The Uncertainty Bellman Equation and Exploration

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Abstract

We consider the exploration/exploitation problem in reinforcement learning. For exploitation, it is well known that the Bellman equation connects the value at any time-step to the expected value at subsequent time-steps. In this paper we consider a similar uncertainty Bellman equation (UBE), which connects the uncertainty at any time-step to the expected uncertainties at subsequent time-steps, thereby extending the potential exploratory benefit of a policy beyond individual time-steps. We prove that the unique fixed point of the UBE yields an upper bound on the variance of the estimated value of any fixed policy. This bound can be much tighter than traditional count-based bonuses that compound standard deviation rather than variance. Importantly, and unlike several existing approaches to optimism, this method scales naturally to large systems with complex generalization. Substituting our UBE-exploration strategy for $\epsilon$-greedy improves DQN performance on 51 out of 57 games in the Atari suite.

1 Introduction

We consider the reinforcement learning (RL) problem of an agent interacting with its environment to maximize cumulative rewards through time [35]. We model the environment as a Markov decision process (MDP), but where the agent is initially uncertain of the true dynamics of the MDP [4, 5]. At each time-step, the agent performs an action, receives a reward, and moves to the next state; from these data it can learn which actions lead to higher payoffs. This leads to the exploration versus exploitation trade-off: Should the agent investigate poorly understood states and actions to improve future performance or instead take actions that maximize rewards given its current knowledge?

Separating estimation and control in RL via ‘greedy’ algorithms can lead to premature and suboptimal exploitation. To offset this, the majority of practical implementations introduce some random noise or dithering into their action selection (such as $\epsilon$-greedy). These algorithms will eventually explore every reachable state and action infinitely often, but can take exponentially long to learn the optimal policy [12]. By contrast, for any set of prior beliefs the optimal exploration policy can be computed directly by dynamic programming in the Bayesian belief space. However this approach can be computationally intractable for even very small problems [9] while direct computational approximations can fail spectacularly badly [22].

For this reason, most provably-efficient approaches to reinforcement learning rely upon the optimism in the face of uncertainty (OFU) heuristic [14, 13, 7]. These algorithms give a bonus to poorly-understood states and actions and subsequently follow the policy that is optimal for this augmented optimistic MDP. This optimism incentivises exploration but, as the agent learns more about the environment, the scale of the bonus should decrease and the agent’s performance should approach optimality. At a high level these approaches to OFU-RL build up confidence sets that contain the true MDP with high probability [33, 16].
These techniques can provide performance guarantees that are ‘near-optimal’ in terms of the problem parameters. However, apart from the simple ‘multi-armed bandit’ setting with only one state, there is still a significant gap between the upper and lower bounds for these algorithms [15][11][27].

One inefficiency in these algorithms is that, although the concentration may be tight at each state and action independently, the combination of simultaneously optimistic estimates may result in an extremely over-optimistic estimate for the MDP as a whole [28]. Other works have suggested that a Bayesian posterior sampling approach may not suffer from these inefficiencies and can lead to performance improvements over OFU methods [34][25]. In this paper we explore an alternative approach that harnesses the simple relationship of the uncertainty Bellman equation (UBE), where we define uncertainty to be the variance of the value estimator the agent is learning, in a sense similar to the parametric variance of Mannor et. al. [17]. Intuitively speaking, if the agent has high uncertainty (as measured by high estimator variance) in a region of the state-space then it should explore there, in order to get a better estimate of those Q-values. We show that, just as the Bellman equation relates the value of a policy beyond a single time-step, so too does the uncertainty Bellman equation propagate uncertainty values over multiple time-steps, thereby facilitating ‘deep exploration’ [26].

The benefit of our approach (which learns the solution to the UBE and uses this to guide exploration) is that we can harness the existing machinery for deep reinforcement learning with minimal change to existing network architectures. The resulting algorithm shares an intimate connection to the existing literature of both OFU and intrinsic motivation [31][30]. Recent work has further connected these approaches through the notion of ‘pseudo-count’ [2][29] or some generalization of the number of visits to a state and action. Rather than pseudo-count, our work builds upon the idea that the more fundamental quantity relates to the uncertainty of the estimated value function and that naively compounding count-based bonuses may lead to inefficient confidence sets [28]. The key difference is that the UBE compounds the sum of the variances at each step, rather than standard deviation.

The observation that the higher moments of a value function also satisfy a form of Bellman equation is not new and has been observed by some of the early papers on the subject [32]. Unlike most prior work, we focus upon the epistemic uncertainty over the mean of the value function, rather than the higher moments of the reward-to-go [16][11][18]. For application to rich environments with complex generalization we will use a deep learning architecture to learn a solution to the UBE according to our observed data, in the style of [37].

