

Function Approximation, Deep Q Network

Milan Straka

EXECUTE: October 26, 2020

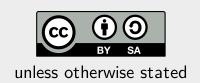








Charles University in Prague Faculty of Mathematics and Physics Institute of Formal and Applied Linguistics



Where Are We



2/34

- Until now, we have solved the tasks by explicitly calculating expected return, either as v(s) or as q(s,a).
 - Finite number of states and actions.
 - We do not share information between different states or actions.
 - \circ We use q(s,a) if we do not have the environment model (a *model-free* method); if we do, it is usually better to estimate v(s) and choose actions as $rg \max_a \mathbb{E}[R+v(s')]$.
- The methods we know differ in several aspects:
 - $^{\circ}$ Whether they compute return by simulating whole episode (Monte Carlo methods), or by using bootstrapping (temporal difference, i.e., $G_t pprox R_t + v(S_t)$, possibly n-step).
 - TD methods more noisy and unstable, but can learn immediately and explicitly assume Markovian property of value function.
 - Whether they estimate the value function of the same policy they use to generate episodes (on-policy) or not (off-policy).
 - The off-policy methods are more noisy and unstable, but more flexible.

Function Approximation



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

We will denote the approximations as

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

Weights are usually shared among states. Therefore, we need to define state distribution $\mu(s)$ to allow an objective for finding the best function approximation (if we give preference to some states, improving their estimates might worsen estimates in other states).

The state distribution $\mu(s)$ gives rise to a natural objective function called *Mean Squared Value Error*, denoted \overline{VE} :

$$\overline{VE}(oldsymbol{w}) \stackrel{ ext{ iny def}}{=} \sum_{s \in \mathcal{S}} \mu(s) \left[v_{\pi}(s) - \hat{v}(s;oldsymbol{w})
ight]^2.$$

Function Approximation



4/34

For on-policy algorithms, $\mu(s)$ is often the on-policy distribution (fraction of time spent in s).

• For **continuing tasks**, μ is the stationary distribution under π , if it exists (i.e., a distribution which does not change after one step):

$$\mu(s) = \sum
olimits_{s'} \mu(s') \sum
olimits_a \pi(a|s') p(s|s',a).$$

• For **episodic tasks**, let h(s) be a probability that an episodes starts in state s, and let $\eta(s)$ denote the number of time steps spent, on average, in state s in a single episode:

$$\eta(s) = h(s) + \sum
olimits_{s'} \eta(s') \sum
olimits_a \pi(a|s') p(s|s',a).$$

The on-policy distribution is then obtained by normalizing: $\mu(s) \stackrel{ ext{def}}{=} rac{\eta(s)}{\sum_{s'} \eta(s')}$.

If there is discounting ($\gamma < 1$), it should be treated as a form of termination, by including a factor γ to the second term of the $\eta(s)$ equation.

Gradient and Semi-Gradient Methods



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

$$egin{aligned} oldsymbol{w}_{t+1} &\leftarrow oldsymbol{w}_t - rac{1}{2} lpha
abla_{oldsymbol{w}_t} \left[v_\pi(S_t) - \hat{v}(S_t; oldsymbol{w}_t)
ight]^2 \ &\leftarrow oldsymbol{w}_t + lpha \left[v_\pi(S_t) - \hat{v}(S_t; oldsymbol{w}_t)
ight]
abla_{oldsymbol{w}_t} \hat{v}(S_t; oldsymbol{w}_t). \end{aligned}$$

As usual, the $v_{\pi}(S_t)$ is estimated by a suitable sample. In Monte Carlo methods, we use episodic return G_t , and in temporal difference methods, we employ bootstrapping and use $R_{t+1} + \gamma \hat{v}(S_{t+1}; \boldsymbol{w})$.

