Function Approximation, Deep Q Network

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Where Are We

- 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.
  - 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 $\arg\max_a \mathbb{E} R + v(s')$.
- The methods we know differ in several aspects:
  - Whether they compute return by simulating whole episode (Monte Carlo methods), or by using bootstrapping (temporal difference, i.e., $G_t \approx R_t + v(S_t)$, 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) of not (off-policy)
    - off-policy methods again more noisy and unstable, but more flexible

Function Approximation

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

We will denote the approximations as

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

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.

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

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

Function Approximation

For on-policy algorithms, μ is usually on-policy distribution. That is the stationary distribution under π for continuous tasks, and for the episodic case it is defined as

$$\eta(s) = h(s) + \sum_{s'} \eta(s') \sum_a \pi(a|s') p(s|s', a),$$

$$\mu(s) = \frac{\eta(s)}{\sum_{s'} \eta(s')},$$

where $h(s)$ is a probability that an episodes starts in state s.

Gradient and Semi-Gradient Methods

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

$$\begin{aligned} \boldsymbol{w}_{t+1} &\leftarrow \boldsymbol{w}_t - \frac{1}{2}\alpha\nabla_{\boldsymbol{w}_t}\left[v_\pi(S_t) - \hat{v}(S_t, \boldsymbol{w}_t)\right]^2 \\ &\leftarrow \boldsymbol{w}_t + \alpha\left[v_\pi(S_t) - \hat{v}(S_t, \boldsymbol{w}_t)\right]\nabla_{\boldsymbol{w}_t}\hat{v}(S_t, \boldsymbol{w}_t). \end{aligned}$$

As usual, the $v_\pi(S_t)$ is estimated by a suitable sample. For example 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 $\hat{v} : \mathcal{S} \times \mathbb{R}^d \to \mathbb{R}$
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, $t = 0, 1, \ldots, T-1$:
        $\mathbf{w} \leftarrow \mathbf{w} + \alpha \big[G_t - \hat{v}(S_t,\mathbf{w})\big] \nabla \hat{v}(S_t,\mathbf{w})$

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

Linear Methods

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

$$\hat{v}(\boldsymbol{x}(s), \boldsymbol{w}) \stackrel{\text{def}}{=} \boldsymbol{x}(s)^T \boldsymbol{w} = \sum x(s)_i w_i.$$

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

The SGD update rule then becomes

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

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 go 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:

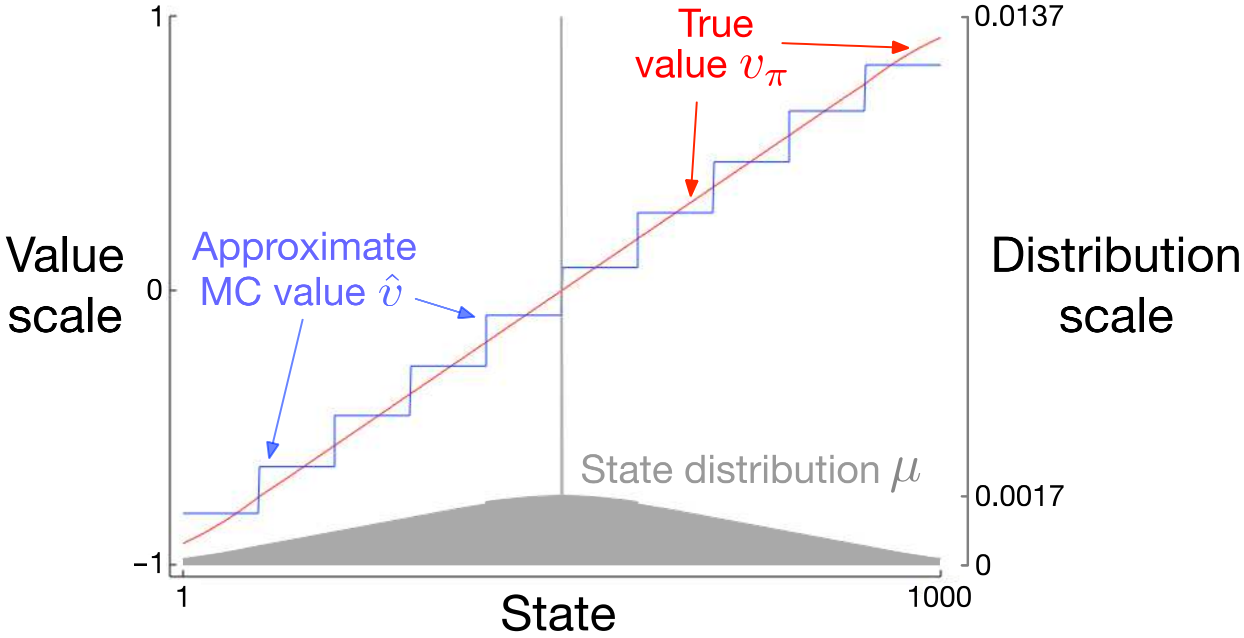


Figure 9.1 of "Reinforcement Learning: An Introduction, Second Edition".

