Elastic Step DQN: A novel multi-step algorithm to alleviate overestimation in Deep Q-Networks

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Abstract

Deep Q-Networks algorithm (DQN) was the first reinforcement learning algorithm using deep neural network to successfully surpass human level performance in a number of Atari learning environments. However, divergent and unstable behaviour have been long standing issues in DQNs. The unstable behaviour is often characterised by overestimation in the Q-values, commonly referred to as the overestimation bias. To address the overestimation bias and the divergent behaviour, a number of heuristic extensions have been proposed. Notably, multi-step updates have been shown to drastically reduce unstable behaviour while improving agent’s training performance. However, agents are often highly sensitive to the selection of the multi-step update horizon \(n\), and our empirical experiments show that a poorly chosen static value for \(n\) can in many cases lead to worse performance than single-step DQN. Inspired by the success of \(n\)-step DQN and the effects that multi-step updates have on overestimation bias, this paper proposes a new algorithm that we call ‘Elastic Step DQN’ (ES-DQN). It dynamically varies the step size horizon in multi-step updates based on the similarity of states visited. Our empirical evaluation shows that ES-DQN out-performs \(n\)-step with fixed \(n\) updates, Double DQN and Average DQN in several OpenAI Gym environments while at the same time alleviating the overestimation bias.
1 Introduction

One of the most prominent reinforcement learning algorithms is Q-learning (Watkins and Dayan, 1992), which has been shown to converge to optimal policies when used with lookup tables. However, tabular Q-learning is limited to small sized and toy environments, and lookup tables are computationally inefficient when environments have large state action spaces. To address the scalability of Q-learning, deep neural networks became a viable alternative to lookup tables to approximate state-action values in large continuous spaces. One of the most popular algorithms is the Deep Q-Network (DQN) (Mnih, Kavukcuoglu, Silver, Graves, Antonoglou, Wierstra and Riedmiller, 2013; Mnih, Kavukcuoglu, Silver, Rusu, Veness, Bellemare, Graves, Riedmiller, Fidjeland, Ostrovski et al., 2015) which uses neural networks and introduced the concept of a target network and replay memory with great success in the Atari games environment. In spite of the success, training instability and divergent behaviour is regularly observed in DQN (Sutton and Barto, 2018; Van Hasselt, Guez and Silver, 2016). The divergent behaviour itself was not specific to DQN, and has also been heavily investigated for function approximators in the past (Sutton and Barto, 2018; Baird, 1995; Tsitsiklis and Van Roy, 1997) with a number of linear solutions having been proposed to address the problem (Maei, Szepesvari, Bhatnagar, Precup, Silver and Sutton, 2009; Baird, 1995). Overestimation of the $Q$-values has frequently been identified as one of the key reasons that causes sub-optimal learning and divergent behaviour – this was thoroughly investigated by Thrun and Schwartz (1993) who attributed the issue to noise generated through function approximation. On the other hand, Hasselt (2010) theorised that the overestimation originated from the max operator used as part $Q$ value updates which tends estimations towards larger values and a more optimistic outlook. Van Hasselt et al. (2018) and Van Hasselt et al. (2016) have suggested that by correcting for overestimation, an agent is much less susceptible to divergent behaviours.

Empirical observations by Van Hasselt et al. (2018) and Hasselt, Modayil, Van Hasselt, Schaul, Ostrovski, Dabney, Horgan, Piot, Azar and Silver (2018) characterised a number of plausible architectural and algorithmic mechanics that may lead to divergent behaviour as well as suggestions that may alleviate divergence. Van Hasselt et al. (2016) also hypothesised that multi-step returns are likely to reduce the occurrence of divergence. This idea that multi-step DQN updates can regulate and reduce divergent behaviour while at the same time return stronger training performance is not without merit. Multi-step implementations like the Rainbow agent (Hessel et al., 2018) and Mixed Multi-step DDPG (Meng, Gorbet and Kulić, 2021) have shown empirically that multi-step updates under certain conditions are more stable, and in many circumstances can circumvent the divergence problem that exists in single-step DQN. However, studies have also shown that multi-step DQN updates are highly sensitive to the selection of the value $n$ which if incorrectly selected can be detrimental to learning (Hessel et al. 2018; Chiang, Yang, Hong and Lee, 2020; Horgan, Quan, Budden, Barth-Maron, Hessel, Van Hasselt and Silver, 2018; Deng, Yin, Deng and Li, 2020; Fedus, Ramachandran, Agarwal, Bengio, Larochelle, Rowland and Dabney, 2020). This raises the question then, is a static value of $n$ the best approach to multi-step updates or is it possible to dynamically select the $n$ parameter and take advantage of the special properties that multi-step updates provide.

One possible approach is inspired by the work of Dazeley, Vamplew and Bignold (2015), who identified an issue where agents may diverge in a grid world setting under linear approximation due to a self-referential learning loop problem. It was suggested that the consolidation of consecutive states and the treatment of them as sub-states of larger state, can encourage more stable algo-
rithmic performance. However the ideas were limited to a grid world setting under linear function approximation. In this paper, we extend the ideas of Dazeley et al. (2015) into a deep reinforcement learning context by leveraging a multi-step update.

As a combination of these ideas, this paper will introduce Elastic Step DQN (ES-DQN) – a novel multi-step update that dynamically selects the step size horizon based on consecutive state similarity. The intuition behind the idea of consolidating similar states together is in general inspired by spatial information theory which identified that people have a natural inclination to use landmarks to provide route directions (Michon and Denis, 2001; Klippel and Winter, 2005). When providing directions, individuals tend to summarise the instructions based on broader objectives and use landmarks to anchor and help generate mental images (e.g. ‘walk down the end of the hallway and turn left once you see the toilet’, in comparison to more detailed step by step descriptions – ‘take one step then another step until you reach the end of the hallway’). Our experimental results indicate that the systematic accumulation of experiences that are similar is able to achieve comparable performance to the well established DQN extensions and superior performance to n-step updates. Furthermore to achieve statistical significance for the experiments, this paper will primarily use three small sized environments as its test bed for this investigation.

