30.2
BinarySearch	0	1	4	5.2	8.6	9.1

tasks, but it makes little headway on the harder tasks. We believe that entropy regularization for policy gradient and ϵ-greedy for Q-learning are relatively weak exploration strategies in long episodic tasks with delayed rewards. On such tasks, one random exploratory step in the wrong direction can take the agent off the optimal policy, hampering its ability to learn. In contrast, UREX provides a form of adaptive and smart exploration. In fact, we observe that the variance of the importance weights decreases as the agent approaches the optimal policy, effectively reducing exploration when it is no longer necessary; see Appendix E.

7.3 Generalization to longer sequences

To confirm whether our method is able to find the correct algorithm for multi-digit addition, we investigate its generalization to longer input sequences than provided during training. We evaluate the trained models on inputs up to a length of 2000 digits, even though training sequences were at most 33 characters. For each length, we test the model on 100 randomly generated inputs, stopping when the accuracy falls below 100%. Out of the 60 models trained on addition with UREX, we find that 5 models generalize to numbers up to 2000 digits without any observed mistakes. On the best UREX hyper-parameters, 2 out of the 5 random restarts are able to generalize successfully. For more detailed results on the generalization performance on 3 different tasks including Copy, DuplicatedInput, and ReversedAddition, see Appendix C. During these evaluations, we take the action with largest probability from $\pi_\theta(\mathbf{a} \mid \mathbf{h})$ at each time step rather than sampling randomly.

We also looked into the generalization of the models trained on the BinarySearch task. We found that none of the agents perform proper binary search. Rather, those that solved the task perform a hybrid of binary and linear search: first actions follow a binary search pattern, but then the agent switches to a linear search procedure once it narrows down the search space; see Appendix D for some execution traces for BinarySearch and ReversedAddition. Thus, on longer input sequences, the agent's running time complexity approaches linear rather than logarithmic. We hope that future work will make more progress on this task. This task is especially interesting because the reward signal should incorporate both correctness and efficiency of the algorithm.

7.4 Implementation details

In all of the experiments, we make use of curriculum learning. The environment begins by only providing small inputs and moves on to longer sequences once the agent achieves close to maximal reward over a number of steps. For policy gradient methods including MENT and UREX, we only provide the agent with a reward at the end of the episode, and there is no notion of intermediate reward. For the value-based baseline, we implement one-step Q-learning as described in Mnih et al. (2016)-Alg. 1, employing double Q-learning with ϵ-greedy exploration. We use the same RNN in our policy-based approaches to estimate the Q values. A grid search over exploration rate, exploration rate decay, learning rate, and sync frequency (between online and target network) is conducted to find the best hyper-parameters. Unlike our other methods, the Q-learning baseline

uses intermediate rewards, as given by the OpenAI Gym on a per-step basis. Hence, the Q-learning baseline has a slight advantage over the policy gradient methods.

In all of the tasks except Copy, our stochastic optimizer uses mini-batches comprising 400 policy samples from the model. These 400 samples correspond to 40 different random sequences drawn from the environment, and 10 random policy trajectories per sequence. In other words, we set $K = 10$ and $N = 40$ as defined in (3) and (12). For MENT, we use the 10 samples to subtract the mean of the coefficient of $\frac{\mathrm{d}}{\mathrm{d}\boldsymbol{\theta}} \log \pi_\theta(\mathbf{a} \mid \mathbf{h})$ which includes the contribution of the reward and entropy regularization. For UREX, we use the 10 trajectories to subtract the mean reward and normalize the importance sampling weights. We do not subtract the mean of the normalized importance weights. For the Copy task, we use mini-batches with 200 samples using $K = 10$ and $N = 20$. Experiments are conducted using Tensorflow (Abadi et al., 2016).

8 Conclusion

We present a variant of policy gradient, called UREX, which promotes exploring action sequences that yield rewards larger than what the model expects. This exploration strategy is the result of importance sampling from the optimal policy. Our experimental results demonstrate that UREX significantly outperforms other value and policy based methods, while being more robust to changes of hyper-parameters. By using UREX, we can solve algorithmic tasks like multi-digit addition, which other methods cannot reliably solve even given the best hyper-parameters. We introduce a new algorithmic task based on binary search to advocate more research in this area, especially when the computational complexity of the solutions matters too. Solving these tasks is not only important to develop human like intelligence to enable learning algorithms, but also important for generic reinforcement learning, where smart and efficient exploration is the key to successful methods.