Feature Construction for Linear Methods

Many methods developed in the past:

- polynomials
- Fourier basis
- tile coding
- radial basis functions

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

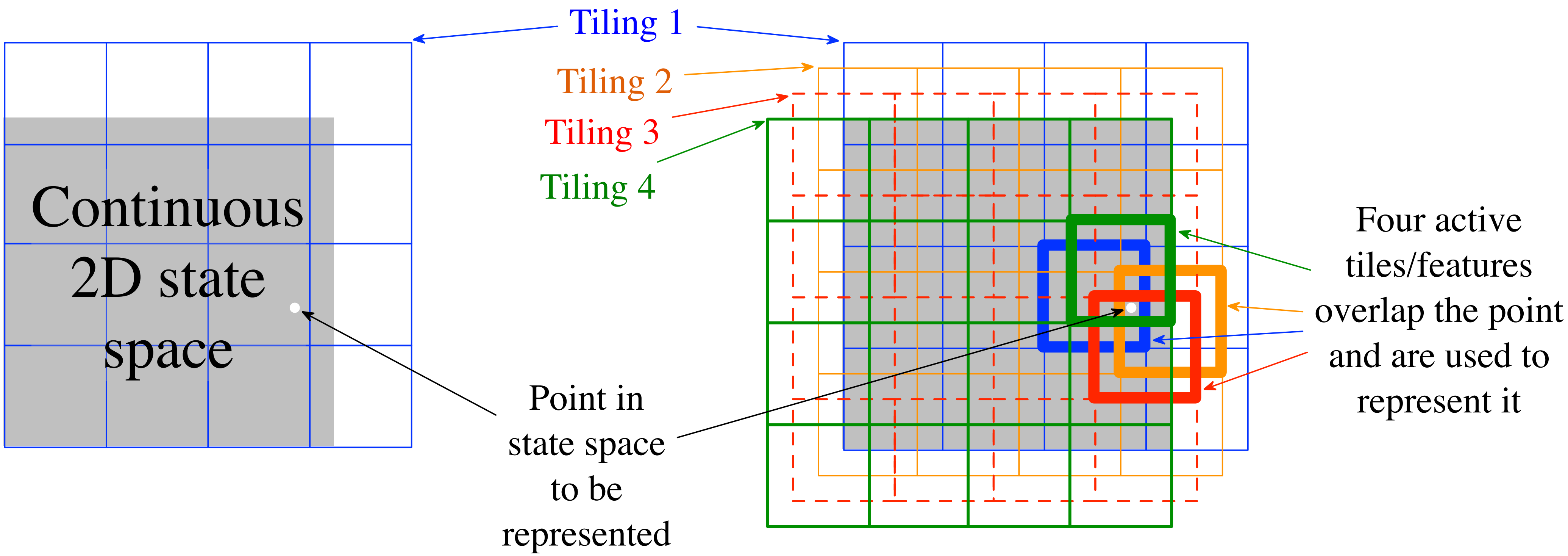


Figure 9.9 of "Reinforcement Learning: An Introduction, Second Edition".

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

Tile Coding

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

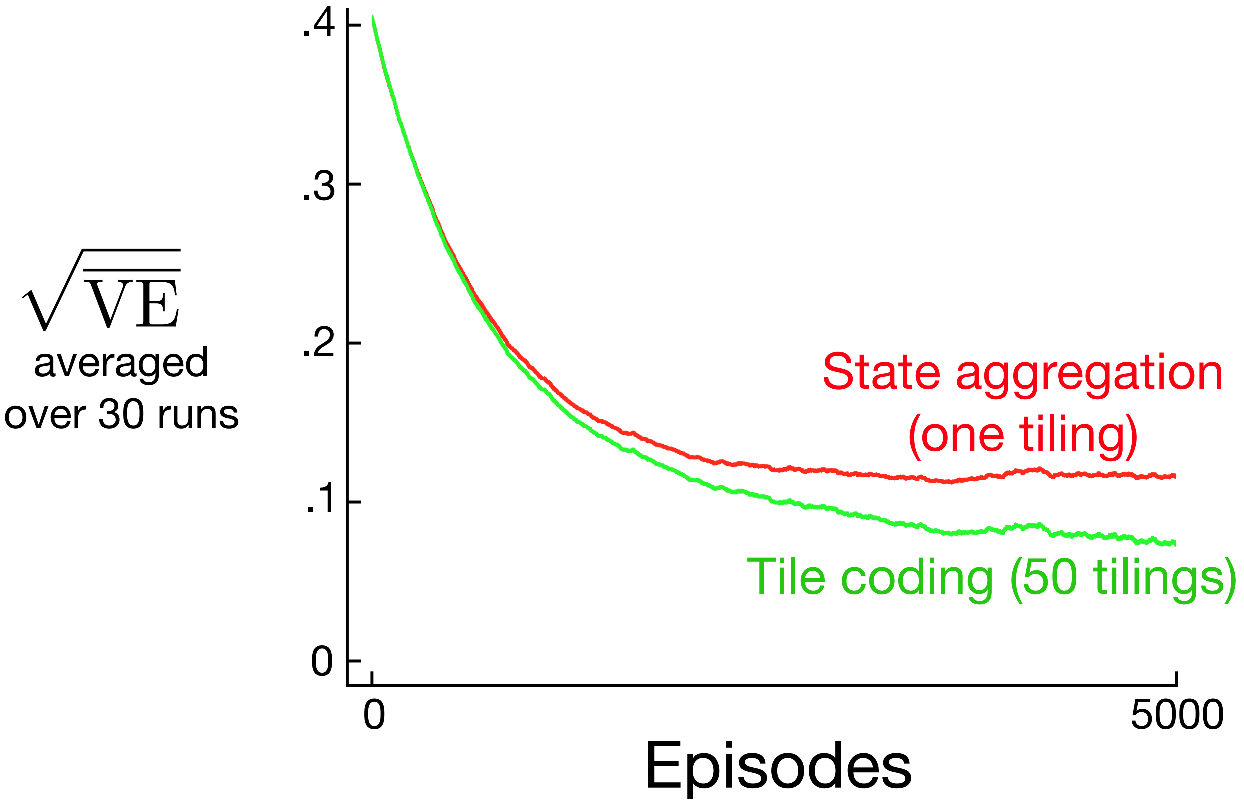


Figure 9.10 of "Reinforcement Learning: An Introduction, Second Edition".