The following sections will investigate the efficacy of multi-step updates, against single-step DQN as well as introduce a novel multi-step DQN update that automates the selection of the step size horizon. The algorithm will also be compared against DoubleDQN and Average DQN which are well established methods of reducing overestimation. This paper makes four key contributions:

• introduce the idea of dynamic multi-step updates based on state similarity
• the introduction of ES-DQN to select the n step horizon dynamically
• an in-depth empirical exploration of n-step DQN against ES-DQN
• and an in-depth empirical analysis of algorithmic stability when grouping together similar states.

2 Related works

2.1 Background

The training of a reinforcement learning agent is typically unguided and is characterised by a Markov decision process where the agent would at each time step \( t \) observe a particular state \( S_t \) before it takes an action \( A_t \). The agent would receive some sort of reward \( R_{t+1} \) and enter into a new state \( S_{t+1} \) – the main objective is for the agent to learn an optimal policy that maximises the expected discounted accumulation of rewards \( G_t \) at time \( t \) to \( k \) steps into the future, at the discount factor \( \gamma \).

\[
G_t \equiv \sum_{k=1}^{k-1} \gamma^k R_{t+k+1}
\]

Classical reinforcement learning algorithms rely largely on lookup tables to store state action values to learn an optimal policy – one such algorithm is Q-learning which was first introduced by Watkins and Dayan (1992) and has since been a focal point of value based reinforcement learning approaches. As a Q-learning agent navigates its environment and receives responses from the
environment, the lookup table is updated at every time step where $Q$ is the state-action value function, $\alpha$ is the learning rate, $R$ is the reward, and $A'$ is an action selected from a policy derived from $Q$ [Sutton and Barto, 2018].

$$Q^{new}(S, A) \leftarrow Q(S, A) + \alpha[R + \gamma \max_{A'} Q(S', A') - Q(S, A)]$$

Multi-step updates (Sutton and Barto, 2018) expand on single-step by temporally extending the step size horizon of the target by the value of $n$, traditionally multi-step updates were infrequently used because it was inconvenient to implement and were more used as an intermediate step to eligibility traces. However, multi-step updates have shown to allow for faster convergence (Sutton and Barto, 2018; Ceron and Castro, 2021) when the value of $n$ is well-tuned.

### 2.2 Related literature

Conceptually the proposed multi-step updates in this paper extends on the ideas introduced in Options (Sutton, Precup and Singh, 1999) and Coarse Q-learning (Dazeley et al., 2015). Options were first formalized as a framework to allow agents to take sub-actions under a single policy until a termination condition is activated. The termination condition can come in the form of a sub-goal being achieved or when a certain temporal range is met. Similarly Coarse Q-learning builds on the Options framework and explores the issue of a wandering agent in a coarsely quantised environment. Dazeley et al. (2015) showed that divergence under quantisation can be explained by a wandering phenomenon where an agent when trapped in the same state for multiple updates may wander aimlessly and exhibit unstable learning. To address the behaviour, Dazeley et al. (2015) introduces clamped actions which force the agent to take the same action until the quantised state is exited, and the $Q$-function is only updated once this occurs. While conceptually both Options and Coarse Q-learning is similar to our approach, both frameworks extend largely to linear function approximators.

Interestingly, while our idea is relatively simple, the concept of consolidating experiences based on state similarity to address value-based divergence has been relatively unexplored in deep reinforcement learning. Early works like the Rainbow agent incorporated multi-step updates into DQN (Hessel et al., 2018; Van Hasselt et al., 2018) which surpassed super-human performance benchmarks set by the DQN and Double DQN agents. While the study indicated that the incorporation of multi-step methods had a strong positive impact on overall agent performance, it was limited in sample size due to the computational intensity of the Atari games. Ceron and Castro (2021) further investigated this with a large exploratory set of experiments and was able to show in an ablation study that the inclusion of multi-step update in DQN yielded strong performance gains, but the study was limited, as it only compared single-step DQN and $n$-step DQN based on the same set of hyper-parameters. As single-step and $n$-step DQN are different algorithms, they may have a different set of optimal hyper-parameters. Meng et al. (2021) showed empirically that a step size where $n = 1$ was comparatively more prone to inaccurate estimations of the $q$-value in comparison to values where $n > 1$. The authors also observed an improvement in training performance when the target was abstracted by an aggregate function over a set time horizon. A similar conclusion was again reached by Chiang et al. (2020) who experimented with a mixture of different step sizes and achieved stronger agent performance across a series of Atari test beds than single-step DQN. The authors hypothesised that the incremental improvement of agent performance was a result from an increased level of heterogeneity from the samples collected in the replay memory. While the study
in general was limited by sample size having had only 3 random seeds as empirical evidence, it provided interesting insights into the potential of mixing step sizes to address both performance and estimation deficiencies experienced with single-step DQN. Other papers like (Deng et al., 2020) also recognised the value of multi-step updates but their approach focused on discount rates that further regularises the reward accumulated to moderate the overestimation potential in multi-step updates.

Moreover, there also exists a wide body of work ((Van Hasselt et al., 2016; Hasselt, 2010; Anschel, Baram and Shimkin, 2017; Wang, Schaul, Hessel, Hasselt, Lanctot and Freitas, 2016; Colas, Sigaud and Oudeyer, 2018; Dabney, Rowland, Bellemare and Munos, 2018; Lan, Pan, Fyshe and White, 2019)) that while indirectly related to our investigation should be noted as they are widely used approaches to address divergent behaviours exhibited by DQN and serves as good benchmarks for our analysis. Of the large body of work, Double DQN and Average DQN will be used as benchmark algorithms in this paper, both algorithms have shown efficacy with tempering overestimation in DQN. Double DQN argues that the max operator used in DQN to both select and evaluate actions inadvertently leads the agent to be over optimistic in its value estimations. To address the problem of overestimation induced the max operator, Double DQN decouples the use of the max operator in action and selection and evaluation. In contrast, Average DQN was also able to achieve a much more stable agent by taking the average of $k$ previous state action value estimates. This allowed the agent to produce more conservative and moderate state action values over time, thus reducing the overestimation. It is also possible as explored by (Sabry and Khalifa, 2019) that overestimation can be addressed through altering the neural network structure. Sabry and Khalifa (2019) through their empirical investigations showed that the use of dropout layers may help alleviate overestimation.