2 Problem formulation

We consider an infinite horizon, discounted, finite state and action space MDP, with state space $S$, action space $A$ and rewards at each time period denoted by $r_t \in \mathbb{R}$. A policy $\pi : S \times A \rightarrow \mathbb{R}_+$ is a mapping from state-action pair to the probability of taking that action at that state. At each time-step $t$ the agent receives a state $s_t$ and a reward $r_t$ and selects an action $a_t$ from the policy $\pi_t$, and the agent moves to the next state $s_{t+1} \sim P(\cdot, s_t, a_t)$. Here $P(s', s, a)$ is the probability of transitioning from state $s$ to state $s'$ after taking action $a$. The goal of the agent is to maximize the expected total discounted return $J$ under its policy $\pi$, where $J(\pi) = \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t r_t \mid \pi \right]$. Here the expectation is with respect to the initial state distribution, the state-transition probabilities, and the policy $\pi$. The discount factor $\gamma \in (0, 1)$ controls how much the agent prioritizes long-term versus short-term rewards.

The action-value, or Q-value, of a particular state under policy $\pi$ is the expected total discounted return from taking that action at that state and following $\pi$ thereafter, $Q^\pi(s, a) = \mathbb{E} \left[ \sum_{t=0}^{\infty} \gamma^t r_t \mid s_0 = s, a_0 = a, \pi \right]$. The value of state $s$ under policy $\pi$, $V^\pi(s) = \mathbb{E} \left[ Q^\pi(s, a) \mid a \sim \pi \right]$ is the expected total discounted return
of policy \( \pi \) from state \( s \). The optimal action-value function \( Q^\star(s, a) = \max_\pi Q^\pi(s, a) \) for each \((s, a)\). The policy that achieves the maximum is the optimal policy \( \pi^\star \).

The Bellman operator \( T^\pi \) for policy \( \pi \), relates the value at each time-step to the value at subsequent time-steps via dynamic programming,

\[
T^\pi Q^\pi(s, a) = \mathbb{E}_r r(s, a) + \gamma \mathbb{E}_{s', a'} Q^\pi(s', a'),
\]

where this expectation is taken over next state \( s' \sim P(\cdot, s, a) \), the reward \( r(s, a) \), and the action \( a' \) from policy \( \pi_{s'} \). For \( \gamma \in (0, 1) \) the Bellman operator is contraction and therefore \( Q^\pi \) is the unique fixed point of \( T^\pi Q^\pi = Q^\pi \). Several reinforcement learning algorithms have been designed around minimizing Bellman residual to propagate knowledge of immediate rewards to long term value \([35, 40]\). In the next section we examine a similar relationship for propagating the uncertainties in an estimator, we call this relationship the uncertainty Bellman equation.

3 The uncertainty Bellman equation

In this section we derive a Bellman-style relationship that propagates the uncertainty (variance) of any Q-value estimator across multiple time-steps. Propagating the potential value of exploration over many timesteps, or deep exploration, is important for statistically efficient RL \([13, 26]\). Our main result, which we state in Theorem \([1]\), is based upon nothing more than the dynamic programming recursion \((1)\) and some crude upper bounds of several intermediate terms. We will show that even in very simple settings this approach can result in well-calibrated uncertainty estimates where common count-based bonuses are inefficient \([28]\).

3.1 Interval estimation via variance estimates

We begin by motivating why the uncertainty (or variance) of the estimator is useful for exploration \([33]\). Consider the problem of learning the value of a policy \( \pi \) from some data \( d \). The true, but unknown, values \( Q^\pi \) satisfy the Bellman equation \((1)\) while our estimate from \( \hat{Q}^\pi = \hat{Q}^\pi(d) \) is a random variable with potentially both bias and variance. We write \( \epsilon(s, a) \) for the Bellman residual,

\[
\epsilon(s, a) := (\hat{Q}^\pi - T^\pi \hat{Q}^\pi)(s, a) = \hat{Q}^\pi(s, a) - \mathbb{E}_r r(s, a) - \gamma \mathbb{E}_{s', a'} \hat{Q}^\pi(s', a').
\]

If we denote by \( \delta(s, a) = \hat{Q}^\pi(s, a) - Q^\pi(s, a) \) the error at \((s, a)\) then we have

\[
\delta(s, a) = \epsilon(s, a) + \gamma \mathbb{E}_{s', a'} \delta(s', a').
\]

If we could calculate \( \epsilon \) exactly everywhere, then we could solve the Bellman equation \((3)\) and obtain the true Q-values. However the true \( \epsilon \) is intractable to calculate, since it requires an exact application of the Bellman operator. Instead we consider the case where we can estimate the moments of the Bellman residual easily, even though we can’t calculate it exactly.

The mean-squared error of the estimator at any state-action pair is given by

\[
m(s, a) := \mathbb{E}_d [(\hat{Q}^\pi(s, a) - Q^\pi(s, a))^2] = \text{var} \hat{Q}^\pi(s, a) + (\text{bias} \hat{Q}^\pi(s, a))^2.
\]

Markov’s inequality \([10]\) implies that

\[
\text{Prob} \left( |\hat{Q}^\pi(s, a) - Q^\pi(s, a)| > \alpha m(s, a)^{1/2} \right) \leq 2/\alpha^2.
\]
Therefore if we know, or can bound, the variance and bias of an estimator then we can use them to construct intervals that contain the true Q-values with high-probability. An agent can then apply the OFU-principle to prioritize its exploration towards potentially rewarding policies [13, 22]. We argue that, for many settings of interest, this error is dominated by the variance term and that, in this case, several simplifying relationships emerge.