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

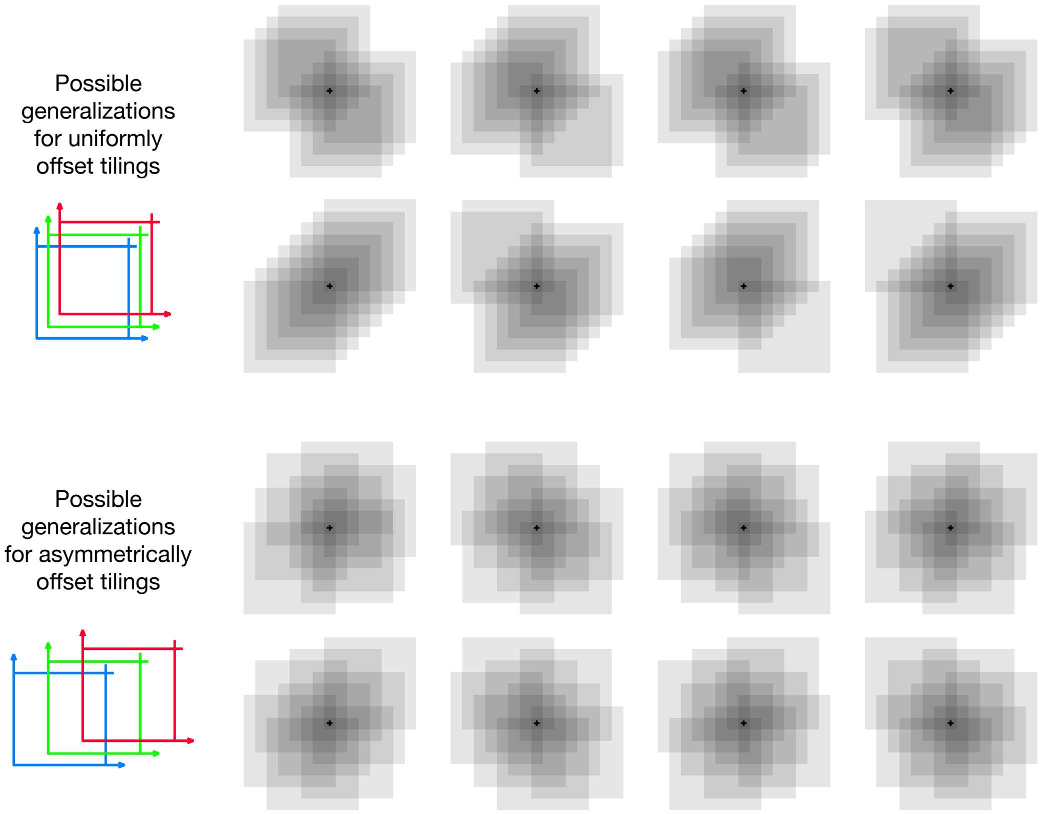


Figure 9.11 of "Reinforcement Learning: An Introduction, Second Edition".

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 π to be evaluated
Input: a differentiable function $\hat v : \mathcal{S}^+ \times \mathbb{R}^d \rightarrow \mathbb{R}$ 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'
        $\mathbf{w} \leftarrow \mathbf{w} + \alpha\big[R + \gamma \hat v(S',\mathbf{w}) - \hat v(S,\mathbf{w})\big]\nabla \hat v(S,\mathbf{w})$
        $S \leftarrow S'$
    until S is terminal

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

Note that such algorithm is called *semi-gradient*, because it does not backpropagate through $\hat v(S', \boldsymbol w)$.

Temporal Difference Semi-Gradient Policy Evaluation

An important fact is that linear semi-gradient TD methods do not converge to $\overline{VE}$. Instead, they converge to a different *TD fixed point* $\boldsymbol{w}_\mathrm{TD}$.

It can be proven that

$$\overline{VE}(\boldsymbol{w}_\mathrm{TD}) \leq \frac{1}{1-\gamma} \min_{\boldsymbol{w}} \overline{VE}(\boldsymbol{w}).$$