Another related area similar to our approach are algorithmic methods that use contrastive learning and representation learning to remove noise and extract low-dimensional features from the observational space (Laskin, Srinivas and Abbeel, 2020; Misra, Henaff, Krishnamurthy and Langford, 2020; Pathak, Agrawal, Efros and Darrell, 2017; Efroni, Misra, Krishnamurthy, Agarwal and Langford, 2021). A major difference between the contrastive and representation learning approaches applied in a reinforcement learning context is that algorithms such as CURL (Laskin et al., 2020) act as prepossessing techniques that extract features from high-dimensional observation spaces and projects it to a more enriched lower dimensional space. On the other hand our algorithm builds a mechanism into the DQN to extract intermediate feature outputs from feed-forward layers to be used as training observations for an unsupervised learning algorithm, this component while non-trivial, represents a small portion of the algorithm.

Across the literature, overestimation is typically measured in terms of how far the $Q$-value diverges from the realisable true value of $Q$. In (Fujimoto, Hoof and Meger, 2018), the true value is calculated as the average discounted return when the agent follows the current policy. In contrast, Hasselt (2010); Van Hasselt et al. (2016) measured overestimation based on how far it deviated from the realisable range of the true absolute $Q$ value ($|Q|$) - this was made possible because the rewards in the environment was bounded between $[-1, 1]$ and the gamma used was 0.99.

### 3 Elastic Step Deep Q-Networks

The objective of Elastic Step DQN is to incorporate the ideas from Coarse Q-learning and multi-step DQN to reduce overestimation and improve the overall performance of DQN. To achieve this there needs to be a method of identifying whether two states are similar or dissimilar that is agnostic to
Figure 1: (1) the DQN agent observes $s_t$ and takes $a_t$ (2) receives $s_{t+1}$ and $r$ (3) output from $Q_h(s_{t+1})$ is stored in the state memory (4) a dataset is sampled from the state memory, (5) this is normalised to unit variance and the clustering algorithm is fitted to the dataset (5a) cluster labels between $s_t$ and $s_{t+1}$ are compared. (6) If they are different then the tuple $(s_t, a_t, s_{t+1}, r)$ is added to the replay memory, if the cluster labels are not different, then the tuple is not added to the replay, the reward is accumulated. (7) Agent samples from replay and the primary network is trained.

State input structures or data type. One approach of doing this is through unsupervised clustering algorithms. Unsupervised clustering algorithms [Károly, Fullér and Galambos 2018] are a class of algorithms designed to identify patterns in data without labels – in this paper we use an algorithm known as HDBSCAN [McInnes, Healy and Astels 2017; McInnes and Healy 2017; Hinneburg and Keim 1999] which has been shown to be very effective at identifying non-even transductive clusters. HDBSCAN is a clustering algorithm that extends on DBSCAN and was selected due to its robustness towards parameter selection, the algorithm performs well out of the box and required no parameter tuning of its own during the experiments. The algorithm much like its base variant, DBSCAN is also robust to the existence of outliers. KMeans and spectral clustering were also considered however both required the user to pre-determine the number of clusters which is unknown in the environments we experimented on (Hamerly and Elkan 2003; Von Luxburg 2007; Ng, Jordan and Weiss 2001). The lack of hyper-parameter tuning naturally lent itself well to our experiments which needed to be transferable across different environments.

There are two main components to this extension of DQN – the first component is state information extraction and storage, here the aim is to find a suitable representation of the state to be used in the clustering algorithm. The second component involves the clustering and how its outputs are used to select the step horizon, which includes the reward accumulation.
3.1 State information extraction and storage

3.1.1 State information extraction

A core component of Elastic Step DQN is the use of HDBSCAN to assign cluster labels to states. Previous research has indicated that Talavera (1999) high quality features generally plays a large role in the quality of clusters produced. Consequently we considered extracting the hidden node outputs as feature inputs into the unsupervised algorithm as previous research by Çayir, Yenidoğan and Dağ (2018) have indicated that it could be effective method to improve classifier performance. We experimented between an Elastic Step DQN variant that used raw state values as input against one that used outputs from the hidden node of the primary network and discovered that in both Cartpole and Mountain Car, we achieved much stronger training performance using the hidden node outputs as shown in Figure 2. The performance difference between the use of raw state values vs hidden node outputs \( Q_h(s) \) led us to choose the hidden node outputs as feature inputs into HDBSCAN.

3.1.2 State information storage

Prior to the main algorithm loop a time-step counter \( d \) is initialised at \( d = 0 \), the agent will observe the current state \( s_t \) and take an action \( a_t \) (label (1) in Figure 1). The agent will receive \( s_{t+1} \) and \( r_t \) (label (2) in Figure 1) and parse both \( s_t \) and \( s_{t+1} \) through the primary DQN network through to the hidden layer \( Q_h \). The hidden layer output is extracted (label (3)) and stored in a state memory bank \( B \) (label (4) in Figure 1). The state memory bank \( B \) is populated with the outputs from the hidden node \( Q_h(s_t) \) generated from a uniform policy before any update has been applied. This early component is to ensure there is enough data to train the clustering algorithm in the initial stages. The state memory bank \( B \) has a capacity of \( H \), as new transformed states are added to the state memory bank, the older states are gradually replaced over time, this is to encourage diversity of more recent samples in the state memory bank. 
Figure 2: The blue line represents the training performance of Elastic Step DQN when the raw state is used while the red line represents the training performance when $Q(h)$ is used as input into the clustering algorithm. The training performance is averaged over 30 seeds, and the shaded region represents the 95 percent confidence interval.