**Lemma 1.** For any policy $\pi$ and any state-action pair $(s, a)$, the biases satisfy a Bellman equation

$$\text{bias } \hat{Q}^\pi(s, a) = E_d \epsilon(s, a) + \gamma \pi_{s',a'} \text{ bias } \hat{Q}^\pi(s', a').$$

**Proof.** Take the expectation of (3) with respect to $d$ and note that $E_d \delta(s, a) = \text{bias } \hat{Q}^\pi(s, a)$. \hfill \Box

For the purposes of our analysis we will assume that the Bellman residuals at any state-action pair are uncorrelated. This property will certainly not hold in all settings, but may be a reasonable approximation in many settings of interest.

**Assumption 1.** For any $s, s' \in S$, $a, a' \in A$,

$$\text{cov}(\epsilon(s, a), \epsilon(s', a')) \leq \min(\text{var } \epsilon(s, a), \text{var } \epsilon(s', a')),$$  

where $\text{cov}$ denotes the covariance.

Assumption 1 implies that the variance of the Q-value estimate satisfies a Bellman inequality.

**Lemma 2.** For any policy $\pi$ and any estimator that satisfies assumption[1] the variance satisfies a Bellman inequality at all $(s, a)$,

$$\text{var } \hat{Q}^\pi(s, a) \leq \beta \text{var } \epsilon(s, a) + \gamma^2 \pi_{s',a'} \text{ var } \hat{Q}^\pi(s', a'),$$

for some $\beta \in [1, \frac{1 + \gamma}{1 - \gamma}]$ and we write $\beta^*$ for the minimum such $\beta$ that satisfies this relationship.

**Proof.** Let $\text{var } \epsilon(s, a) = E_d [(\epsilon(s, a) - E_d \epsilon(s, a))^2]$ be the variance of the Bellman residual at $(s, a)$. We will refer to this quantity as the local (or shallow) uncertainty from finite data. We now consider the variance of the estimator:

\[
\text{var } \hat{Q}^\pi(s, a) = E_d \left[ (\hat{Q}^\pi(s, a) - E_d \hat{Q}^\pi(s, a))^2 \right] \\
= E_d \left[ (\hat{Q}^\pi(s, a) - Q^\pi(s, a) - \text{bias } \hat{Q}^\pi(s, a))^2 \right] \\
= E_d \left[ (\hat{Q}^\pi(s, a) - E_d r(s, a) - \gamma \pi_{s',a'} \hat{Q}^\pi(s', a') - \text{bias } \hat{Q}^\pi(s, a))^2 \right] \\
= E_d \left[ (\epsilon(s, a) - E_d \epsilon(s, a) + \gamma \pi_{s',a'}[\hat{Q}^\pi(s', a') - E_d \hat{Q}^\pi(s', a')])^2 \right],
\]

where in the last line we used lemma[1] Expanding the square we obtain

\[
\text{var } \hat{Q}^\pi(s, a) = \text{var } \epsilon(s, a) + \gamma^2 E_d \left[ (E_d \epsilon(s', a') - E_d \hat{Q}^\pi(s', a'))^2 \right] + 2 \gamma c(s, a),
\]

where $c(s, a)$ is the cross-term. In the appendix, we prove that under assumption[1] this can be bounded

\[
c(s, a) \leq \alpha \text{ var } \epsilon(s, a),
\]

(8)
where $0 \leq \alpha \leq \frac{1}{1-\gamma}$ is a constant that might depend on the MDP, the policy, and the estimator. By Jensen’s inequality we have that

$$E_d[(E_{s',a'}[\hat{Q}^\pi(s',a') - \hat{Q}^\pi(s',a')])^2] \leq E_d, s',a'[(\hat{Q}^\pi(s',a') - \hat{Q}^\pi(s',a'))^2] = E_{s',a'} \text{var } \hat{Q}^\pi(s',a').$$

Combining this result with (8) we can then say,

$$\text{var } \hat{Q}^\pi(s,a) \leq \beta \text{var } \epsilon(s,a) + \gamma^2 E_{s',a'} \text{var } \hat{Q}^\pi(s',a'), \quad (9)$$

for some $1 \leq \beta \leq \frac{1 + \gamma}{(1 - \gamma)}$.

With these lemmas we are ready to prove our main theorem.

**Theorem 1** (Solution of the uncertainty Bellman equation). Under Assumption [7] for any policy $\pi$, let $\beta^* \in [1, \frac{1 + \gamma}{1 - \gamma}]$ be the smallest $\beta$ that satisfies the conditions for Lemma [2]. Then there exists a unique $u^*$ that satisfies the uncertainty Bellman equation

$$u^*(s,a) = (T^\pi u^*)(s,a) := \beta^* \text{var } \epsilon(s,a) + \gamma^2 E_{s',a'} u^* (s',a') \quad (10)$$

for each $(s,a)$, and $u^* \geq \text{var } \hat{Q}^\pi$ pointwise.

