Function Approximation, Deep Q Network, Rainbow

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Function Approximation

We will approximate value function $v$ and/or action-value function $q$, selecting it from a family of functions parametrized by a weight vector $w \in \mathbb{R}^d$.

We denote the approximations as

$$\hat{v}(s; w),$$
$$\hat{q}(s, a; w).$$

We utilize the *Mean Squared Value Error* objective, denoted $\overline{VE}$:

$$\overline{VE}(w) \overset{\text{def}}{=} \sum_{s \in S} \mu(s) \left[ v_\pi(s) - \hat{v}(s, w) \right]^2,$$

where the state distribution $\mu(s)$ is usually on-policy distribution.
Gradient and Semi-Gradient Methods

The functional approximation (i.e., the weight vector $w$) is usually optimized using gradient methods, for example as

$$w_{t+1} \leftarrow w_t - \frac{1}{2} \alpha \nabla w_t \left( v_{\pi}(S_t) - \hat{v}(S_t; w_t) \right)^2$$

As usual, the $v_{\pi}(S_t)$ is estimated by a suitable sample of a return:

- in Monte Carlo methods, we use episodic return $G_t$,
- in temporal difference methods, we employ bootstrapping and use one-step return

$$R_{t+1} + [-\text{done}] \cdot \gamma \hat{v}(S_{t+1}; w)$$

or an $n$-step return.
In TD methods, we again bootstrap the estimate $v_\pi(S_t)$ as $R_{t+1} + [-\text{done}] \cdot \gamma \hat{v}(S_{t+1}; w)$.
Why Semi-Gradient TD

Note that the above algorithm is called semi-gradient, because it does not backpropagate through \( \hat{v}(S_{t+1}; w) \):

\[
w \leftarrow w + \alpha (R_{t+1} + [-\text{done}] \cdot \gamma \hat{v}(S_{t+1}; w) - \hat{v}(S_t; w)) \nabla_w \hat{v}(S_t; w).
\]

In other words, the above rule is in fact not an SGD update, because there does not exist a function \( J(w) \), for which we would get the above update.

To sketch a proof, consider a linear \( \hat{v}(S_t; w) = \sum_i x(S_t)_i w_i \) and assume such a \( J(w) \) exists. Then

\[
\frac{\partial}{\partial w_i} J(w) = (R_{t+1} + \gamma \hat{v}(S_{t+1}; w) - \hat{v}(S_t; w)) x(S_t)_i.
\]

Now considering second derivatives, we see they are not equal, which is a contradiction:

\[
\frac{\partial}{\partial w_i} \frac{\partial}{\partial w_j} J(w) = (\gamma x(S_{t+1})_i - x(S_t)_i) x(S_t)_j = \gamma x(S_{t+1})_i x(S_t)_j - x(S_t)_i x(S_t)_j
\]

\[
\frac{\partial}{\partial w_j} \frac{\partial}{\partial w_i} J(w) = (\gamma x(S_{t+1})_j - x(S_t)_j) x(S_t)_i = \gamma x(S_{t+1})_j x(S_t)_i - x(S_t)_i x(S_t)_j
\]
It can be proven (by using separate theory than for SGD) that the linear semi-gradient TD methods do converge. However, they do not converge to the optimum of $\overline{VE}$. Instead, they converge to a different TD fixed point $w_{TD}$.

It can be proven that

$$\overline{VE}(w_{TD}) \leq \frac{1}{1 - \gamma} \min_w \overline{VE}(w).$$

However, when $\gamma$ is close to one, the multiplication factor in the above bound is quite large.
As before, we can utilize $n$-step TD methods.