Monte Carlo Gradient Policy Evaluation



Gradient Monte Carlo Algorithm for Estimating $\hat{v} \approx v_{\pi}$

Input: the policy π to be evaluated

Input: a differentiable function $\hat{v}: \mathbb{S} \times \mathbb{R}^d \to \mathbb{R}$

Algorithm parameter: step size $\alpha > 0$

Initialize value-function weights $\mathbf{w} \in \mathbb{R}^d$ arbitrarily (e.g., $\mathbf{w} = \mathbf{0}$)

Loop forever (for each episode):

Generate an episode $S_0, A_0, R_1, S_1, A_1, \ldots, R_T, S_T$ using π

Loop for each step of episode, $t = 0, 1, \dots, T - 1$:

$$\mathbf{w} \leftarrow \mathbf{w} + \alpha \left[G_t - \hat{v}(S_t, \mathbf{w}) \right] \nabla \hat{v}(S_t, \mathbf{w})$$

Algorithm 9.3 of "Reinforcement Learning: An Introduction, Second Edition".

Linear Methods



A simple special case of function approximation are linear methods, where

$$\hat{v}ig(oldsymbol{x}(s);oldsymbol{w}ig) \stackrel{ ext{def}}{=} oldsymbol{x}(s)^Toldsymbol{w} = \sum x(s)_i w_i.$$

The x(s) is a representation of state s, which is a vector of the same size as w. It is sometimes called a *feature vector*.

The SGD update rule then becomes

$$\boldsymbol{w}_{t+1} \leftarrow \boldsymbol{w}_t + \alpha \left[v_{\pi}(S_t) - \hat{v}(\boldsymbol{x}(S_t); \boldsymbol{w}_t) \right] \boldsymbol{x}(S_t).$$

This rule is the same as in tabular methods, if $m{x}(s)$ is one-hot representation of state s.

State Aggregation



8/34

Simple way of generating a feature vector is **state aggregation**, where several neighboring states are grouped together.

For example, consider a 1000-state random walk, where transitions lead uniformly randomly to any of 100 neighboring states on the left or on the right. Using state aggregation, we can partition the 1000 states into 10 groups of 100 states. Monte Carlo policy evaluation then computes the following:

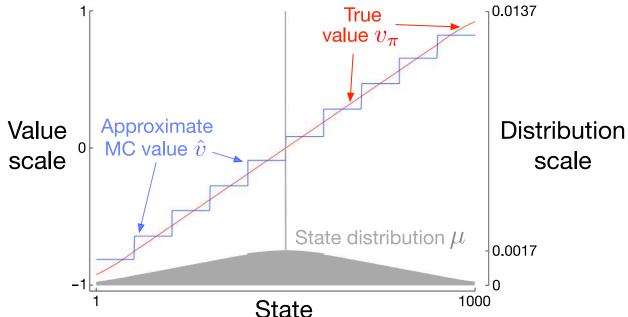


Figure 9.1 of "Reinforcement Learning: An Introduction, Second Edition".

Feature Construction for Linear Methods



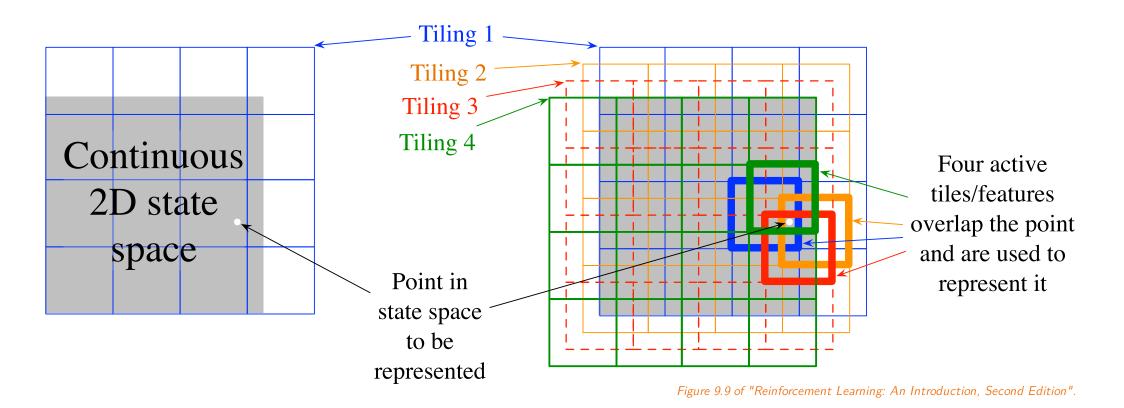
Many methods developed in the past:

- polynomials,
- Fourier bases,
- radial basis functions,
- tile coding, ...