**Proof.** To show this we use three essential properties of the Bellman operator for a fixed policy [5]. First, the Bellman operator is a $\gamma$-contraction in the $\ell_\infty$ norm and so the fixed point $u^*$ exists and is unique. Second, value iteration converges in that $(T^\pi u^*)^k x \to u^*$ for any starting $x$. Finally, the Bellman operator is monotonically increasing in its arguments, i.e., if $x \geq y$ pointwise then $T^\pi u^* x \geq T^\pi u^* y$ pointwise. As the the variance satisfies a Bellman inequality [9], we have

$$\text{var } \hat{Q}^\pi \leq T^\pi \text{var } \hat{Q}^\pi \leq \lim_{k \to \infty} (T^\pi u^*)^k \text{var } \hat{Q}^\pi = u^*. \quad (11)$$

3.2 Comparison to traditional exploration bonus

Consider a simple decision problem with known deterministic transitions, unknown rewards and two actions. We imagine an agent has gathered some data $d$ and produces some unbiased value estimates. According to these estimates, the first action leads to a single reward with expectation zero and variance $\sigma^2$. The second action leads to an infinite chain of independent states with expectation zero and variance $\sigma^2(1 - \gamma^2)$. These numbers are chosen so that the variance of the estimated value of each action is mean zero and variance $\sigma^2$. An optimistic agent motivated by (5) has no reason to value one action over the other. Nonetheless, most existing approaches to optimism that work via exploration bonus would lead to an inconsistent decision rule in this setting [28].

Rather than consider the variance of the value as a whole, the majority of existing approaches to OFU provide exploration bonuses at each state and action independently and then combine these estimates via union bound. In this context, even a state of the art algorithm such as UCRL2 [11] would afford each state a bonus proportional to its standard deviation of estimate. For action one this would be proportional to $\sigma$, but for action two this would be proportional to,

$$\text{ExplorationBonus}(a_2) \propto \sum_{t=0}^T \gamma^t \sigma \sqrt{1 - \gamma^2} = \sigma \sqrt{\frac{1 + \gamma}{1 - \gamma}}. \quad (12)$$
In the tabular setting, the variance of the estimated reward at each state can be approximated by the inverse ‘count’ \( N(s, a) \) of visits to each state and action \([2]\). Effectively, this means that action two would be visited \( \frac{1 + \gamma}{1} \) more often to obtain the same level of confidence as an estimation via the uncertainty Bellman equation \([10]\). The essential issue that, unlike the variance, the classic exploration bonus based upon the standard deviation does not obey a Bellman-style relationship.

### 4 Local uncertainty

Section \([3]\) outlines how the uncertainty Bellman equation can be used to propagate local estimates of the variance of \( \hat{Q}^\pi \) to global estimates for the uncertainty. In this section we present some pragmatic approaches to estimating local uncertainty that we can then use for practical learning algorithms inspired by Theorem 1. We do not claim that these approaches are the only approaches to estimating local uncertainty, or even that these simple approximations are in any sense the ‘best’. Investigating these choices is an important area of future research, but outside the scope of this short paper. We present a simple progression from tabular representations, to linear function approximation and then to non-linear neural network architectures.

**Tabular value estimate.** Consider the setting where each \( \hat{Q}^\pi(s, a) \) is learned separately. If we model the Bellman error as IID with variance bounded by \( \sigma^2 \), we can apply \([5]\) to bound \( \text{var} \epsilon(s, a) \leq \sigma^2/N(s, a) \), where \( N(s, a) \) is the count of the number of visits to state \( s \) taking action \( a \) \([11]\). We can then use \( \sigma^2/N(s, a) \) as a proxy for the local uncertainty in Theorem 1.

**Linear value estimate.** Let us consider a linear value function estimator \( \hat{Q}^\pi(s, a) = \phi(s)^T w_a \) for each state and action with fixed basis functions \( \phi(s) : S \to \mathbb{R}^D \) and learned weights \( w_a \in \mathbb{R}^D \), one for each action. This setting allows for some generalization between states and actions through the basis functions. For any fixed dataset we can find the least squares solution for each action \( a \) \([6]\),

\[
\min_{w_a} \sum_{i=1}^N (\phi(s_i)^T w_a - y_i)^2,
\]

where each \( y_i \in \mathbb{R} \) is a regression target (e.g., a Monte Carlo return from that state-action). The solution to this problem is \( w_a^* = (\Phi_a^T \Phi_a)^{-1} \Phi_a^T y \), where \( \Phi_a \) is the matrix consisting of the \( \phi(s_i) \) vectors stacked row-wise (we use the subscript \( a \) to denote the fact that action \( a \) was taken at these states). We can consider the variance of the estimator, if we model the targets \( y_i \) as IID with variance \( \sigma^2 \), then \( \text{var} w_a^* = E[w_a^* w_a^{T}] = \sigma^2 (\Phi_a^T \Phi_a)^{-1} \). Given a new state vector \( \phi_s \), the variance of the Q-value estimate at \( (s, a) \) is then \( \text{var} \hat{Q}_s^\pi = \sigma^2 \phi_s^T (\Phi_a^T \Phi_a)^{-1} \phi_s \). The local uncertainty is also then just

\[
\text{var} \epsilon(s, a) = E_a(\phi_s^T w_a^* - E_{r, s', a'} y(s, a) - E_a \epsilon(s, a))^2
= \sigma^2 \phi_s^T (\Phi_a^T \Phi_a)^{-1} \phi_s
\]

where \( E_a(\epsilon(s, a)) = E_a \phi_s^T w_a^* - E_{r, s', a'} y(s, a) \) is the bias introduced by the fact that the linear approximation might not be able to represent exactly the average of the targets everywhere. Note that in the tabular case the quantity \( \sigma^2 \phi_s^T (\Phi_a^T \Phi_a)^{-1} \phi_s \) is equal to \( \sigma^2/N(s, a) \), as might be expected.