$n$-step semi-gradient TD for estimating $\hat{v} \approx v_\pi$

Input: the policy $\pi$ to be evaluated
Input: a differentiable function $\hat{v} : S^+ \times \mathbb{R}^d \to \mathbb{R}$ such that $\hat{v}(\text{terminal}, \cdot) = 0$
Algorithm parameters: step size $\alpha > 0$, a positive integer $n$
Initialize value-function weights $w$ arbitrarily (e.g., $w = 0$)
All store and access operations ($S_t$ and $R_t$) can take their index mod $n + 1$

Loop for each episode:
  Initialize and store $S_0 \neq \text{terminal}$
  $T \leftarrow \infty$
  Loop for $t = 0, 1, 2, \ldots$:
    If $t < T$, then:
      Take an action according to $\pi(\cdot|S_t)$
      Observe and store the next reward as $R_{t+1}$ and the next state as $S_{t+1}$
      If $S_{t+1}$ is terminal, then $T \leftarrow t + 1$
    $\tau \leftarrow t - n + 1$ (\tau is the time whose state’s estimate is being updated)
    If $\tau \geq 0$:
      $G \leftarrow \sum_{i=\tau+1}^{\min(\tau+n,T)} \gamma^{i-\tau-1} R_i$  
      If $\tau + n < T$, then: $G \leftarrow G + \gamma^n \hat{v}(S_{\tau+n}, w)$
      $w \leftarrow w + \alpha (G - \hat{v}(S_\tau, w)) \nabla \hat{v}(S_\tau, w)$
  Until $\tau = T - 1$

Algorithm 9.5 of "Reinforcement Learning: An Introduction, Second Edition".
On the left, the results of one-step TD(0) algorithm are presented. The effect of increasing \( n \) in an \( n \)-step variant is displayed on the right.

**Figure 9.2 of “Reinforcement Learning: An Introduction, Second Edition”**.
Until now, we talked only about policy evaluation. Naturally, we can extend it to a full Sarsa algorithm:

**Episodic Semi-gradient Sarsa for Estimating $\hat{q} \approx q_*$**

Input: a differentiable action-value function parameterization $\hat{q} : S \times A \times \mathbb{R}^d \rightarrow \mathbb{R}$
Algorithm parameters: step size $\alpha > 0$, small $\varepsilon > 0$
Initialize action-value function weights $w \in \mathbb{R}^d$ arbitrarily (e.g., $w = 0$)

Loop for each episode:

- $S, A \leftarrow$ initial state and action of episode (e.g., $\varepsilon$-greedy)

Loop for each step of episode:

- Take action $A$, observe $R, S'$
- If $S'$ is terminal:
  - $w \leftarrow w + \alpha [R - \hat{q}(S, A, w)] \nabla \hat{q}(S, A, w)$
  - Go to next episode
- Choose $A'$ as a function of $\hat{q}(S', \cdot, w)$ (e.g., $\varepsilon$-greedy)

$w \leftarrow w + \alpha [R + \gamma \hat{q}(S', A', w) - \hat{q}(S, A, w)] \nabla \hat{q}(S, A, w)$

$S \leftarrow S'$

$A \leftarrow A'$

*Modified from Algorithm 10.1 of "Reinforcement Learning: An Introduction, Second Edition".*
Additionally, we can incorporate $n$-step returns:

Episodic semi-gradient $n$-step Sarsa for estimating $\hat{q} \approx q_\pi$ or $q_\pi$

- **Input:** a differentiable action-value function parameterization $\hat{q} : S \times A \times \mathbb{R}^d \rightarrow \mathbb{R}$
- **Input:** a policy $\pi$ (if estimating $q_\pi$)
- **Algorithm parameters:** step size $\alpha > 0$, small $\epsilon > 0$, a positive integer $n$
- **Initialize action-value function weights $w \in \mathbb{R}^d$ arbitrarily (e.g., $w = 0$)**
- **All store and access operations ($S_t$, $A_t$, and $R_t$) can take their index mod $n + 1$**

**Loop for each episode:**
- Initialize and store $S_0 \neq$ terminal
- Select and store an action $A_0 \sim \pi(\cdot|S_0)$ or $\epsilon$-greedy wrt $\hat{q}(S_0, \cdot, w)$
- $T \leftarrow \infty$
- Loop for $t = 0, 1, 2, \ldots$
  - If $t < T$, then:
    - Take action $A_t$
    - Observe and store the next reward as $R_{t+1}$ and the next state as $S_{t+1}$
    - If $S_{t+1}$ is terminal, then:
      - $T \leftarrow t + 1$
    - else:
      - Select and store $A_{t+1} \sim \pi(\cdot|S_{t+1})$ or $\epsilon$-greedy wrt $\hat{q}(S_{t+1}, \cdot, w)$
      - $\tau \leftarrow t - n + 1$ ( $\tau$ is the time whose estimate is being updated)
    - If $\tau \geq 0$:
      - $G \leftarrow \sum_{i=\tau+1}^{\min(\tau+n,T)} \gamma^{i-\tau-1} R_i$
      - If $\tau + n < T$, then $G \leftarrow G + \gamma^n \hat{q}(S_{\tau+n}, A_{\tau+n}, w)$
      - $w \leftarrow w + \alpha [G - \hat{q}(S_\tau, A_\tau, w)] \nabla \hat{q}(S_\tau, A_\tau, w)$
  - Until $\tau = T - 1$