But of course, nowadays we use deep neural networks, which construct a suitable feature vector automatically as a latent variable (the last hidden layer).

Tile Coding





If t overlapping tiles are used, the learning rate is usually normalized as lpha/t.

Tile Coding



11/34

For example, on the 1000-state random walk example, the performance of tile coding surpasses state aggregation:

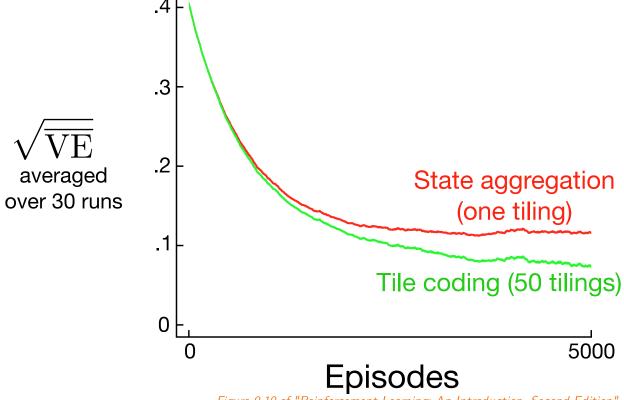


Figure 9.10 of "Reinforcement Learning: An Introduction, Second Edition".

Asymmetrical Tile Coding



12/34

In higher dimensions, the tiles should have asymmetrical offsets, with a sequence of $(1,3,5,\ldots,2d-1)$ proposed as a good choice.

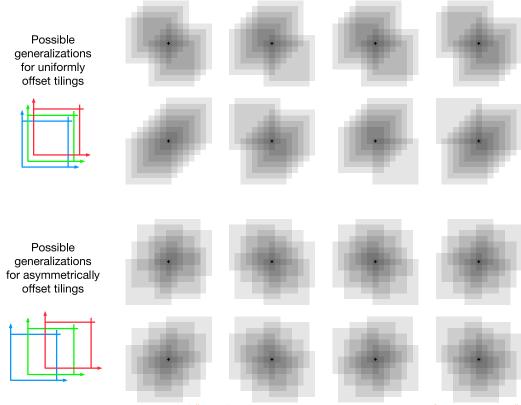


Figure 9.11 of "Reinforcement Learning: An Introduction, Second Edition".

Temporal Difference Semi-Gradient Policy Evaluation



In TD methods, we again use bootstrapping to estimate $v_{\pi}(S_t)$ as $R_{t+1} + \gamma \hat{v}(S_{t+1}; \boldsymbol{w})$.

```
Semi-gradient TD(0) for estimating \hat{v} \approx v_{\pi}
Input: the policy \pi to be evaluated
Input: a differentiable function \hat{v}: \mathbb{S}^+ \times \mathbb{R}^d \to \mathbb{R} such that \hat{v}(\text{terminal}, \cdot) = 0
Algorithm parameter: step size \alpha > 0
Initialize value-function weights \mathbf{w} \in \mathbb{R}^d arbitrarily (e.g., \mathbf{w} = \mathbf{0})
Loop for each episode:
    Initialize S
    Loop for each step of episode:
        Choose A \sim \pi(\cdot|S)
        Take action A, observe R, S'
        \mathbf{w} \leftarrow \mathbf{w} + \alpha [R + \gamma \hat{v}(S', \mathbf{w}) - \hat{v}(S, \mathbf{w})] \nabla \hat{v}(S, \mathbf{w})
        S \leftarrow S'
    until S is terminal
```

Algorithm 9.3 of "Reinforcement Learning: An Introduction, Second Edition".