An agent using this notion of local uncertainty must maintain and update the matrix \( \Sigma_a = (\Phi_a^T \Phi_a)^{-1} \) as it receives new data. Given new sample \( \phi \), the updated matrix \( \Sigma_a^+ \) is given by

\[
\Sigma_a^+ = \left( \begin{bmatrix} \Phi_a
\phi_T \end{bmatrix}^T \begin{bmatrix} \Phi_a
\phi_T \end{bmatrix} \right)^{-1} = (\Phi_a^T \Phi_a + \phi \phi^T)^{-1}
= \Sigma_a - (\Sigma_a \phi \phi^T \Sigma_a) / (1 + \phi^T \Sigma_a \phi)
\]

(14)
by the Sherman-Morrison-Woodbury formula \[8\], the cost of this update is one matrix multiply and one matrix-matrix subtraction per step.

**Neural networks value estimate.** If we are approximating our Q-value function using a neural network then the above analysis does not hold. However if the last layer of the network is linear, then the Q-values are approximated as

\[ Q^\pi(s, a) = \phi(s)^Tw_a, \]

where \( w_a \) are the weights of the last layer associate with action \( a \) and \( \phi(s) \) is the output of the network up to the last layer for state \( s \). In other words we can think of a neural network as learning a useful set of basis functions such that a linear combination of them approximates the Q-values. Then, if we ignore the uncertainty in the \( \phi \) mapping, we can reuse the analysis for the purely linear case to derive an approximate measure of local uncertainty that might be useful in practice.

This scheme has some advantages. As the agent progresses it is learning a state representation that helps it achieve the goal of maximizing the return. The agent will learn to pay attention to small but important details (e.g., the ball in Atari ‘breakout’) and learn to ignore large but irrelevant changes (e.g., if the background suddenly changes). This is a desirable property from the point of view of using these features to drive exploration, because the states that differ only in irrelevant ways will be aliased to (roughly) the same state representation, and states that differ is small but important ways will be mapped to quite different state vectors, permitting a more task-relevant measure of local uncertainty.

## 5 Algorithm for Deep Reinforcement Learning

In this section we describe an exploration heuristic for deep reinforcement learning whereby we attempt to learn both the Q-values and the uncertainties associated with them simultaneously (we assume the biases are small enough to ignore). The goal is for the agent to explore areas where it learns that it has higher uncertainty. This is in contrast to the commonly used \( \epsilon \)-greedy [20] and Boltzmann exploration strategies [19, 23] which simply inject noise into the agents actions. Our policy uses Thompson sampling [38], where the action is selected as

\[
a = \arg\max_b (\hat{Q}^\pi(s, b) + \alpha \zeta(b)u(s, b)^{1/2})
\]

where \( \zeta(b) \sim \mathcal{N}(0, 1) \) and \( \alpha > 0 \) is a hyper-parameter. In this case the probability of selecting action \( a \) is the probability that \( a \) has the maximum value if each action \( b \) was distributed normally with mean \( \hat{Q}^\pi(s, b) \) and variance \( \alpha^2u(s, b) \).

The technique is described in pseudo-code in algorithm 1. We refer to the technique as one-step since the uncertainty values are updated using a one-step SARSA Bellman backup, but it is easily extendable to the \( n \)-step case. The algorithm takes as input a neural network which has two output heads, one which is attempting to learn the optimal Q-values as normal, the other is attempting to learn the uncertainty values of the current policy (which is constantly changing). We do not allow the gradients from the uncertainty head to flow into the trunk; this ensures the Q-value estimates are not perturbed by the changing uncertainty signal. For the local uncertainty measure we use the linear basis approximation described previously. We have dropped the constant \( \beta \) from the uncertainty Bellman equation (10) and the unknown \( \sigma^2 \) term from the local-uncertainty in equation (13) because they are both absorbed by the hyper-parameter \( \alpha \) in the policy.

Most of the assumptions that allowed us to bound the true Q-values in equation (5) are violated by this scheme, in particular we have ignored the bias term, and the policy is changing as the Q-values change. However, we might expect this strategy to provide a useful signal of novelty to the agent and therefore perform well in practice.
Algorithm 1 One-step UBE exploration with linear uncertainty estimates.

```
// Input: Neural network outputting Q and u estimates
// Input: Q-value learning subroutine qlearn
// Input: Thompson sampling hyper-parameter α > 0

Initialize Σ_a = μI for each a, where μ > 0

Get initial state s, take initial action a

repeat
  Retrieve feature mapping φ(s) from input to last layer of Q-head
  Receive new state s' and reward r
  Calculate Q-value estimates Q(s', ·), uncertainty estimates u(s', ·)
  Calculate action a' = argmax_b(Q(s', b) + αζ(b)u(s', b)^1/2), where ζ(b) ~ N(0, 1)
  Calculate y = \{ φ(s)^TΣ_aφ(s), for terminal s'
                    φ(s)^TΣ_aφ(s) + γ^2u(s', a'), o.w. \}
  Take gradient step in u subnetwork with respect to error (y - u(s, a))^2
  Update Q-values using qlearn(s, a, r, s', a')
  Update Σ_{a'} according to eq. (14)
  Take action a'

until T > T_{max}
```