The performances are for semi-gradient Sarsa(\(\lambda\)) algorithm (which we did not talk about yet) with tile coding of 8 overlapping tiles covering position and velocity, with offsets of (1, 3).
Mountain Car Example

Figure 10.3 of “Reinforcement Learning: An Introduction, Second Edition”.

Figure 10.4 of “Reinforcement Learning: An Introduction, Second Edition”.
Off-policy Divergence With Function Approximation

Consider a deterministic transition between two states whose values are computed using the same weight:

![Diagram](attachment:image.png)

*Figure from Section 11.2 of “Reinforcement Learning: An Introduction, Second Edition”.*

- If initially $w = 10$, the TD error will be also 10 (or nearly 10 if $\gamma < 1$).
- If for example $\alpha = 0.1$, $w$ will be increased to 11 (by 10%).
- This process can continue indefinitely.

However, the problem arises only in off-policy setting, where we do not decrease value of the second state from further observation.
The previous idea can be implemented for instance by the following **Baird's counterexample**:

![Diagram](image)

\[ \pi(\text{solid} | \cdot) = 1 \]
\[ b(\text{dashed} | \cdot) = 6/7 \]
\[ b(\text{solid} | \cdot) = 1/7 \]
\[ \gamma = 0.99 \]

The rewards are zero everywhere, so the value function is also zero everywhere. We assume the initial values of weights are 1, except for \( w_7 = 10 \), and that the learning rate \( \alpha = 0.01 \).
For off-policy semi-gradient Sarsa, or even for off-policy dynamic-programming update (where we compute expectation over all following states and actions), the weights diverge to $+\infty$.

Using on-policy distribution converges fine.

$$w \leftarrow w + \frac{\alpha}{|S|} \sum_s \left( E_\pi [R_{t+1} + \gamma \hat{v}(S_{t+1}; w) | S_t = s] - \hat{v}(s; w) \right) \nabla \hat{v}(s; w)$$
The divergence can happen when all following elements are combined:

- functional approximation;
- bootstrapping;
- off-policy training.

In the Sutton's and Barto's book, these are called the **deadly triad**.

Training can be extremely brittle (and can even diverge as shown earlier).
Deep Q Network

Figure 1 of "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.
Deep Q Networks

- Preprocessing: 210 × 160 128-color images are converted to grayscale and then resized to 84 × 84.
- **Frame skipping** technique is used, i.e., only every 4\textsuperscript{th} frame (out of 60 per second) is considered, and the selected action is repeated on the other frames.
- **Frame stacking** is utilized – the input to the network are the last 4 frames (considering only the frames kept by frame skipping), i.e., the network input is an image with 4 channels.
- The network is fairly standard, performing
  - 32 filters of size 8 × 8 with stride 4 and ReLU,
  - 64 filters of size 4 × 4 with stride 2 and ReLU,
  - 64 filters of size 3 × 3 with stride 1 and ReLU,
  - fully connected layer with 512 units and ReLU,
  - output layer with 18 output units (one for each action)
Deep Q Networks

- Network is trained with RMSProp to minimize the following loss:

\[
L \overset{\text{def}}{=} \mathbb{E}_{(s,a,r,s') \sim \text{data}} \left[ (r + \neg \text{done}) \cdot \gamma \max_a Q(s', a'; \bar{\theta}) - Q(s, a; \theta) \right]^2.
\]

- An \( \varepsilon \)-greedy behavior policy is utilized (starts at \( \varepsilon = 1 \) and gradually decreases to 0.1).