Why Semi-Gradient TD



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

$$oldsymbol{w} \leftarrow oldsymbol{w} + lpha ig[R_{t+1} + \gamma \hat{v}(S_{t+1}; oldsymbol{w}) - \hat{v}(S_t; oldsymbol{w})ig]
abla_{oldsymbol{w}_t} \hat{v}(S_t; oldsymbol{w}).$$

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

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

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

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

$$egin{aligned} rac{\partial}{\partial w_i}rac{\partial}{\partial w_j}J(oldsymbol{w}) &= ig[\gamma x(S_{t+1})_i - x(S_t)_iig]x(S_t)_j = \gamma x(S_{t+1})_i x(S_t)_j - x(S_t)_i x(S_t)_j \ rac{\partial}{\partial w_i}rac{\partial}{\partial w_i}J(oldsymbol{w}) &= ig[\gamma x(S_{t+1})_j - x(S_t)_jig]x(S_t)_i = \gamma x(S_{t+1})_j x(S_t)_i - x(S_t)_i x(S_t)_j \end{aligned}$$

Temporal Difference Semi-Gradient Convergence



It can be proven (by using separate theory than for SGD) that the linear semi-gradient TD methods 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

$$\overline{VE}(oldsymbol{w}_{ ext{TD}}) \leq rac{1}{1-\gamma} \min_{oldsymbol{w}} \overline{VE}(oldsymbol{w}).$$

However, when γ is close to one, the multiplication factor in the above bound is quite large.

Temporal Difference Semi-Gradient Policy Evaluation



16/34

As before, we can utilize n-step TD methods.

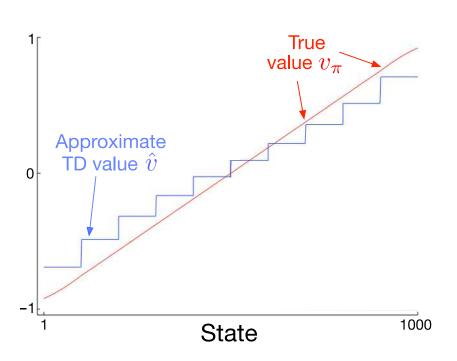
```
n-step semi-gradient TD for estimating \hat{v} \approx v_{\pi}
Input: the policy \pi to be evaluated
Input: a differentiable function \hat{v}: \mathbb{S}^+ \times \mathbb{R}^d \to \mathbb{R} such that \hat{v}(\text{terminal},\cdot) = 0
Algorithm parameters: step size \alpha > 0, a positive integer n
Initialize value-function weights \mathbf{w} arbitrarily (e.g., \mathbf{w} = \mathbf{0})
All store and access operations (S_t \text{ 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, ...:
       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 > 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}, \mathbf{w})
            \mathbf{w} \leftarrow \mathbf{w} + \alpha \left[ G - \hat{v}(S_{\tau}, \mathbf{w}) \right] \nabla \hat{v}(S_{\tau}, \mathbf{w})
    Until \tau = T - 1
```

Algorithm 9.5 of "Reinforcement Learning: An Introduction, Second Edition"

Temporal Difference Semi-Gradient Policy Evaluation



On the left, the results of one-step TD(0) algorithm is presented. The effect of increasing n in an n-step variant is displayed on the right.



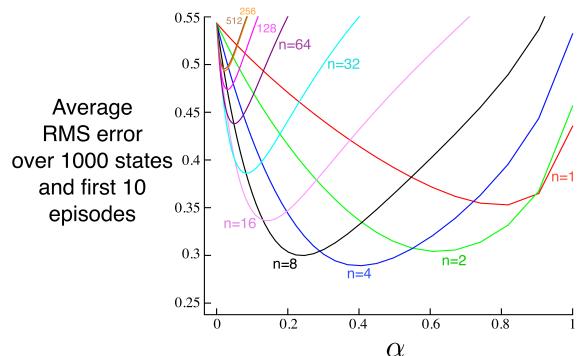


Figure 9.2 of "Reinforcement Learning: An Introduction, Second Edition".