5.1 Experimental results

Here we present results of algorithm (1) on the Atari suite of games [3], where the network is attempting to learn the Q-values as in DQN [20, 21] and the uncertainties simultaneously. The only change to vanilla DQN we made was to replace the ε-greedy policy with Thompson sampling over the learned uncertainty values, where the α constant in (15) was chosen to be 0.01 for all games, by a parameter sweep. We used the exact same network architecture, learning rate, optimizer, pre-processing and replay scheme as [21]. For the uncertainty head we used a single fully connected hidden layer with 512 hidden units followed by the output layer. We trained the uncertainty head using a separate RMSProp optimizer [39] with learning rate 10^{-3}. The addition of the uncertainty head and the computation associated with it, only reduced the frame-rate compared to vanilla DQN by about 10% on a GPU, so the speed cost of the approach is negligible.

We compare two versions of our approach: a 1-step method and an n-step method where we set n to 150. The n-step method accumulates the uncertainty signal over n time-steps before performing an update which should lead to the uncertainty signal propagating to earlier encountered states faster, at the expense of increased variance of the signal. Note that in all cases the Q-learning update is always 1-step; our n-step implementation only affects the uncertainty update.

We compare our approaches to vanilla DQN, and also to an exploration bonus intrinsic motivation approach, where the agent receives an augmented reward consisting of the extrinsic reward and the square root of the linear uncertainty (13), which was scaled by a hyper-parameter chosen to be 0.1 by a sweep. In this case a stochastic policy was still required for good performance and so we used ε-greedy with the DQN annealing schedule.

In the recent work by Bellemare et al. [2], and the follow-up work [29], the authors add an intrinsic motivation signal to a DQN-style agent that has been modified to use the full Monte Carlo return of the episode when learning the Q-values. Using Monte Carlo returns dramatically improves the performance of DQN in a way unrelated to exploration, and due to that change we can’t compare the numerical results directly. In order to have a point of comparison we implemented our own intrinsic motivation exploration signal, as
discussed above. Similarly, we can’t compare directly to the numerical results obtained by Bootstrap DQN \cite{24} since that agent is using Double-DQN, a variant of DQN that achieves a higher performance in a way unrelated to exploration. However, we note that our approach achieves a higher evaluation score in 27 out of the 48 games tested in the Bootstrap DQN paper despite using an inferior base DQN implementation, and it runs at a significantly lower computational and memory cost.

We trained all strategies for 200M frames (about 8 days on a GPU). Each game and strategy was tested three times per method with the same hyper-parameters but with different random seeds, and all plots and scores correspond to an average over the seeds. All scores were normalized by subtracting the average score achieved by an agent that takes actions uniformly at random. Every 1M frames the agents were saved and evaluated (without learning) on 0.5M frames, where each episode is started from the random start condition described in \cite{21}. The final scores presented correspond to first averaging the evaluation score in each period across seeds, then taking the max average episodic score observed during any evaluation period. Of the tested strategies the \( n \)-step UBE approach was the highest performer in 32 out of 57 games, the 1-step UBE approach in 14 games, DQN in 1 game, the exploration bonus strategy in 7 games, and there were 3 ties. In table 1 we give the mean and median normalized scores as percentage of an expert human normalized score across all games, and the number of games where the agent is ‘super-human’, for each tested algorithm. Note that the mean scores are significantly affected by a single outlier with very high score (‘Atlantis’), and therefore the median score is a better indicator of agent performance. In Figure 1 we plot the number of games at super-human performance against frames for each method, and in Figure 2 we plot the median performance across all games against frames for all methods. The results across all 57 games, as well as the learning curves for all 57 games, are given in the appendix.

Of particular interest is the game ‘Montezuma’s Revenge’, a notoriously difficult exploration game where no one-step algorithm has managed to learn anything. Our 1-step strategy learns in 200M frames a policy that is able to consistently get about 500 points, which is the score the agent gets for picking up the first key and moving into the second room. In Figure 3 we show the learning progress of the agents for 500M frames where we set the Thompson sampling parameter slightly higher; 0.016 instead of 0.01 (since this game is a challenging exploration task it stands to reason that a higher exploration parameter is required). By the end of 500M frames the \( n \)-step agent is consistently getting around 3000 points, which is several rooms of progress. These scores are close to state-of-the-art, and are state-of-the-art for one-step methods (like DQN) to the best of our knowledge.

|                      | mean   | median | > human |
|----------------------|--------|--------|---------|
| DQN                  | 688.60 | 79.41  | 21      |
| DQN Intrinsic Motivation | 472.93 | 76.73  | 24      |
| DQN UBE 1-step       | 776.40 | 94.54  | 26      |
| DQN UBE n-step       | 439.88 | 126.41 | 35      |

Table 1: Scores for the Atari suite, as a percentage of human score.