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A Optimal Policy for the UREX Objective

To derive the form of the optimal policy for the UREX objective (11), note that for each $\mathbf{h}$ one would like to maximize

$$\sum_{\mathbf{a}\in\mathcal{A}} \Big[\pi_\theta(\mathbf{a})\, r(\mathbf{a}) + \tau\, \pi^*_\tau(\mathbf{a}) \log \pi_\theta(\mathbf{a})\Big] \,, \tag{13}$$

subject to the constraint $\sum_{\mathbf{a}\in\mathcal{A}} \pi_\theta(\mathbf{a}) = 1$. To enforce the constraint, we introduce a Lagrange multiplier α and aim to maximize

$$\sum_{\mathbf{a}\in\mathcal{A}} \Big[\pi_\theta(\mathbf{a})\, r(\mathbf{a}) + \tau\, \pi^*_\tau(\mathbf{a}) \log \pi_\theta(\mathbf{a}) - \alpha\pi_\theta(\mathbf{a})\Big] + \alpha \,. \tag{14}$$

Since the gradient of the Lagrangian (14) with respect to $\boldsymbol{\theta}$ is given by

$$\sum_{\mathbf{a}\in\mathcal{A}} \frac{\mathrm{d}\pi_\theta(\mathbf{a})}{\mathrm{d}\boldsymbol{\theta}} \Big[r(\mathbf{a}) + \tau\, \frac{\pi^*_\tau(\mathbf{a})}{\pi_\theta(\mathbf{a})} - \alpha\Big] \,, \tag{15}$$

the optimal choice for π_θ is achieved by setting

$$\pi_\theta(\mathbf{a}) = \frac{\tau\, \pi^*_\tau(\mathbf{a})}{\alpha - r(\mathbf{a})} \quad \text{for all} \quad \mathbf{a} \in \mathcal{A} \,, \tag{16}$$

forcing the gradient to be zero. The Lagrange multiplier α can then be chosen so that $\sum_{\mathbf{a}\in\mathcal{A}} \pi_\theta(\mathbf{a}) = 1$ while also satisfying $\alpha > \max_{\mathbf{a}\in\mathcal{A}} r(\mathbf{a})$; see *e.g.* (Golub, 1987).

B Robustness to Hyper-parameters

Tables 3–8 provide more details on different cells of Table 1. Each table presents the results of MENT using the best temperature τ *vs.* UREX with $\tau = 0.1$ on a variety of learning rates and clipping values. Each cell is the number of trials out of 5 random restarts that succeed at solving the task using a specific η and c.

Table 3: Copy – number of successful attempts out of 5.

	MENT ($\tau = 0.01$)			UREX ($\tau = 0.1$)		
	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$
$c = 1$	3	5	5	5	5	2
$c = 10$	5	4	5	5	5	3
$c = 40$	3	5	5	4	4	1
$c = 100$	4	5	5	4	5	2

Table 4: DuplicatedInput – number of successful attempts out of 5.

	MENT ($\tau = 0.01$)			UREX ($\tau = 0.1$)		
	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$
$c = 1$	3	5	3	5	5	5
$c = 10$	2	5	3	5	5	5
$c = 40$	4	5	3	5	5	5
$c = 100$	2	5	4	5	5	5

Table 5: RepeatCopy – number of successful attempts out of 5.

	MENT ($\tau = 0.01$)			UREX ($\tau = 0.1$)		
	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$
$c = 1$	0	1	0	0	2	0
$c = 10$	0	0	2	0	4	0
$c = 40$	0	0	1	0	2	0
$c = 100$	0	0	3	0	3	0

Table 6: Reverse – number of successful attempts out of 5.

	MENT ($\tau = 0.1$)			UREX ($\tau = 0.1$)		
	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$
$c = 1$	1	1	0	0	0	0
$c = 10$	0	1	0	0	4	0
$c = 40$	0	2	0	0	2	1
$c = 100$	1	0	0	0	2	1

Table 7: ReversedAddition – number of successful attempts out of 5.

	MENT ($\tau = 0.01$)			UREX ($\tau = 0.1$)		
	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$
$c = 1$	0	0	0	0	0	4
$c = 10$	0	0	0	0	3	2
$c = 40$	0	0	0	0	0	5
$c = 100$	0	0	1	0	1	3

Table 8: BinarySearch – number of successful attempts out of 5.

	MENT ($\tau = 0.01$)			UREX ($\tau = 0.1$)		
	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$	$\eta = 0.1$	$\eta = 0.01$	$\eta = 0.001$
$c = 1$	0	0	0	0	4	0
$c = 10$	0	1	0	0	3	0
$c = 40$	0	0	0	0	3	0
$c = 100$	0	0	0	0	2	0

C Generalization to Longer Sequences

Table 9 provides a more detailed look into the generalization performance of the trained models on Copy, DuplicatedInput, and ReversedAddition. The tables show how the number of models which can solve the task correctly drops off as the length of the input increases.

Table 9: Generalization results. Each cell includes the number of runs out of 60 different hyperparameters and random initializations that achieve 100% accuracy on input of length up to the specified length. The bottom row is the maximal length (≤ 2000) up to which at least one model achieves 100% accuracy.

	Copy		DuplicatedInput		ReversedAddition	
	MENT	UREX	MENT	UREX	MENT	UREX
30	54	45	44	60	1	18
100	51	45	36	56	0	6
500	27	22	19	25	0	5
1000	3	2	12	17	0	5
2000	0	0	6	9	0	5
Max	1126	1326	2000	2000	38	2000

D Example Execution Traces

We provide the traces of two trained agents on the ReversedAddition task (Figure 2) and the BinarySearch task (Table 10).