Sarsa with Function Approximation



18/34

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 $\hat{q}: \mathbb{S} \times \mathcal{A} \times \mathbb{R}^d \to \mathbb{R}$ Algorithm parameters: step size $\alpha > 0$, small $\varepsilon > 0$ Initialize value-function weights $\mathbf{w} \in \mathbb{R}^d$ arbitrarily (e.g., $\mathbf{w} = \mathbf{0}$) Loop for each episode: $S, A \leftarrow \text{initial state}$ and action of episode (e.g., ε -greedy) Loop for each step of episode: Take action A, observe R, S'If S' is terminal: $\mathbf{w} \leftarrow \mathbf{w} + \alpha [R - \hat{q}(S, A, \mathbf{w})] \nabla \hat{q}(S, A, \mathbf{w})$ Go to next episode Choose A' as a function of $\hat{q}(S', \cdot, \mathbf{w})$ (e.g., ε -greedy) $\mathbf{w} \leftarrow \mathbf{w} + \alpha [R + \gamma \hat{q}(S', A', \mathbf{w}) - \hat{q}(S, A, \mathbf{w})] \nabla \hat{q}(S, A, \mathbf{w})$ $S \leftarrow S'$ $A \leftarrow A'$

Algorithm 10.1 of "Reinforcement Learning: An Introduction, Second Edition".

Sarsa with Function Approximation



19/34

Additionally, we can incorporate n-step returns:

```
Episodic semi-gradient n-step Sarsa for estimating \hat{q} \approx q_* or q_{\pi}
Input: a differentiable action-value function parameterization \hat{q}: \mathbb{S} \times \mathcal{A} \times \mathbb{R}^d \to \mathbb{R}
Input: a policy \pi (if estimating q_{\pi})
Algorithm parameters: step size \alpha > 0, small \varepsilon > 0, a positive integer n
Initialize value-function weights \mathbf{w} \in \mathbb{R}^d arbitrarily (e.g., \mathbf{w} = \mathbf{0})
All store and access operations (S_t, A_t, \text{ and } R_t) can take their index mod n+1
Loop for each episode:
   Initialize and store S_0 \neq \text{terminal}
    Select and store an action A_0 \sim \pi(\cdot|S_0) or \varepsilon-greedy wrt \hat{q}(S_0,\cdot,\mathbf{w})
    T \leftarrow \infty
    Loop for t = 0, 1, 2, ...:
        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 \varepsilon-greedy wrt \hat{q}(S_{t+1}, \cdot, \mathbf{w})
        \tau \leftarrow t - n + 1 (\tau is the time whose estimate is being updated)
        If \tau > 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}, \mathbf{w})

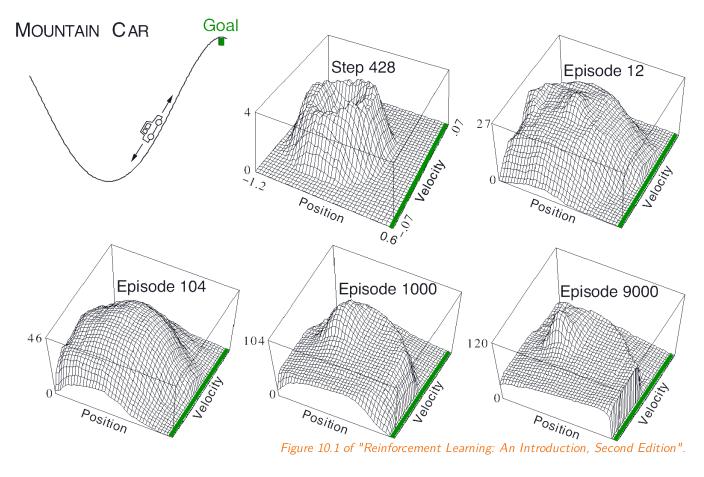
\mathbf{w} \leftarrow \mathbf{w} + \alpha \left[ G - \hat{q}(S_{\tau}, A_{\tau}, \mathbf{w}) \right] \nabla \hat{q}(S_{\tau}, A_{\tau}, \mathbf{w})
    Until \tau = T - 1
```

Algorithm 10.2 of "Reinforcement Learning: An Introduction, Second Edition".