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

Temporal Difference Semi-Gradient Policy Evaluation

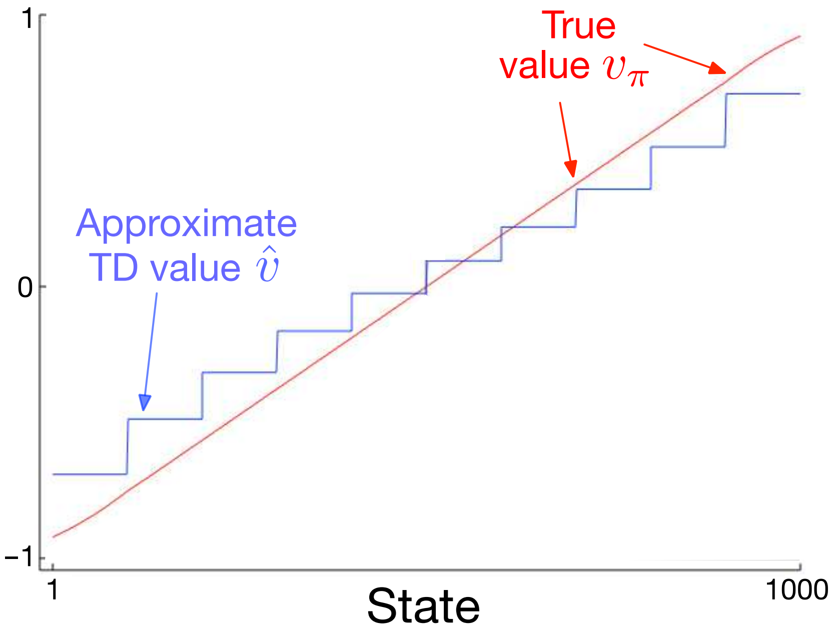
As before, we can utilize n-step TD methods.

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

Input: the policy π to be evaluated
Input: a differentiable function $\hat{v} : \mathcal{S}^+ \times \mathbb{R}^d \to \mathbb{R}$ 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 and R_t) can take their index mod $n+1$

Loop for each episode:
    Initialize and store $S_0 \neq$ 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 $T \leftarrow t+1$
    | $\tau \leftarrow t - n + 1$ (τ 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: $G \leftarrow G + \gamma^n \hat{v}(S_{\tau+n},\mathbf{w})$ $(G_{\tau:\tau+n})$
    | $\mathbf{w} \leftarrow \mathbf{w} + \alpha \left[G - \hat{v}(S_\tau,\mathbf{w})\right] \nabla \hat{v}(S_\tau,\mathbf{w})$
    Until $\tau = T - 1$

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



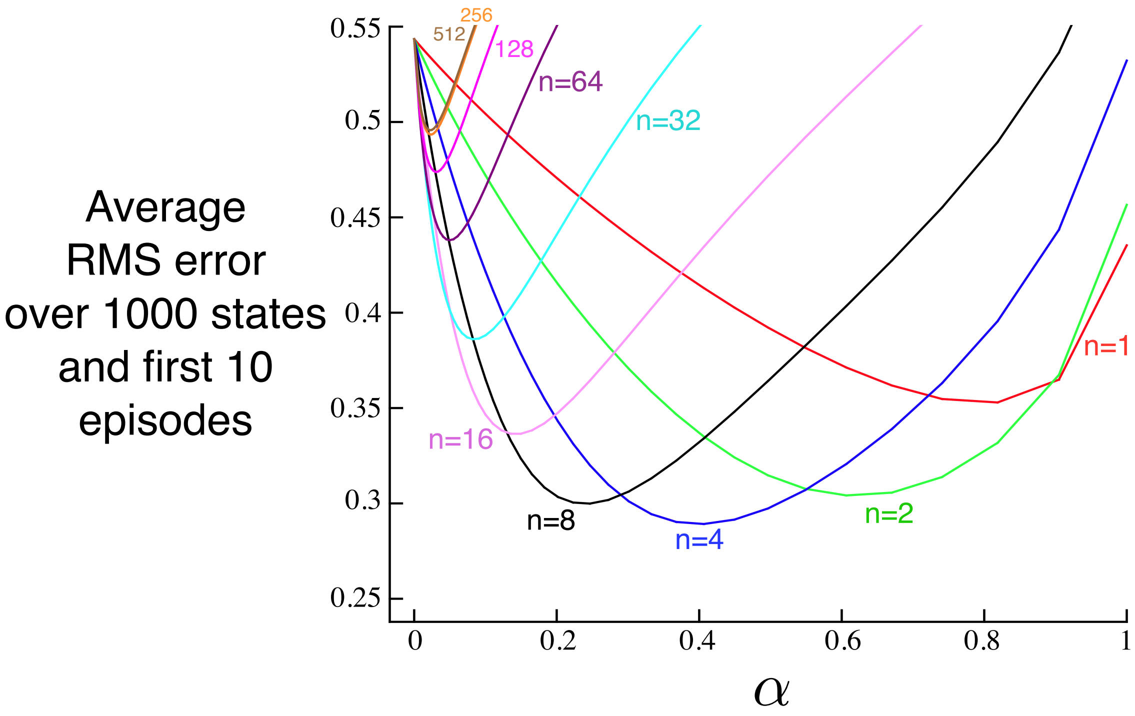


Figure 9.2 of "Reinforcement Learning: An Introduction, Second Edition".