Important improvements:

- **experience replay**: the generated episodes are stored in a buffer as \( (s, a, r, s') \) quadruples, and for training a transition is sampled uniformly (off-policy training);
- **separate target network \( \bar{\theta} \)**: to prevent instabilities, a separate target network is used to estimate one-step returns. The weights are not trained, but copied from the trained network after a fixed number of gradient updates;
- **reward clipping**: because rewards have wildly different scale in different games, all positive rewards are replaced by +1 and negative by −1; life loss is used as an end of episode.
  - furthermore, \((r + \neg \text{done}) \cdot \gamma \max_a Q(s', a'; \bar{\theta}) - Q(s, a; \theta)\) is also clipped to \([-1, 1]\) (i.e., a smooth \(L_1\) loss or Huber loss).
Algorithm 1: deep Q-learning with experience replay.
Initialize replay memory $D$ to capacity $N$
Initialize action-value function $Q$ with random weights $\theta$
Initialize target action-value function $\hat{Q}$ with weights $\theta^- = \theta$

For episode $= 1, M$ do
  Initialize sequence $s_1 = \{x_1\}$ and preprocessed sequence $\phi_1 = \phi(s_1)$
  For $t = 1, T$ do
    With probability $\epsilon$ select a random action $a_t$
    otherwise select $a_t = \arg \max_a Q(\phi(s_t), a; \theta)$
    Execute action $a_t$ in emulator and observe reward $r_t$ and image $x_{t+1}$
    Set $s_{t+1} = s_t, a_t, x_{t+1}$ and preprocess $\phi_{t+1} = \phi(s_{t+1})$
    Store transition $(\phi_t, a_t, r_t, \phi_{t+1})$ in $D$
    Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from $D$
    Set $y_j = \begin{cases} r_j & \text{if episode terminates at step } j+1 \\ r_j + \gamma \max_{a'} \hat{Q}(\phi_{j+1}, a'; \theta^-) & \text{otherwise} \end{cases}$
    Perform a gradient descent step on $\left(y_j - Q(\phi_j, a_j; \theta)\right)^2$ with respect to the network parameters $\theta$
  End For
End For

Algorithm 1 of “Human-level control through deep reinforcement learning” by Volodymyr Mnih et al.
Figure 3 of "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.
Deep Q Network

Extended Data Figure 2a of "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.
Deep Q Network

Extended Data Figure 2b of "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.
# Deep Q Networks Hyperparameters

<table>
<thead>
<tr>
<th>Hyperparameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>minibatch size</td>
<td>32</td>
</tr>
<tr>
<td>replay buffer size</td>
<td>1M</td>
</tr>
<tr>
<td>target network update frequency</td>
<td>10k</td>
</tr>
<tr>
<td>discount factor</td>
<td>0.99</td>
</tr>
<tr>
<td>training frames</td>
<td>50M</td>
</tr>
<tr>
<td>RMSProp learning rate and both momentums</td>
<td>0.00025, 0.95</td>
</tr>
<tr>
<td>initial $\epsilon$, final $\epsilon$ (linear decay) and frame of final $\epsilon$</td>
<td>1.0, 0.1, 1M</td>
</tr>
<tr>
<td>replay start size</td>
<td>50k</td>
</tr>
<tr>
<td>no-op max</td>
<td>30</td>
</tr>
</tbody>
</table>
There have been many suggested improvements to the DQN architecture. In the end of 2017, the *Rainbow: Combining Improvements in Deep Reinforcement Learning* paper combines 6 of them into a single architecture they call **Rainbow**.

![Figure 1 of "Rainbow: Combining Improvements in Deep Reinforcement Learning" by Matteo Hessel et al.](image)
Q-learning and Maximization Bias

Because behaviour policy in Q-learning is $\varepsilon$-greedy variant of the target policy, the same samples (up to $\varepsilon$-greedy) determine both the maximizing action and estimate its value.