Mountain Car Example



20/34



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

Mountain Car Example



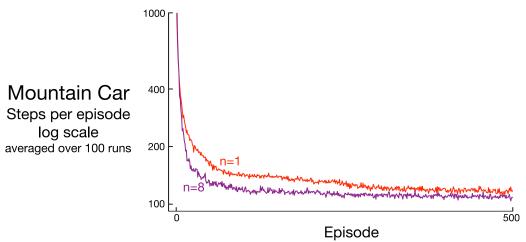


Figure 10.3 of "Reinforcement Learning: An Introduction, Second Edition".

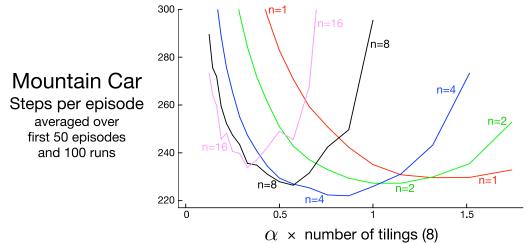


Figure 10.4 of "Reinforcement Learning: An Introduction, Second Edition".



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



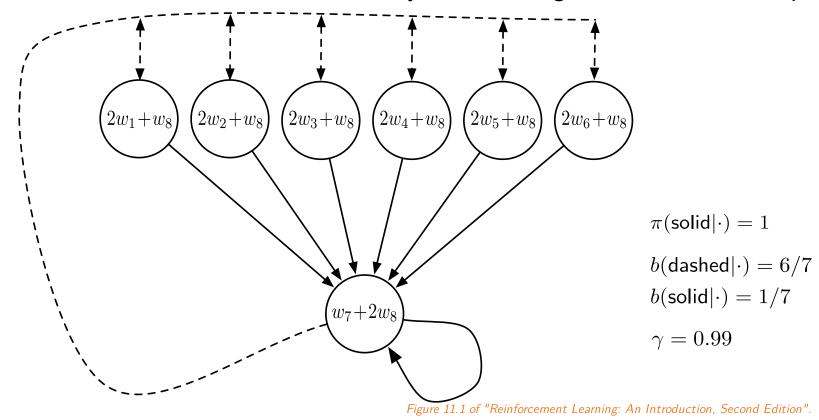
Figure from Section 11.2 of "Reinforcement Learning: An Introduction, Second Edition".

- ullet If initially w=10, TD error will be also 10 (or nearly 10 if $\gamma < 1$).
- ullet If for example lpha=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 realized for instance by the following *Baird's counterexample*:



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 $\alpha = 0.01$.



However, 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 $+\infty$ (while using on-policy distribution converges fine).

$$oldsymbol{w} \leftarrow oldsymbol{w} + rac{lpha}{|\mathcal{S}|} \sum_s \left(\mathbb{E}_{\pi} ig[R_{t+1} + \gamma \hat{v}(S_{t+1}; oldsymbol{w}) | S_t = s ig] - \hat{v}(s; oldsymbol{w})
ight)
abla \hat{v}(s; oldsymbol{w})$$

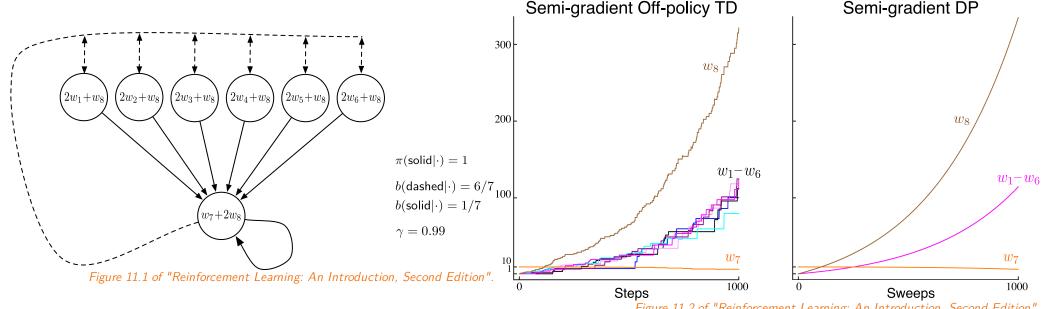


Figure 11.2 of "Reinforcement Learning: An Introduction, Second Edition".



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**.