Sarsa with Function Approximation

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 $\hat{q} : \mathcal{S} \times \mathcal{A} \times \mathbb{R}^d \to \mathbb{R}$
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:
- $S, A \leftarrow$ 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:
    - $\mathbf{w} \leftarrow \mathbf{w} + \alpha\big[R - \hat{q}(S, A, \mathbf{w})\big]\nabla\hat{q}(S, A, \mathbf{w})$
    - Go to next episode
  - Choose A' as a function of $\hat{q}(S', \cdot, \mathbf{w})$ (e.g., ε-greedy)
  - $\mathbf{w} \leftarrow \mathbf{w} + \alpha\big[R + \gamma\hat{q}(S', A', \mathbf{w}) - \hat{q}(S, A, \mathbf{w})\big]\nabla\hat{q}(S, A, \mathbf{w})$
  - $S \leftarrow S'$
  - $A \leftarrow A'$

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

Sarsa with Function Approximation

Additionally, we can incorporate n-step returns:

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

Input: a differentiable action-value function parameterization $\hat{q} : \mathcal{S} \times \mathcal{A} \times \mathbb{R}^d \to \mathbb{R}$
Input: a policy π (if estimating q_π)
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, 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 ε-greedy wrt $\hat{q}(S_0, \cdot, \mathbf{w})$
  $T \leftarrow \infty$
  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 ε-greedy wrt $\hat{q}(S_{t+1}, \cdot, \mathbf{w})$
  | $\tau \leftarrow t - n + 1$ (τ 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 $G \leftarrow G + \gamma^n \hat{q}(S_{\tau+n}, A_{\tau+n}, \mathbf{w})$ $(G_{\tau:\tau+n})$
  | $\mathbf{w} \leftarrow \mathbf{w} + \alpha \left[G - \hat{q}(S_\tau, A_\tau, \mathbf{w})\right] \nabla \hat{q}(S_\tau, A_\tau, \mathbf{w})$
  Until $\tau = T - 1$

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

Mountain Car Example

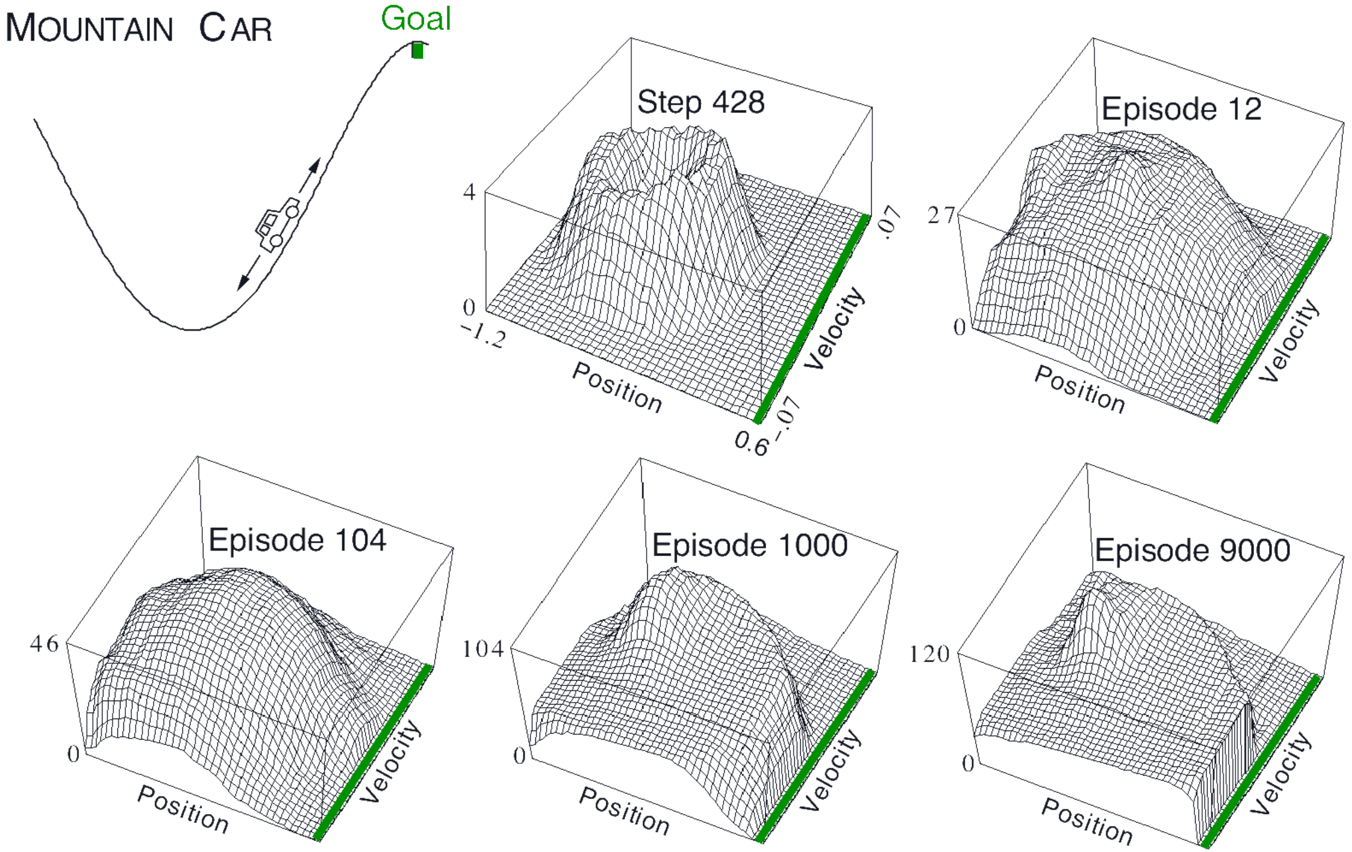


Figure 10.1 of "Reinforcement Learning: An Introduction, Second Edition".