Figure 6.5 of "Reinforcement Learning: An Introduction, Second Edition".
Double Q-learning

Algorithm parameters: step size $\alpha \in (0, 1]$, small $\varepsilon > 0$

Initialize $Q_1(s, a)$ and $Q_2(s, a)$, for all $s \in S$, $a \in A(s)$, such that $Q(\text{terminal}, \cdot) = 0$

Loop for each episode:
- Initialize $S$
- Loop for each step of episode:
  - Choose $A$ from $S$ using the policy $\varepsilon$-greedy in $Q_1 + Q_2$
  - Take action $A$, observe $R$, $S'$
  - With 0.5 probability:
      $$Q_1(S, A) \leftarrow Q_1(S, A) + \alpha \left( R + \gamma Q_2(S', \arg\max_a Q_1(S', a)) - Q_1(S, A) \right)$$
  - else:
      $$Q_2(S, A) \leftarrow Q_2(S, A) + \alpha \left( R + \gamma Q_1(S', \arg\max_a Q_2(S', a)) - Q_2(S, A) \right)$$
  - $S \leftarrow S'$
- until $S$ is terminal

**Double Q-learning**

Similarly to double Q-learning, instead of

\[
    r + \gamma \max_{a'} Q(s', a'; \bar{\theta}) - Q(s, a; \theta),
\]

we minimize

\[
    r + \gamma Q(s', \arg\max_{a'} Q(s', a'; \theta); \bar{\theta}) - Q(s, a; \theta).
\]

![Figure 1](image-url)
Rainbow DQN Extensions

**Double Q-learning**

True value and an estimate

All estimates and max

Bias as function of state

Average error

Figure 2 of "Deep Reinforcement Learning with Double Q-learning" by Hado van Hasselt et al.
Double Q-learning

Figure 3 of "Deep Reinforcement Learning with Double Q-learning" by Hado van Hasselt et al.
Rainbow DQN Extensions

Double Q-learning

Performance on episodes taking at most 5 minutes and no-op starts on 49 games:

<table>
<thead>
<tr>
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<th>DQN</th>
<th>Double DQN</th>
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</thead>
<tbody>
<tr>
<td>Median</td>
<td>93.5%</td>
<td>114.7%</td>
</tr>
<tr>
<td>Mean</td>
<td>241.1%</td>
<td>330.3%</td>
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</table>

*Table 1 of "Deep Reinforcement Learning with Double Q-learning" by Hado van Hasselt et al.*

Performance on episodes taking at most 30 minutes and using human starts on 49 games:

<table>
<thead>
<tr>
<th></th>
<th>DQN</th>
<th>Double DQN</th>
<th>Double DQN (tuned)</th>
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</thead>
<tbody>
<tr>
<td>Median</td>
<td>47.5%</td>
<td>88.4%</td>
<td>116.7%</td>
</tr>
<tr>
<td>Mean</td>
<td>122.0%</td>
<td>273.1%</td>
<td>475.2%</td>
</tr>
</tbody>
</table>

*Table 2 of "Deep Reinforcement Learning with Double Q-learning" by Hado van Hasselt et al.*
Prioritized Replay

Instead of sampling the transitions uniformly from the replay buffer, we instead prefer those with a large TD error. Therefore, we sample transitions according to their probability

\[ p_t \propto |r + \gamma \max_{a'} Q(s', a'; \bar{\theta}) - Q(s, a; \theta)|^\omega, \]

where \( \omega \) controls the shape of the distribution (which is uniform for \( \omega = 0 \) and corresponds to TD error for \( \omega = 1 \)).

New transitions are inserted into the replay buffer with maximum probability to support exploration of all encountered transitions.

When combined with DDQN, the probabilities are naturally computed as

\[ p_t \propto |r + \gamma Q(s', \arg \max_{a'} Q(s', a'; \theta); \bar{\theta}) - Q(s, a; \theta)|^\omega, \]
Prioritized Replay

Because we now sample transitions according to $p_t$ instead of uniformly, on-policy distribution and sampling distribution differ. To compensate, we therefore utilize importance sampling with ratio

$$
\rho_t = \left( \frac{1/N}{p_t} \right)^\beta.
$$

The authors utilize in fact “for stability reasons”