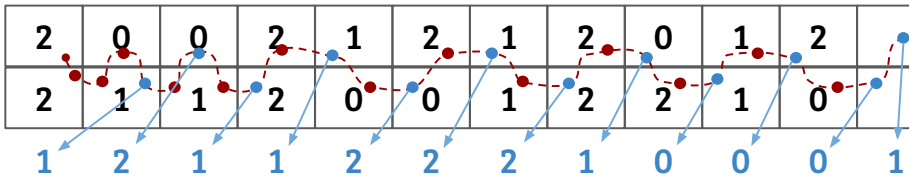

Figure 2: A graphical representation of a trained addition agent. The agent begins at the top left corner of a $2 \times n$ grid of ternary digits. At each time step, it may move to the left, right, up, or down (observing one digit at a time) and optionally write to output.

Table 10: Example trace on the BinarySearch task where $n = 512$ and the number to find is at position 100. At time t the agent observes $\mathbf{s}_t$ from the environment and samples an action $\mathbf{a}_t$. We also include the inferred range of indices to which the agent has narrowed down the position of x. We see that the first several steps of the agent follow a binary search algorithm. However, at some point the agent switches to a linear search

R_0	R_1	R_2	$\mathbf{s}_t$	$\mathbf{a}_t$	Inferred range
512	0	0	–	AVG(2)	$[0, 512)$
512	0	256	–	CMP(2)	$[0, 512)$
512	0	256	$<$	DIV(0)	$[0, 256)$
256	0	256	–	AVG(2)	$[0, 256)$
256	0	128	–	CMP(2)	$[0, 256)$
256	0	128	$<$	DIV(0)	$[0, 128)$
128	0	128	–	AVG(2)	$[0, 128)$
128	0	64	–	CMP(2)	$[0, 128)$
128	0	64	$>$	AVG(1)	$(64, 128)$
128	96	64	–	CMP(1)	$(64, 128)$
128	96	64	$>$	AVG(2)	$(96, 128)$
128	96	112	–	CMP(2)	$(96, 128)$
128	96	112	$<$	AVG(1)	$(96, 112)$
128	120	112	–	CMP(2)	$(96, 112)$
128	120	112	$<$	DIV(1)	$(96, 112)$
128	60	112	–	AVG(2)	$(96, 112)$
128	60	94	–	CMP(2)	$(96, 112)$
128	60	94	$>$	AVG(1)	$(96, 112)$
128	111	94	–	CMP(1)	$(96, 112)$
128	111	94	$<$	INC(1)	$(96, 111)$
128	112	94	–	INC(2)	$(96, 111)$
128	112	95	–	CMP(2)	$(96, 111)$
128	112	95	$>$	INC(2)	$(96, 111)$
128	112	96	–	CMP(2)	$(96, 111)$
128	112	96	$>$	INC(2)	$(96, 111)$
128	112	97	–	CMP(2)	$(96, 111)$
128	112	97	$>$	INC(2)	$(97, 111)$
128	112	98	–	CMP(2)	$(97, 111)$
128	112	98	$>$	INC(2)	$(98, 111)$
128	112	99	–	CMP(2)	$(98, 111)$
128	112	99	$>$	INC(2)	$(99, 111)$
128	112	100	–	CMP(2)	$(99, 111)$
128	112	100	$=$	–	–

E VARIANCE OF IMPORTANCE WEIGHTS

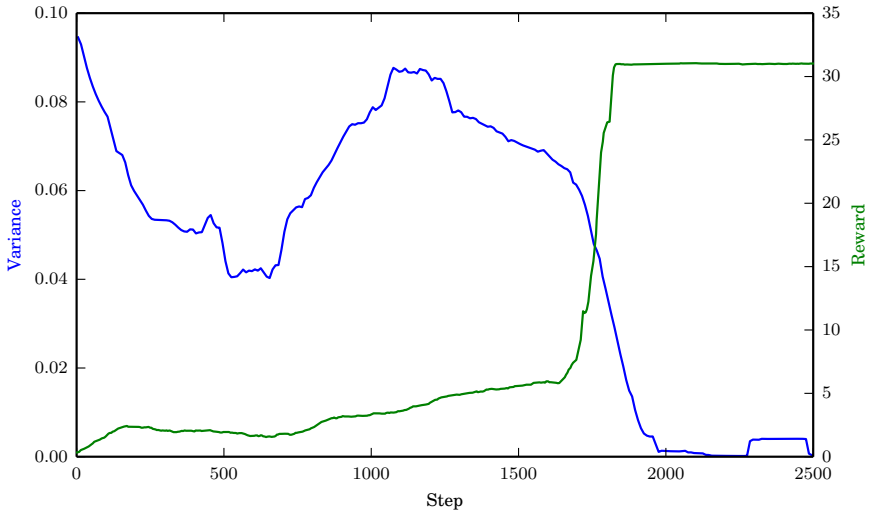

Figure 3: This plot shows the variance of the importance weights in the UREX updates as well as the average reward. We see that the variance starts off high and reaches near 0 towards the end when the optimal policy is found. In between, we see a dip and rise in the variance which corresponds to a plateau and then increase in the average reward.