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

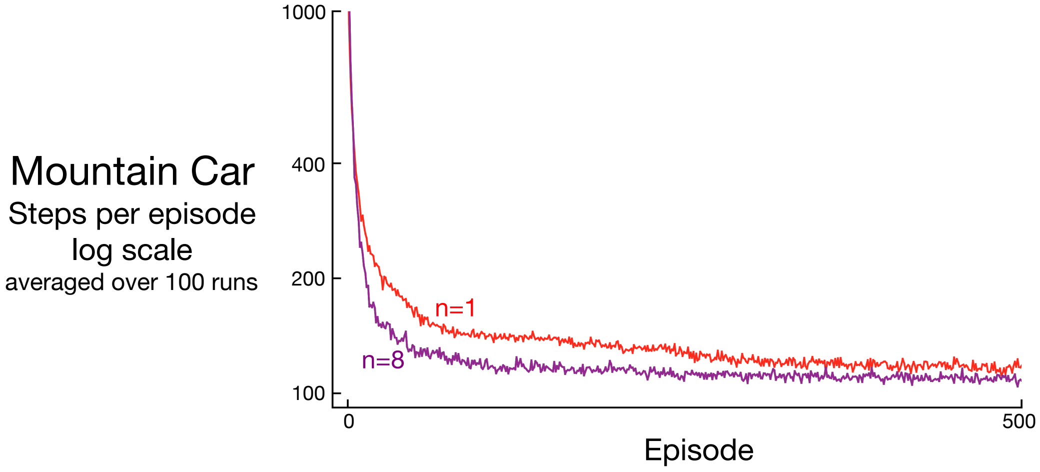


Figure 10.3 of "Reinforcement Learning: An Introduction, Second Edition".

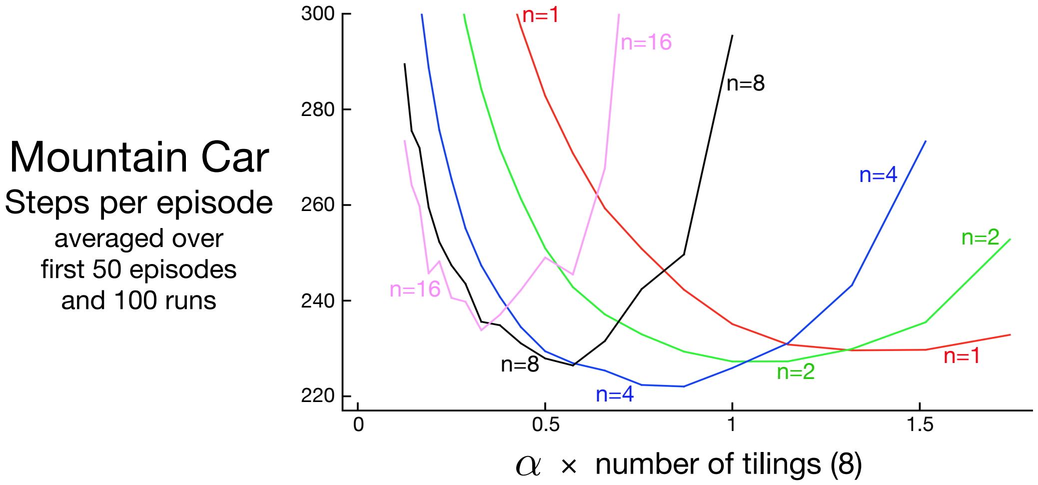


Figure 10.4 of "Reinforcement Learning: An Introduction, Second Edition".

Off-policy Divergence With Function Approximation

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

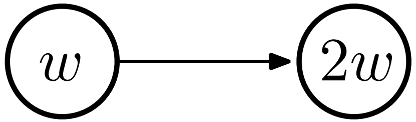


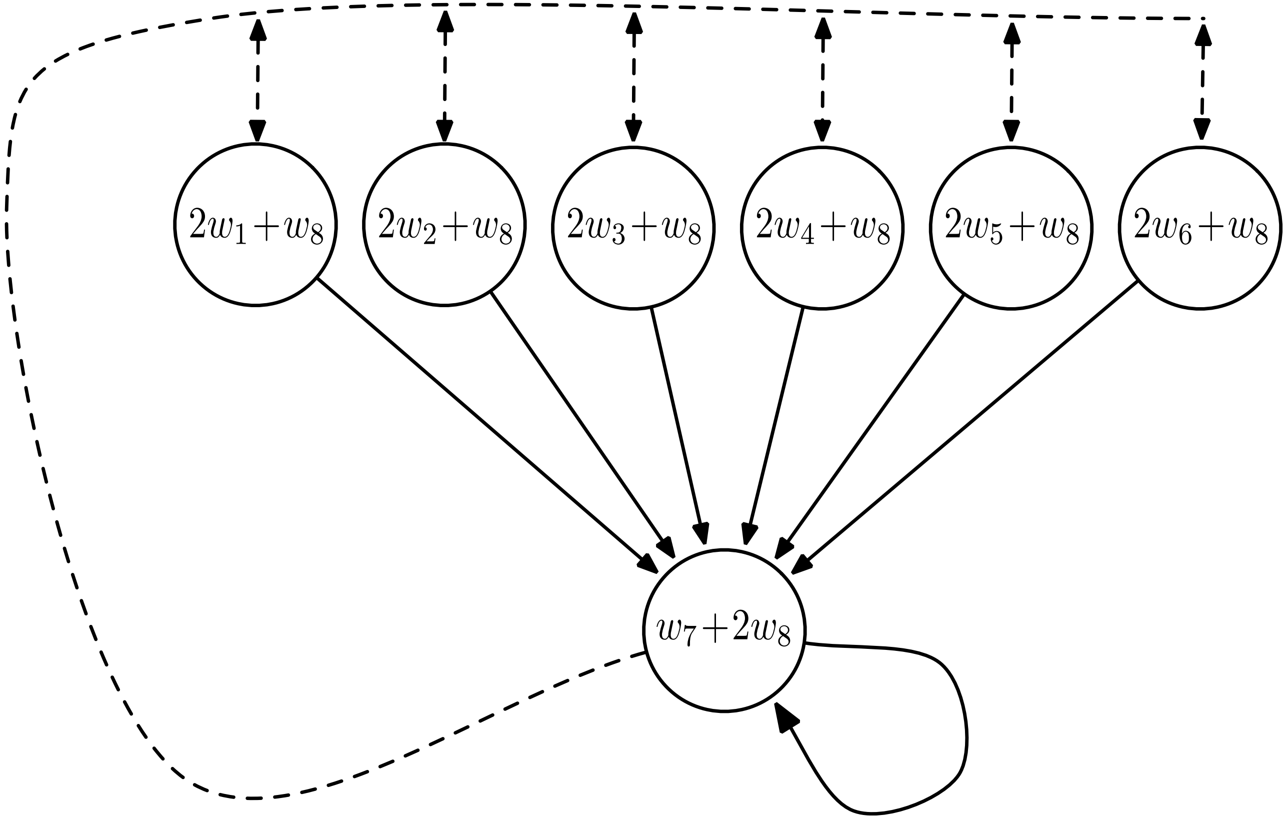
Figure from Section 11.2 of "Reinforcement Learning: An Introduction, Second Edition".