$$
\frac{\rho_t}{\max_i \rho_i}.
$$
Rainbow DQN Extensions

Prioritized Replay

**Algorithm 1** Double DQN with proportional prioritization

1: **Input:** minibatch $k$, step-size $\eta$, replay period $K$ and size $N$, exponents $\alpha$ and $\beta$, budget $T$.
2: Initialize replay memory $\mathcal{H} = \emptyset$, $\Delta = 0$, $p_1 = 1$
3: Observe $S_0$ and choose $A_0 \sim \pi_\theta(S_0)$
4: for $t = 1$ to $T$ do
5: Observe $S_t, R_t, \gamma_t$
6: Store transition $(S_{t-1}, A_{t-1}, R_t, \gamma_t, S_t)$ in $\mathcal{H}$ with maximal priority $p_t = \max_{i < t} p_i$
7: if $t \equiv 0 \mod K$ then
8: for $j = 1$ to $k$ do
9: Sample transition $j \sim P(j) = p_j^\alpha / \sum_i p_i^\alpha$
10: Compute importance-sampling weight $w_j = (N \cdot P(j))^{-\beta} / \max_i w_i$
11: Compute TD-error $\delta_j = R_j + \gamma_j Q_{\text{target}}(S_j, \arg\max_a Q(S_j, a)) - Q(S_{j-1}, A_{j-1})$
12: Update transition priority $p_j \leftarrow |\delta_j|$.
13: Accumulate weight-change $\Delta \leftarrow \Delta + w_j \cdot \delta_j \cdot \nabla_\theta Q(S_{j-1}, A_{j-1})$
14: end for
15: Update weights $\theta \leftarrow \theta + \eta \cdot \Delta$, reset $\Delta = 0$
16: From time to time copy weights into target network $\theta_{\text{target}} \leftarrow \theta$
17: end if
18: Choose action $A_t \sim \pi_\theta(S_t)$
19: end for

*Algorithm 1 of "Prioritized Experience Replay" by Tom Schaul et al.*
Dueling Networks

Instead of computing directly $Q(s, a; \theta)$, we compose it from the following quantities:

- average return in a given state $s$, $V(s; \theta) = \frac{1}{|A|} \sum_a Q(s, a; \theta)$,
- advantage function computing an advantage $Q(s, a; \theta) - V(s; \theta)$ of action $a$ in state $s$.

\[
Q(s, a) \overset{\text{def}}{=} V(f(s; \zeta); \eta) + A(f(s; \zeta), a; \psi) - \frac{\sum_{a' \in A} A(f(s; \zeta), a'; \psi)}{|A|}
\]
Rainbow DQN Extensions

Dueling Networks

**CORRIDOR ENVIRONMENT**

![COrridor Environment Diagram]

Figure 3. (a) The corridor environment. The star marks the starting state. The redness of a state signifies the reward the agent receives upon arrival. The game terminates upon reaching either reward state. The agent’s actions are going up, down, left, right and no action. Plots (b), (c) and (d) show squared error for policy evaluation with 5, 10, and 20 actions on a log-log scale. The dueling network (Duel) consistently outperforms a conventional single-stream network (Single), with the performance gap increasing with the number of actions.

*Figure 3 of "Dueling Network Architectures for Deep Reinforcement Learning" by Ziyu Wang et al.*
Rainbow DQN Extensions

Dueling Networks

Figure 2 of “Dueling Network Architectures for Deep Reinforcement Learning” by Ziyu Wang et al.
Dueling Networks

Results on all 57 games (retraining the original DQN on the 8 missing games). Single refers to DDQN with a direct computation of $Q(s, a; \theta)$, Clip corresponds to additional gradient clipping to norm at most 10 and larger first hidden layer (so that duelling and single have roughly the same number of parameters).

<table>
<thead>
<tr>
<th></th>
<th>30 no-ops</th>
<th>Human Starts</th>
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<tbody>
<tr>
<td></td>
<td>Mean</td>
<td>Median</td>
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<tr>
<td>Prior. Duel Clip</td>
<td>591.9%</td>
<td>172.1%</td>
</tr>
<tr>
<td>Prior. Single</td>
<td>434.6%</td>
<td>123.7%</td>
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<tr>
<td>Duel Clip</td>
<td>373.1%</td>
<td>151.5%</td>
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<tr>
<td>Single Clip</td>
<td>341.2%</td>
<td>132.6%</td>
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<tr>
<td>Single</td>
<td>307.3%</td>
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<tr>
<td>Nature DQN</td>
<td>227.9%</td>
<td>79.1%</td>
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</table>

Table 1 of "Dueling Network Architectures for Deep Reinforcement Learning" by Ziyu Wang et al.