3.2 State clustering

Once the state memory bank $B$ is filled, the agent samples a dataset with replacement from $B$ – each feature from this data-set is then standardised by removing the mean and scaled to unit variance. The data is sampled with replacement to ensure that the selected batch used to train the unsupervised algorithm is representative. Like most unsupervised clustering algorithm, HDBSCAN is less effective when the dataset is high dimensional [McInnes et al. (2017); McInnes and Healy (2017); Hinneburg and Keim (1999)], as a result if the number of features is greater than 30, then principal component analysis [Ding and He (2004)] is applied to the dataset and only the top 30 components are taken. HDBSCAN is then trained on the dataset. Cluster labels are then assigned to $Q_h(s_t)$ and $Q_h(s_{t+1})$ (there is no limit set to the number of labels assigned to the particular dataset), if the cluster labels between $Q_h(s_t)$ and $Q_h(s_{t+1})$ are the same (i.e., they are similar states), then the reward and $\gamma$ are accumulated $\sum \gamma^d r_{t+d+1}$ and the time step counter $d$ is also incremented.

If the cluster labels for $Q_h(s_t)$ and $Q_h(s_{t+d+1})$ are different or either of them represents the
terminal state, then the tuple \((s_t, a_t, r_{t+d+1}, s_{t+d+1}, \gamma^d)\) is then stored in the replay memory. In the instance where HDBSCAN detects outliers, each outlier is treated as a separate label, which means if both \(s_t\) and \(s_{t+d+1}\) are assigned an outlier label they are considered dissimilar. The performance of the algorithm is highly dependent on the quality of clusters generated, as a result it is important to retrieve a heterogeneous but representative sample of the environment for training. While HDBSCAN was the unsupervised clustering algorithm of choice for this paper, in theory any algorithm can be used as long as it generalises well to the environment.

**Algorithm 1** Elastic Step Deep Q-Network: \(u, M\) and \(T\) are all constants defined at the beginning of the algorithm, while \(Q_h\) denotes the hidden layer of \(Q\)

1: Initialize a step counter \(d = 0\), sample value \(u\), max of episodes \(M\), max of time-steps \(T\), and target update interval
2: Initialize primary network \(Q\) with weight \(\theta\), target network \(\hat{Q}\) with weight \(\theta^- = \theta\) and replay buffer \(D\) with capacity \(N\)
3: Initialize state memory bank \(B\) with capacity \(H\) and clustering algorithm \textit{Clusterer}
4: Pre-fill \(D\) with random experiences and \(B\) with the hidden layer outputs of the same experiences
5: for episode = 1 to \(M\) do
6: Reset the environment and observe the initial states
7: for each time step to \(T\) do
8: Select action \(a_t\) using \(\epsilon-greedy\)
9: Execute action in the environment and
10: observe the next state \(s_{t+d+1}\) and reward \(r_t\)
11: Pass \(s_t\) and \(s_{t+d+1}\) into \(Q_h\)
12: Extract output and store in \(B\)
13: With sample value \(u\), randomly sample from \(B\)
14: Train \textit{Clusterer} and assign cluster labels to \(Q_h(s_t)\) and \(Q_h(s_{t+d+1})\)
15: if cluster labels are not equal then
16: Store transition \((s_t, a_t, R_t, s_{t+d+1}, \gamma^d)\) in \(D\)
17: Reset counter step counter \(d = 0\)
18: else
19: Increment step counter \(d\)
20: \(R_t + = \gamma^d r_{t+d+1}\)
21: end if
22: Randomly sample mini-batch from \(D\)
23: \(y_{t+d+1} = \begin{cases} R_t & \text{for terminal } s_{t+d+1} \\ R_t + \gamma^d \max \hat{Q}(s_{t+d+1}, a_t) & \text{for non terminal } s_{t+d+1} \end{cases}\)
24: Update \(\theta\) by gradient descent
25: Update target network at each target update interval
26: end for
27: end for
4 Experiments

4.1 Experimental setup

To test the efficacy of Elastic Step DQN, a large number of experiments were run across three separate OpenAI gym environments (Cartpole, Mountain Car and Acrobot) (Brockman, Cheung, Pettersson, Schneider, Schulman, Tang and Zaremba, 2016). For consistency, this paper utilises the MushroomRL framework (D’Eramo, Tateo, Bonarini, Restelli and Peters, 2021) to implement all the algorithm. The use of smaller environments allows for a larger sample size of experiments to be run in comparison to what may be possible with larger environments (Ceron and Castro, 2021).

For each gym environment, eight separate DQN implementations (single-step DQN, 2/3/4/6/8 step DQN, Average DQN, Double DQN and Elastic Step DQN) were trained across 30 seeds for a range of different hyper-parameter settings. The best performing hyper-parameters across the 30 seeds were selected for comparison. Each algorithm was trained on Cartpole, Acrobot, Mountain Car for respectively 40000, 40000 and 30000 time steps. The performance is then evaluated across 100 epochs. Each epoch represents \((\text{timesteps})/100\) (i.e. 400, 400 and 3000 time steps is a single epoch for Cartpole, Acrobot, Mountain Car for respectively) - the reward was captured both at the episodic and epoch level (with standard deviation, median and mean captured at each epoch) while the \(|Q|-\text{values}\) were captured at every 1000 time-step. Across each environment, if the termination condition is not met, the episode will terminate at the 1000th time step.

From a hyper-parameter standpoint the search space for each algorithm was too large to be searched exhaustively, as a results only sensitive parameters were tuned while other parameters were based off of successful implementations of similar sized environments in the MushroomRL official repository. All agents received equal levels of hyper-parameter tuning, and each hyper-parameter set was trained for a full 30 seeds to check for statistical significance – as a result the best hyper-parameters for each algorithm in each environment is different (the hyper-parameters for each algorithm across the test-bed environments can be found in the Appendix A).

Each algorithm was evaluated on both the average final training reward and the average \(|Q|\) achieved. A two sample t-statistic is calculated on the final training reward (as defined as the last 5 epochs) between the benchmark algorithm and Elastic Step DQN. To measure for divergent behaviour, this paper will refer to the true value of \(|Q|\) as shown by (Thrun and Schwartz, 1993; Van Hasselt et al., 2018; Hasselt, 2010) where because the reward is bounded between \([-1, 1]\) across all three environments and the \(\gamma\) is 0.99, the true value of \(|Q|\) is bounded by \(\frac{1}{1-\gamma} = \frac{1}{1-0.99} = 100\). \(|Q|\)-values that exceed the upper bound of 100 are indicative of overestimation.