26/34

Volodymyr Mnih et al.: Playing Atari with Deep Reinforcement Learning (Dec 2013 on arXiv),

In Feb 2015 accepted in Nature, as Human-level control through deep reinforcement learning.

Off-policy Q-learning algorithm with a convolutional neural network function approximation of action-value function.

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



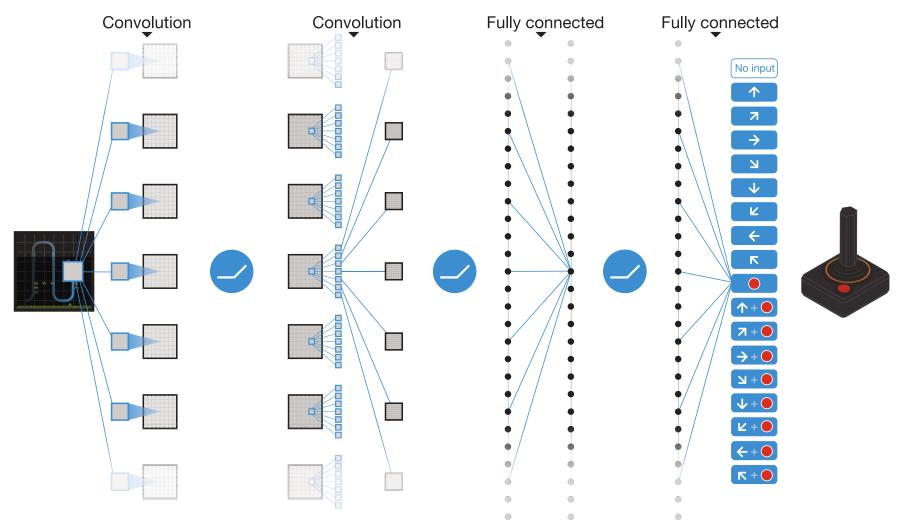


Figure 1 of the paper "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.



28/34

- ullet Preprocessing: 210 imes 160 128-color images are converted to grayscale and then resized to 84×84
- ullet Frame skipping technique is used, i.e., only every 4^{th} frame (out of 60 per second) is considered, and the selected action is repeated on the other frames.
- Input to the network are last 4 frames (considering only the frames kept by frame skipping), i.e., an image with 4 channels.
- The network is fairly standard, performing
 - 32 filters of size 8×8 with stride 4 and ReLU.
 - \circ 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)



Network is trained with RMSProp to minimize the following loss:

$$\mathcal{L} \stackrel{ ext{ iny def}}{=} \mathbb{E}_{(s,a,r,s') \sim ext{data}} \left[(r + [s' ext{ not terminal}] \cdot \gamma \max_{a'} Q(s',a';oldsymbol{ar{ heta}}) - Q(s,a;oldsymbol{ heta}))^2
ight].$$

ullet An arepsilon-greedy behavior policy is utilized (starts at arepsilon=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);
- ullet separate target network $oldsymbol{ heta}$: to prevent instabilities, a separate target network is used to estimate state-value function. The weights are not trained, but copied from the trained network once in a while;
- ullet 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 end of episode.
 - o furthermore, $(r + [s' \text{ not terminal}] \cdot \gamma \max_{a'} Q(s', a'; \overline{\theta}) Q(s, a; \theta))$ is also clipped to [-1, 1] (i.e., a smooth_{L1} loss or Huber loss).



30/34

```
Algorithm 1: deep Q-learning with experience replay.
```

Initialize replay memory D to capacity N

Initialize action-value function Q with random weights θ

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 ε select a random action a_t

otherwise select $a_t = \operatorname{argmax}_a Q(\phi(s_t), a; \theta)$

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 $\left(y_j - Q\left(\phi_j, a_j; \theta\right)\right)^2$ with respect to the network parameters θ

Every C steps reset $\hat{Q} = Q$

End For

End For

Algorithm 1 of the paper "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.