- If initially $w = 10$, 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.

Off-policy Divergence With Function Approximation

The previous idea can be realized for instance by the following *Baird's counterexample*:



$\pi(\text{solid}|\cdot) = 1$

$b(\text{dashed}|\cdot) = 6/7$

$b(\text{solid}|\cdot) = 1/7$

$\gamma = 0.99$

Figure 11.1 of "Reinforcement Learning: An Introduction, Second Edition".

The rewards are zero everywhere, so the value function is also zero everywhere.

Off-policy Divergence With Function Approximation

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 ∞.

$$\boldsymbol{w}_{t+1} \leftarrow \boldsymbol{w}_t + \frac{\alpha}{|\mathcal{S}|} \sum_s \Big(\mathbb{E}_\pi \big[R_{t+1} + \gamma \hat{v}(S_{t+1}, \boldsymbol{w}_k) \big| S_t = s \big] - \hat{v}(s, \boldsymbol{w}_k) \Big) \nabla \hat{v}(s, \boldsymbol{w}_k)$$

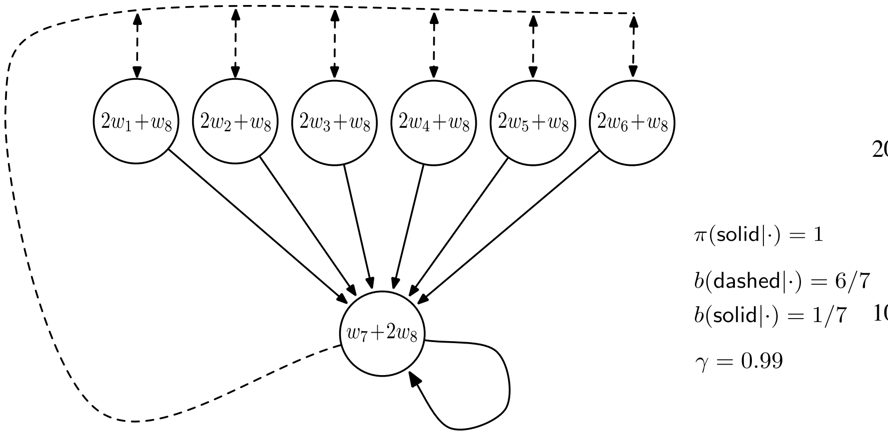


Figure 11.1 of "Reinforcement Learning: An Introduction, Second Edition".