Traditionally, the default upper bound of time-steps before the termination condition for Cartpole, Mountain Car and Acrobot is set at 200 time-steps. However, the upper bound artificially caps the amount of reward that the agent can receive which can obscure how well or poorly an agent can truly perform, consequently the termination condition was set at 1000 steps for all three environments.

4.2 Analysis of the final training performance across \(n\)-step variants and DQN extensions

Elastic Step DQN was developed on the principle that dynamic selection of the value \(n\) can reduce overestimation bias and improve algorithmic training performance. The empirical trials computed across Cartpole, Acrobot and Mountain Car consistently showed statistically significant higher
Figure 3: 3a, 3c and 3e compare the training curves between the 2/3/4/6/8-Step DQN updates against Elastic Step DQN and single-step DQN. They show the average episodic rewards across the training epochs. The solid line represents the average reward while the shaded region represents the 95 percent confidence interval. The scatter plots 3b, 3d and 3f map the relationship between the average reward achieved across each experiment against the average $|Q|$-values from that experiment. The dotted dash line represents the upper bound of the true $|Q|$-value estimate.
Figure 4: Here the Elastic Step DQN algorithm is compared across the three test bed environments against well known variants of DQN that are known to address the divergent and overestimation issue. (a), (c) and (e) plots the training curve for each of the tested environments while (b), (d) and (f) plots the relationship between reward against the $|Q|$-value estimate. The dotted dash vertical line represents the upper bound of the absolute $|Q|$-value.
Table 1: This table outlines the final training reward performance of each algorithm averaged over the 30 seeds. The final reward performance is defined as only the last 10 epochs of each run. A two sample t-test is then calculated on the final performance data between Elastic Step DQN and all benchmark algorithms with the p-value reported for each environment in the table. The algorithms with the highest reward are in bold text.

|                | Cartpole | Acrobot | Mountain Car |
|----------------|----------|---------|--------------|
|                | $\bar{x}$ reward | s | p-value | $\bar{x}$ reward | s | p-value | $\bar{x}$ reward | s | p-value |
| DQN            | 100.7    | 29.6    | <0.05   | -107.6       | 89.4  | 0.22   | -156.8       | 26.5 | <0.05 |
| 2 step         | 74.3     | 31.3    | <0.05   | -121         | 89.4  | 0.12   | -462.9       | 153.5 | <0.05 |
| 3 step         | 76.9     | 40.7    | <0.05   | -110.6       | 28.9  | <0.05  | -880.8       | 161.5 | <0.05 |
| 4 step         | 29       | 20.5    | <0.05   | -93.2        | 20.6  | 0.75   | -753.8       | 180   | <0.05 |
| 6 step         | 9.8      | 1.2     | <0.05   | -91.5        | 16.4  | 0.39   | -513.4       | 226.5 | <0.05 |
| 8 step         | 10       | 1.5     | <0.05   | -213.8       | 70.4  | <0.05  | -891.4       | 191   | <0.05 |
| Double         | 225.7    | 166.6   | <0.05   | -103.3       | 19    | 0.19   | -162.8       | 55.6  | <0.05 |
| Average        | 183.6    | 38.2    | <0.05   | -100.8       | 31.4  | 0.31   | -153.9       | 21.7  | <0.05 |
| Elastic Step   | **413.4**| 112.2   |         | -94.5        | 9.9   |        | **-123.4**   | 19.8  |        |

The final training performance against a majority of the n-step update algorithms. Figure 3a, 3c and 3e compares the training results between Elastic DQN against the n-step variants (2/3/4/6/8) measured in terms of the average rewards ($\bar{x}$) received per epoch along with the standard deviation (s) of each epoch also plotted on the graph. Cartpole has been acknowledged to be very sensitive to hyper-parameter tuning and in our experiments shown itself to be prone to divergent behaviour – as a result it is a good environment to test for training efficacy. In the Cartpole experiments, Elastic Step DQN took an average of 1.05 steps (with a maximum of 297 and a minimum of 1 step per update), and was able to achieve statistically significant higher average final training performance ($\bar{x}$ reward = 413.4) than the n-step variants as well as single-step DQN ($\bar{x}$ reward = 100.7). Observations from Figure 3a showed that while n-step variants exhibited stronger early stage performance in the environments, a majority of the n-step variants struggled to learn any meaningful policy in the Cartpole environment. The optimal value of n for the Cartpole environment was 3, which peaked after the 33rd epoch and suffered periodic degradation of training performance over time. This periodic degradation of training performance can also be observed in single step DQN which went through a period of stability between the 25th epoch to the 70th epoch before collapsing afterwards. This instability is again observed in Double DQN in Figure 4a but not Average DQN. Interestingly, when the termination condition was set much higher in the Cartpole environment, both Average DQN and Double DQN rarely achieved rewards above 200 which was the original default termination condition, while Elastic Step DQN was able to consistently surpass the 200 rewards mark. In the experiments against the DQN extensions, Elastic Step DQN ($\bar{x}$ reward = 413.4), was able to achieve statistically significant improvements against Double DQN ($\bar{x}$ reward = 225.7) and Average DQN ($\bar{x}$ reward = 183.6) as indicated in Table 1.

Of the three environments, Acrobot was the easiest environment for all the algorithmic implementations. The n-step variants performed comparatively well in the Acrobot environment, both 4/6/both (4-step: $\bar{x}$ reward = -93.2, 6-step: $\bar{x}$ reward = -91.5) achieved higher average final training performance than Elastic Step DQN ($\bar{x}$ reward = -94.5). In spite of this, the training curves in
Figure 3c does show that Elastic Step DQN converged much faster than the n-step variants and for a majority of the epochs had sustained higher rewards than the n-step. In this environment, statistically significant improvements was achieved against 3 and 8-step DQN. Single-step DQN ($\bar{x}$ reward = -107.6), Average ($\bar{x}$ reward = -100.8) and Double DQN ($\bar{x}$ reward = -103.3) also had very little issue converging to a decent policy and statistical significance could not be claimed against either. In this environment Elastic Step DQN took an average of 8.59 steps during its run (with a maximum of 923 steps and a minimum of 1 step per updates), demonstrating that this algorithm does indeed adjust the step-size to suit the environment.