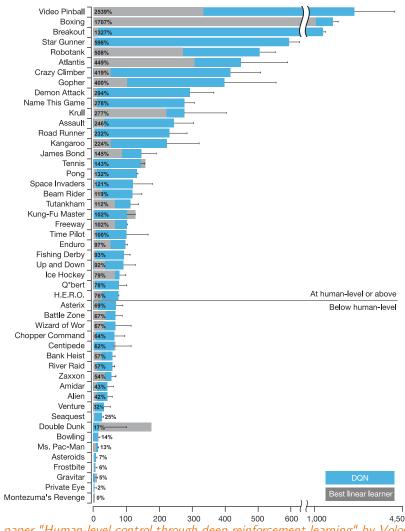
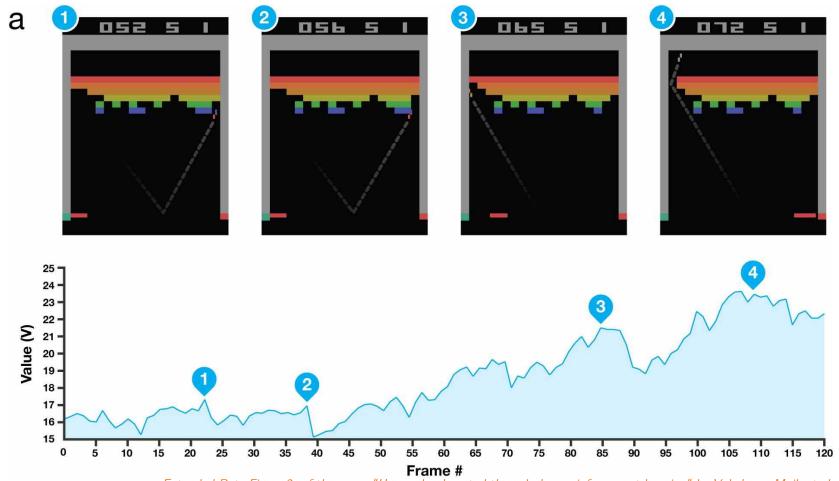


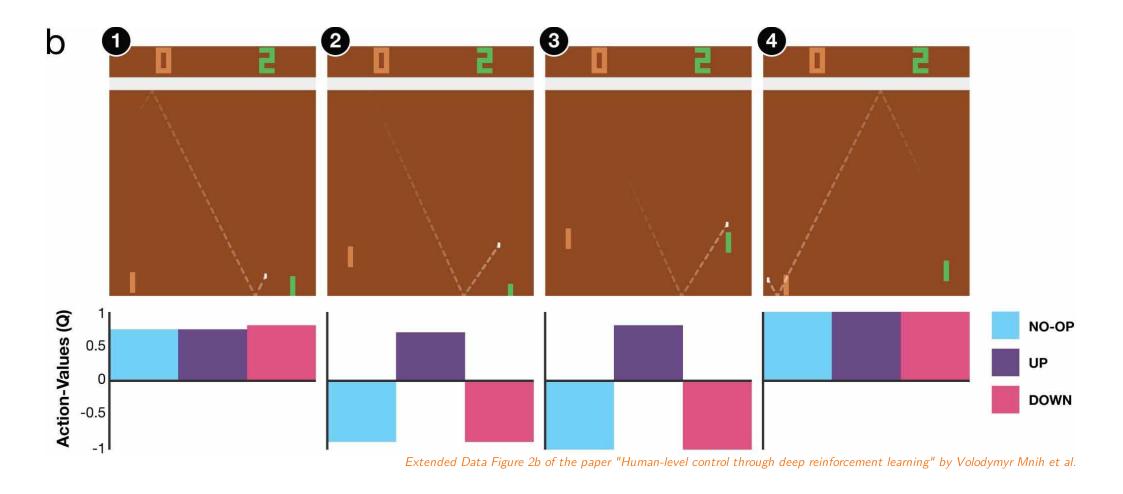
Figure 3 of the paper "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.





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





Deep Q Networks Hyperparameters



Hyperparameter	Value
minibatch size	32
replay buffer size	1M
target network update frequency	10k
discount factor	0.99
training frames	50M
RMSProp learning rate and momentum	0.00025, 0.95
initial $arepsilon$, final $arepsilon$ (linear decay) and frame of final $arepsilon$	1.0, 0.1, 1M
replay start size	50k
no-op max	30

DQN