6 Conclusion

In this paper we derived a Bellman equation on the uncertainties of any estimator of the Q-values of a policy, under some conditions. This allows an agent to propagate uncertainty across many time-steps, so-called ‘deep-exploration’, in the same way that value propagates through time in the standard dynamic
Figure 1: Number of games at super-human performance.

Figure 2: Median performance across all games.

Figure 3: UBE on Montezuma’s Revenge for 500M frames.
programming recursion. This uncertainty can be used by the agent to make decisions about which states and actions to explore, in order to gather more data about the environment and learn a better policy. Since the uncertainty satisfies a Bellman recursion, the agent can learn it using the same reinforcement learning machinery that have been developed for value functions. We showed that an algorithm based on this learned uncertainty can boost the performance of standard deep-RL techniques. Our technique was able to improve the average performance of DQN across the Atari suite of games, when compared against DQN using ϵ-greedy.

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References

[1] M. G. Azar, R. Munos, and B. Kappen, On the sample complexity of reinforcement learning with a generative model, in Proceedings of the 29th International Conference on Machine Learning (ICML), 2012.

[2] M. Bellemare, S. Srinivasan, G. Ostrovski, T. Schaul, D. Saxton, and R. Munos, Unifying count-based exploration and intrinsic motivation, in Advances in Neural Information Processing Systems, 2016, pp. 1471–1479.

[3] M. G. Bellemare, Y. Naddaf, J. Veness, and M. Bowling, The arcade learning environment: An evaluation platform for general agents, Journal of Artificial Intelligence Research, (2012).

[4] R. Bellman, Dynamic programming, Princeton University Press, 1957.

[5] D. P. Bertsekas, Dynamic programming and optimal control, vol. 1, Athena Scientific, 2005.

[6] J. A. Boyan, Least-squares temporal difference learning, in ICML, 1999, pp. 49–56.

[7] R. I. Brafman and M. Tennenholtz, R-max: A general polynomial time algorithm for near-optimal reinforcement learning, Journal of Machine Learning Research, 3 (2002), pp. 213–231.

[8] G. H. Golub and C. F. Van Loan, Matrix computations, vol. 3, JHU Press, 2012.

[9] A. Guez, D. Silver, and P. Dayan, Efficient Bayes-adaptive reinforcement learning using sample-based search, in Advances in Neural Information Processing Systems, 2012, pp. 1025–1033.

[10] G. H. Hardy, J. E. Littlewood, and G. Pólya, Inequalities, Cambridge university press, 1952.

[11] T. Jaksch, R. Ortner, and P. Auer, Near-optimal regret bounds for reinforcement learning, Journal of Machine Learning Research, 11 (2010), pp. 1563–1600.

[12] S. M. Kakade, On the sample complexity of reinforcement learning, PhD thesis, University of London London, England, 2003.
[13] M. Kearns and S. Singh, *Near-optimal reinforcement learning in polynomial time*, Machine Learning, 49 (2002), pp. 209–232.

[14] T. L. Lai and H. Robbins, *Asymptotically efficient adaptive allocation rules*, Advances in Applied Mathematics, 6 (1985), pp. 4–22.

[15] T. Lattimore, *Regret analysis of the anytime optimally confident UCB algorithm*, arXiv preprint arXiv:1603.08661, (2016).

[16] T. Lattimore and M. Hutter, *Pac bounds for discounted MDPs*, in International Conference on Algorithmic Learning Theory, Springer, 2012, pp. 320–334.

[17] S. Mannor, D. Simester, P. Sun, and J. N. Tsitsiklis, *Bias and variance approximation in value function estimates*, Management Science, 53 (2007), pp. 308–322.

[18] S. Mannor and J. Tsitsiklis, *Mean-variance optimization in Markov decision processes*, in Proceedings of the 28th International Conference on Machine Learning (ICML), 2011, pp. 177–184.

[19] V. Mnih, A. P. Badia, M. Mirza, A. Graves, T. Lillicrap, T. Harley, D. Silver, and K. Kavukcuoglu, *Asynchronous methods for deep reinforcement learning*, in Proceedings of the 33rd International Conference on Machine Learning (ICML), 2016, pp. 1928–1937.

[20] V. Mnih, K. Kavukcuoglu, D. Silver, A. Graves, I. Antonoglou, D. Wierstra, and M. Riedmiller, *Playing atari with deep reinforcement learning*, in NIPS Deep Learning Workshop, 2013.

[21] V. Mnih, K. Kavukcuoglu, D. Silver, A. Rusu, J. Veness, M. G. Bellemare, A. Graves, M. Riedmiller, A. K. Fidjeland, G. Ostrovski, S. Petersen, C. Beattie, A. Sadik, I. Antonoglou, H. King, D. Kumaran, D. Wierstra, S. Legg, and D. Hassabis, *Human-level control through deep reinforcement learning*, Nature, 518 (2015), pp. 529–533.

[22] R. Munos, *From bandits to Monte-Carlo tree search: The optimistic principle applied to optimization and planning*, Foundations and Trends® in Machine Learning, 7 (2014), pp. 1–129.