The Mountain Car environment proved also to be a difficult for n-step variants which generally have learned sub-optimal policies. Figure 3c plots the training curve for the n-step variants, single step DQN and Elastic Step DQN. The plot shows that the n-step variants suffered from highly volatile learning with most collapsing after a period of learning like the training curves observed in Figure 3a. From Figure 3a it seems lower step sizes introduce more stability 2/4-step DQN suffer from a much less dramatic collapse of the learning than 6/8-step. On the contrary, Elastic Step DQN took an average of 7.22 steps (with a maximum of 1000 steps and a minimum of 1 step per update) to converge to an optimal policy. In these experiments, Elastic Step DQN achieved statistically significant improvements ($\bar{x}$ reward = -123.4) against the n-step variants (2-step DQN $\bar{x}$ reward = -462.9) and single step DQN ($\bar{x}$ reward = -156.8). n-step variants suffered from highly learning volatility as observed from the standard deviation of the rewards which were at least three times the standard deviation of single-step DQN and five times that of Elastic Step DQN (refer to Table 1). Close inspection into single seed runs of the Mountain Car environment have shown instances where both the 2 and 6 step DQN implementations have outperformed the Elastic Step DQN and single-step DQN algorithm by moderate margins. These results run in contrary to the portrayed image that multi-step DQN are in general more performant than single-step DQN. It is possible that perhaps the step size selection was not suitable, however this validates how difficult it may be to select the correct horizon. When compared against the DQN extensions, we saw that Average DQN and Double DQN algorithm have been able to converge to an optimal policy much faster than Elastic Step DQN in Figure 4c, but on average achieved a statistically significant lower final training performance (Table 1: Double DQN $\bar{x}$ reward = -162.8, Average DQN $\bar{x}$ reward = -153.9) than Elastic Step DQN ($\bar{x}$ reward = -123.4).

One noticeable trend in Figures 4a, 4c and 4e is that Elastic Step DQN is slower to converge to an optimal policy than Double DQN and Average DQN. This slower convergence speed could be attributed to the large step sizes the agent needs to take in the early stages of learning when the data is scarce and the clustering algorithm does not have representative data sample to train on. As the agent accumulates more data, the agent naturally takes smaller step sizes. In spite of this disadvantage, Elastic Step DQN has shown comparable performance against the n-step variants and well established DQN extensions. Whether this is a result of more accurate $Q$ value estimations will be explored in Section 4.3.

4.3 Analysis of overestimation and soft divergence

Given Elastic Step DQN’s strong final training performance observed in Section 4.1 the question is then, is this as a result of the ability of Elastic Step DQN to moderate $Q$ value estimates? As discussed in Section 4.1 we have established that $|Q|$-value estimates greater than 100 can be considered to be suffering from overestimation. Based on this definition, based on the mean $|Q|$-value estimates from Table 3 Elastic Step DQN did not suffer from overestimation, although
Table 2: Summary statistics steps taken during Elastic Step DQN runs.

|                | Cartpole | Acrobot | Mountain Car |
|----------------|----------|---------|--------------|
| $\bar{x}$ steps | 1.05     | 8.59    | 7.22         |
| Min steps      | 1        | 1       | 1            |
| Max steps      | 297      | 923     | 1000         |
| x$_{0.5}$ steps | 1        | 3       | 2            |
| s steps        | 0.84     | 18.99   | 21.11        |

Table 3: This table outlines the average absolute $Q$ value estimate ($\bar{x} |Q|$), the standard deviation of the absolute $Q$ value estimate ($s |Q|$) and the median absolute $Q$ value estimate ($x_{0.5}$) of each algorithm over the 30 seeds. $|Q|$-values that exceed 100 are in bold.

|                | Cartpole | Acrobot | Mountain Car |
|----------------|----------|---------|--------------|
| $\bar{x} |Q|$ | $s$ | $x_{0.5}$ | $\bar{x} |Q|$ | $s$ | $x_{0.5}$ | $\bar{x} |Q|$ | $s$ | $x_{0.5}$ |
| DQN            | 52.6     | 24.1    | 52.4         | 67.4 | 22.8 | 67.6 | 1803.1 | 3445.6 | 549.1 |
| 2 step DQN     | 33.3     | 17.9    | 33.1         | 65   | 19.9 | 66.5 | 98.1   | 98.1   | 10.4 |
| 3 step DQN     | 43.7     | 22.2    | 42.6         | 39.5 | 19.6 | 39.4 | 98.6   | 10.1   | 98.6 |
| 4 step DQN     | 56       | 32.4    | 43.9         | 79.9 | 22.2 | 80.3 | 98.3   | 10.7   | 98.4 |
| 6 step DQN     | **415.2**| 722.5   | 56.7         | 92.1 | 13.6 | 92.7 | 98.5   | 10.6   | 98.5 |
| 8 step DQN     | **2919.6**| 5634.7 | **278.4**    | 97.3 | 4.4  | 97.6 | 98.7   | 10.4   | 98.7 |
| Double DQN     | 52.1     | 24      | 51.9         | 67.7 | 21.3 | 68.2 | **1985.2**| 2701.8 | 612.8 |
| Average DQN    | 39.4     | 19.4    | 39.3         | 75.8 | 14.7 | 76.9 | **1135.5**| 2065   | **154.5**|
| Elastic Step DQN| 52.4     | 23.2    | 65.6         | 78.8 | 13.1 | 79.4 | 81.9   | 14.9   | 79.4 |

Table 4: Maximum average absolute $Q$ value estimate ($\max |Q|$), and the Spearman correlation between training reward and $|Q|$ of each algorithm over the 30 seeds. $|Q|$-values that exceed 100 are in bold.