[23] B. O’Donoghue, R. Munos, K. Kavukcuoglu, and V. Mnih, *Combining policy gradient and Q-learning*, in International Conference on Learning Representations (ICLR), 2017.

[24] I. Osband, C. Blundell, A. Pritzel, and B. Van Roy, *Deep exploration via bootstrapped DQN*, in Advances In Neural Information Processing Systems, 2016, pp. 4026–4034.

[25] I. Osband, D. Russo, and B. Van Roy, *More efficient reinforcement learning via posterior sampling*, in Advances in Neural Information Processing Systems, 2013, pp. 3003–3011.

[26] I. Osband, D. Russo, Z. Wen, and B. Van Roy, *Deep exploration via randomized value functions*, arXiv preprint arXiv:1703.07608, (2017).

[27] I. Osband and B. Van Roy, *On lower bounds for regret in reinforcement learning*, stat, 1050 (2016), p. 9.

[28] —, *Why is posterior sampling better than optimism for reinforcement learning*, arXiv preprint arXiv:1607.00215, (2016).
[39] T. Tieleman and G. Hinton, *Lecture 6.5-rmsprop: Divide the gradient by a running average of its recent magnitude*, COURSERA: Neural Networks for Machine Learning, 4 (2012).

[40] C. J. C. H. Watkins, *Learning from delayed rewards*, PhD thesis, University of Cambridge England, 1989.
8 Appendix

8.1 Bound on the cross-term

Here we prove the bound on the cross-term given in equation (8)

\[
c(s, a) = E_d \left[ (\epsilon(s, a) - E_d \epsilon(s, a)) [\hat{Q}^\pi(s', a') - Q^\pi(s', a') - \text{bias} \hat{Q}^\pi(s', a')] \right]
\]

\[
= E_{s', a'} E_d \left[ (\epsilon(s, a) - E_d \epsilon(s, a)) (\epsilon(s', a') - E_d \epsilon(s', a') \right.
\]

\[
+ \gamma E_{s'', a''} [\hat{Q}(s'', a'') - Q(s'', a'') - \text{bias} \hat{Q}^\pi(s'', a'')] \left. \right] \right]
\]

\[
= E_{s', a', s'', a''} \ldots E_d \left[ (\epsilon(s, a) - E_d \epsilon(s, a)) \right.
\]

\[
\times (\epsilon(s', a') - E_d \epsilon(s', a') + \gamma (\epsilon(s'', a'') - E_d \epsilon(s'', a'')) + \gamma^2 (\ldots)) \left. \right] \right]
\]

\[
\leq \max_{s', a', s'', a''} \ldots E_d \left[ (\epsilon(s, a) - E_d \epsilon(s, a)) \right.
\]

\[
\times (\epsilon(s', a') - E_d \epsilon(s', a') + \gamma (\epsilon(s'', a'') - E_d \epsilon(s'', a'')) + \gamma^2 (\ldots)) \left. \right] \right]
\]

\[
= \text{var} \epsilon(s, a)(1 + \gamma + \gamma^2 + \ldots) = \text{var} \epsilon(s, a)/(1 - \gamma),
\]

where we have repeatedly used the fact that \( \hat{Q}^\pi(t, b) - Q^\pi(t, b) = \gamma E_{t', b'} (\hat{Q}^\pi(t', b') - Q^\pi(t', b')) + \epsilon(t, b) \) for any \((t, b)\), the fact that the biases satisfy a Bellman equation, and assumption 1 which implies that the max over each \( s', a' \) is attained when \((s', a') = (s, a)\).

If we have more knowledge about the policy and the MDP then we can provide tighter bounds. For example, if we know that under the policy the agent cannot visit the same state before \( T \) time-steps then the cross-term can be bounded by \( c(s, a) \leq \gamma^{T-1} \text{var} \epsilon(s, a)/(1 - \gamma^T) \) and the multiplicative factor becomes \((1 + \gamma^T)/(1 - \gamma^T)\). In particular a policy which never visits the same state twice (e.g., where the MDP is acyclic) has \( c(s, a) = 0 \) and the multiplicative factor in the uncertainty Bellman equation is one.

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Table 2: Normalized scores for the Atari suite from random starts, as a percentage of human normalized score.
8.2 Learning curves
Million Frames
0 50 100 150 200
Average Episode Return
venture
DQN
DQN Intrinsic Motivation
DQN UBE 1-step
DQN UBE n-step

Million Frames
0 50 100 150 200
Average Episode Return
video_pinball
DQN
DQN Intrinsic Motivation
DQN UBE 1-step
DQN UBE n-step

Million Frames
0 50 100 150 200
Average Episode Return
wizard_of_wor
DQN
DQN Intrinsic Motivation
DQN UBE 1-step
DQN UBE n-step

Million Frames
0 50 100 150 200
Average Episode Return
yars_revenge
DQN
DQN Intrinsic Motivation
DQN UBE 1-step
DQN UBE n-step

Million Frames
0 50 100 150 200
Average Episode Return
zaxxon
DQN
DQN Intrinsic Motivation
DQN UBE 1-step
DQN UBE n-step