|                | Cartpole | Acrobot | Mountain Car |
|----------------|----------|---------|--------------|
| Spearman max $|Q|$ | Spearman max $|Q|$ | Spearman max $|Q|$ |
| DQN            | -0.4     | 54.5    | -0.8         | 69.9 | 0.5  | 16558.9 |
| 2 step DQN     | 0        | 44.1    | -0.5         | 71.2 | -0.1 | 98.8   |
| 3 step DQN     | 0        | 66.8    | 0.2          | 40.3 | -0.4 | 99.2   |
| 4 step DQN     | -0.3     | **153.9**| -0.1         | 84.4 | 0.1  | 98.9   |
| 6 step DQN     | -0.6     | **5455.3**| -0.5         | 94   | -0.1 | 98.9   |
| 8 step DQN     | -0.8     | **31125.4**| -0.3         | 98.1 | 0.5  | 99.1   |
| Double DQN     | 54.1     | -0.4    | -0.9         | 72.8 | 0.8  | **10918.3**|
| Average DQN    | -0.2     | 40.7    | -1           | 83.2 | 0.7  | **7237.2**|
| Elastic Step DQN| -0.4     | 81.4    | 0.9          | 91   | -0.9 | **102.5**|
examination of the max $|Q|$ from the Mountain Car environment in Table 4 indicates that it breached the $|Q| > 100$ threshold by 2.5. However, this value is negligible when compared to single-step DQN, Double DQN and Average DQN which had an average $|Q|$-value estimate of 1803.1, 1,985.2 and 1,135.5 respectively in the Mountain Car environment. Interestingly, despite the overestimation, Figure 4f seem to show that the runs where the $|Q|$-value estimates were above 100 did very well while runs that were within the [0, 100] bound had mix performances. When we observe Figure 3b, 3d and 3f for the three environments across the $n$-step DQN, we can observe that there exist a visual relationship between poor performance and a overestimated $|Q|$ value. Elastic Step DQN tended to cluster together where the $|Q|$ values are lower and the reward is higher, on the other hand, the $n$-step algorithms had very volatile $|Q|$ values, and the higher $|Q|$ values also visually aligned with poorer performance. In contrast, we saw a contradictory relationship in Figure 4f where despite DQN, Double DQN and Average DQN crossed the upper bound limit, it consistently performed well. The Spearman correlation as stated in Table 4 for single-step DQN, Double DQN and Average DQN were 0.5, 0.8 and 0.7 respectively which indicated there existed a moderate to strong monotonic relationship between reward and $|Q|$-value. An increase in the $|Q|$-value estimates above the upper bound of 100 seem to positively correlate which stronger training performance which seems to indicate that overestimation does not actually guarantee poor performance or instability. One explanation could be that overestimation is only bad when the relative value of the state action value estimates do not encourage optimal action. In Lan et al. (2019) analysis of overestimation indicated that overestimation can be harmful or beneficial depending on the environment. Of course, there were situations where overestimations did correlate with poor performance – in the case of Cartpole, each increase of the step size in the value of $n$ lead to incrementally higher $|Q|$-value estimates – both 6, and 8-step DQN experienced tendencies to over-estimate. Overestimation in multi-step DQN have only been recorded when the step-size horizon was incorrectly tuned, which seems to confirm the idea that correctly tuned multi-step algorithms are able to moderate overestimation bias. In some cases the $|Q|$-value estimates were relatively lower than well-performing algorithms which could be potentially also be harmful as underestimation as explored by He and Hou (2020) Lan et al. (2019) indicated that agents who were prone to underestimation bias tended to incur non-optimal performance.

4.4 Cluster analysis of the Mountain Car environment

The primary objective of the unsupervised clustering algorithm was to leverage its mechanism of similarity detection to assist with the selection of the step size. To validate whether the clusters are rationally assigned, there needs to be a close inspection into the clusters generated from a successful run of the algorithm. The Mountain Car environment is a good environment to analyse the clustering performance because the OpenAI implementation exposes a two element vector state space which can easily be mapped onto a two dimensional plot. Figure 5 displays the cluster results mapped against the observational vectors from a single successful run of Mountain Car, each colour represents a different set of cluster labels and each data point represents a single observation vector. The x-axis is represented by the position of the car at a certain point in time while the y-axis is represented by velocity that the car was travelling at (a negative value indicates the car is moving backwards while a positive value indicates the car is moving towards the goal). The results from the clusters shows that the unsupervised clustering algorithm systematically identified seven main clusters which are all uneven and dense separated by areas of low density data points. Observations into the individual clusters indicate that HDBSCAN has identified and separately clustered varying
state action strategies together. To beat the Mountain Car environment, the agent needs to move back and forth at the bottom of the mountain to gain momentum this is labelled 1 in figure 5. As the car reached middle of the mountain, the momentum builds up and the car gains more velocity over time as indicated by label 2 and 3. These clusters identified by HDBSCAN are inline with the expected behaviour of the algorithm.

5 Conclusion and future work

Overestimation in the $|Q|$-value estimates has been an enduring challenge in Deep Q-networks and overestimation can stifle learning and lead the agent to learn sub-optimal policies. This paper takes a fresh look at two ideas prevalent in the literature that may potentially address the overestimation issue. The first idea centres around a school of thought that multi-step updates can alleviate the overestimation pressures in deep value based reinforcement learning—this idea has been extensively experimented with in the literature and have shown promise. However the application of the approach can be difficult because multi-step updates can be very sensitive to the hyper-parameters. The second idea centres around Coarse Q-learning and the idea that systematic generalisation of similar states can alleviate divergent behaviour.

In this paper a new algorithm called Elastic Step DQN is presented that combines the ideas mentioned to address overestimation in Deep Q-Networks. The Elastic Step Agent utilises a clustering algorithm to systematically discern states that are similar together and belong to a single multi-step update. This allows the agent to automate the step size and leverage the benefits of multi-step updates. The empirical analyses in the paper so far has shown that Elastic Step DQN
can on average achieve comparable or better results than \( n \)-step variants and established DQN extensions while moderate overestimation in \(|Q|\)-value estimates.

One of the disadvantages of Elastic Step DQN is that it is slow in the early stages of learning to converge to an optimal policy, in spite of this it has shown to achieve comparable or better final performance to Average DQN and Double DQN. In addition, observed behaviours of overestimation in Double DQN and Average DQN did not guarantee poor performance and in fact experience consistently stronger performance than instances where the \(|Q|\)-value was estimated within the bounds. In the same vein, a desirable estimation of the Q value does not mean that the algorithm will perform well.

These results highlights its potential for further exploration. So far the environments used in this paper have been small control problems, with vectored inputs, it would be interesting for future work to expand the experimental analyses into larger pixel based environments and perhaps apply the ideas to actor critic based algorithms and explore its impacts. It would also be beneficial to understand whether the algorithm could add incremental benefits when combined with other approaches. Additionally, there is also potential to explore new methods to discern similarity that is more computationally efficient and more accurate.

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A Appendix A

A.1 Hyper-parameters
| Algorithm       | Hyper-parameter       | Cartpole | Acrobot | Mountain Car |
|-----------------|-----------------------|---------|---------|--------------|
|                 | learning rate         | 0.0001  | 0.003   | 0.002        |
|                 | target update horizon | 250     | 20      | 250          |
|                 | replay capacity       | 10000   | 10000   | 10000        |
| Average DQN     | initial replay size   | 500     | 500     | 500          |
|                 | train frequency       | 1       | 1       | 1            |
|                 | gamma                 | 0.99    | 0.99    | 0.99         |
|                 | epsilon min           | 0.1     | 0.1     | 0.1          |
|                 | epsilon start         | 1       | 1       | 1            |
|                 | epsilon decay strategy| linear  | linear  | linear       |
|                 | batch size            | 32      | 32      | 32           |
|                 | hidden units          | 200     | 24      | 24           |
|                 | number of approximators| 2       | 2       | 2            |
| Double DQN      | learning rate         | 0.0001  | 0.003   | 0.0005       |
|                 | target update horizon | 250     | 100     | 20           |
|                 | replay capacity       | 10000   | 10000   | 10000        |
|                 | initial replay size   | 500     | 500     | 500          |
|                 | train frequency       | 1       | 1       | 1            |
|                 | gamma                 | 0.99    | 0.99    | 0.99         |
|                 | epsilon min           | 0.1     | 0.1     | 0.1          |
|                 | epsilon start         | 1       | 1       | 1            |
|                 | epsilon decay strategy| linear  | linear  | linear       |
|                 | batch size            | 32      | 32      | 32           |
|                 | hidden units          | 200     | 24      | 24           |
|                 | hidden units          | 200     | 24      | 24           |
| 2-step DQN      | learning rate         | 0.00025 | 0.0001  | 0.0001       |
|                 | target update horizon | 1000    | 100     | 20           |
|                 | replay capacity       | 10000   | 10000   | 10000        |
|                 | initial replay size   | 500     | 500     | 500          |
|                 | train frequency       | 1       | 1       | 1            |
|                 | gamma                 | 0.99    | 0.99    | 0.99         |
|                 | epsilon min           | 0.1     | 0.1     | 0.1          |
|                 | epsilon start         | 1       | 1       | 1            |
|                 | epsilon decay strategy| linear  | linear  | linear       |
|                 | batch size            | 32      | 32      | 32           |
|                 | hidden units          | 512     | 24      | 24           |
| 4-step DQN      | learning rate         | 0.00025 | 0.0001  | 0.0001       |
|                 | target update horizon | 1000    | 100     | 100          |
|                 | replay capacity       | 10000   | 10000   | 10000        |
|                 | initial replay size   | 500     | 500     | 500          |
|                 | train frequency       | 1       | 1       | 1            |
|                 | gamma                 | 0.99    | 0.99    | 0.99         |
|                 | epsilon min           | 0.1     | 0.1     | 0.1          |
|                 | epsilon start         | 1       | 1       | 1            |
|                 | epsilon decay strategy| linear  | linear  | linear       |
|                 | batch size            | 32      | 32      | 32           |
|                 | hidden units          | 512     | 24      | 24           |
|                        | 6-step DQN                                                                 | 8-step DQN                                                                 | DQN                                                                 | Elastic Step DQN                                                                 |
|------------------------|---------------------------------------------------------------------------|---------------------------------------------------------------------------|---------------------------------------------------------------------|--------------------------------------------------------------------------------|
| learning rate          | 0.00025 0.001 0.00001                                                    | 0.00025 0.003 0.00001                                                    | 0.0001 0.001 0.0005                                                | 0.0001 0.001 0.0005                                                            |
| target update horizon  | 1000 100 100                                                              | 1000 20 100                                                               | 250 100 100                                                         | 250 20 250                                                                     |
| replay capacity        | 10000 10000 10000                                                        | 10000 10000 10000                                                       | 10000 10000 10000                                                  | 10000 10000 10000                                                             |
| initial replay size    | 500 500 500                                                               | 500 500 500                                                              | 500 500 500                                                        | 500 500 500                                                                     |
| train frequency        | 1 1 1                                                                     | 1 1 1                                                                    | 1 1 1                                                               | 1 1 1                                                                           |
| gamma                  | 0.99 0.99 0.99                                                            | 0.99 0.99 0.99                                                           | 0.99 0.99 0.99                                                      | 0.99 0.99 0.99                                                                  |
| epsilon min            | 0.1 0.1 0.1                                                               | 0.1 0.1 0.1                                                              | 0.1 0.1 0.1                                                        | 0.1 0.1 0.1                                                                     |
| epsilon start          | 1 1 1                                                                     | 1 1 1                                                                    | 1 1 1                                                               | 1 1 1                                                                           |
| epsilon decay strategy | linear linear linear                                                      | linear linear linear                                                     | linear linear                                                      | linear linear                                                                  |
| batch size             | 32 32 32                                                                  | 32 32 32                                                                 | 32 32 32                                                           | 32 32 32                                                                        |
| hidden units           | 512 24 24                                                                 | 512 24 24                                                                | 512 24 24                                                          | 512 24 24                                                                       |
|                        |                                                                           |                                                                           |                                                                     |                                                                               |
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|                        |                                                                           |                                                                           |                                                                     |                                                                               |
|                        |                                                                           |                                                                           |                                                                     |                                                                               |
|                       | 1st experiment | 2nd experiment | 3rd experiment |
|-----------------------|----------------|----------------|----------------|
| leaf size             | 40             | 40             | 40             |
| minimum cluster size  | 5              | 5              | 5              |
| metric                | euclidean      | euclidean      | euclidean      |
| state memory bank     | 10000          | 10000          | 1000           |
| state memory batch size | 1000         | 1000           | 1000           |

Table 5: Final hyper-parameters used across all the experiments