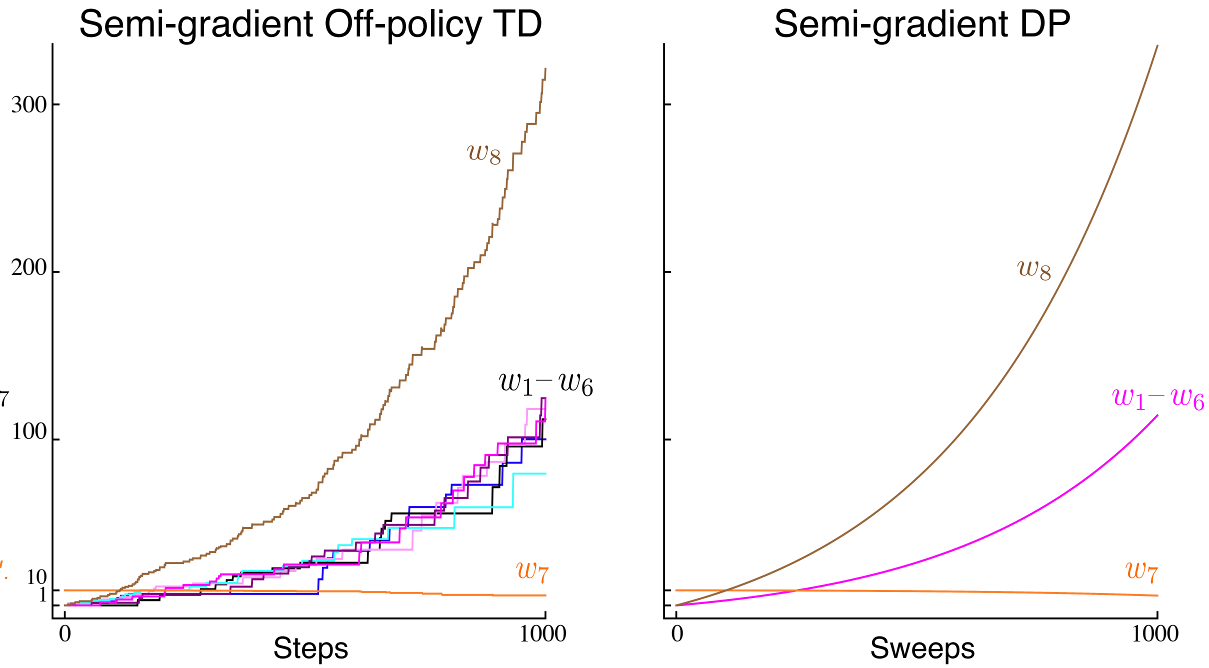


Figure 11.2 of "Reinforcement Learning: An Introduction, Second Edition".

Deep Q Networks

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

In 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).

Deep Q Network

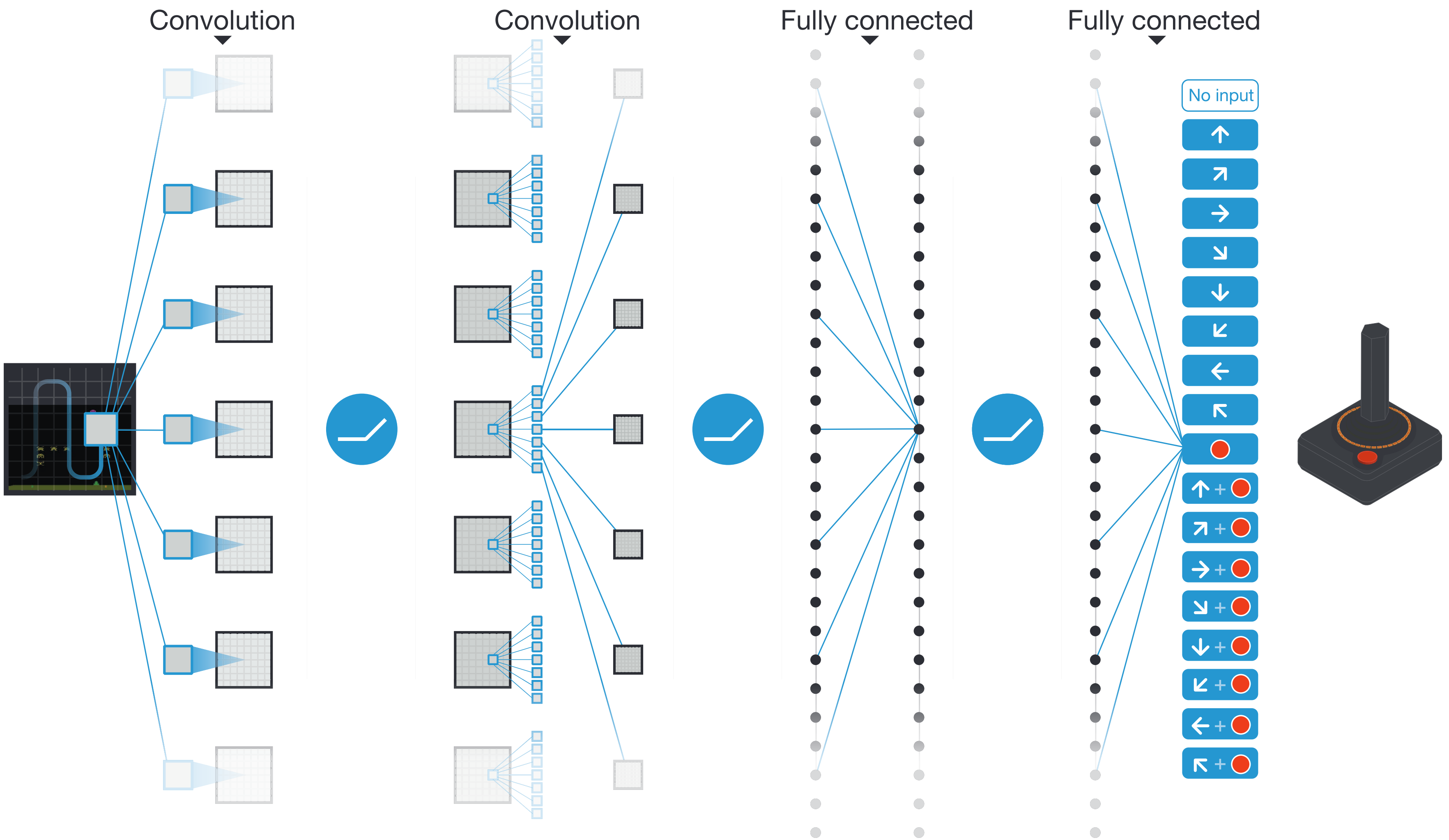


Figure 1 of the paper "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.

Deep Q Network

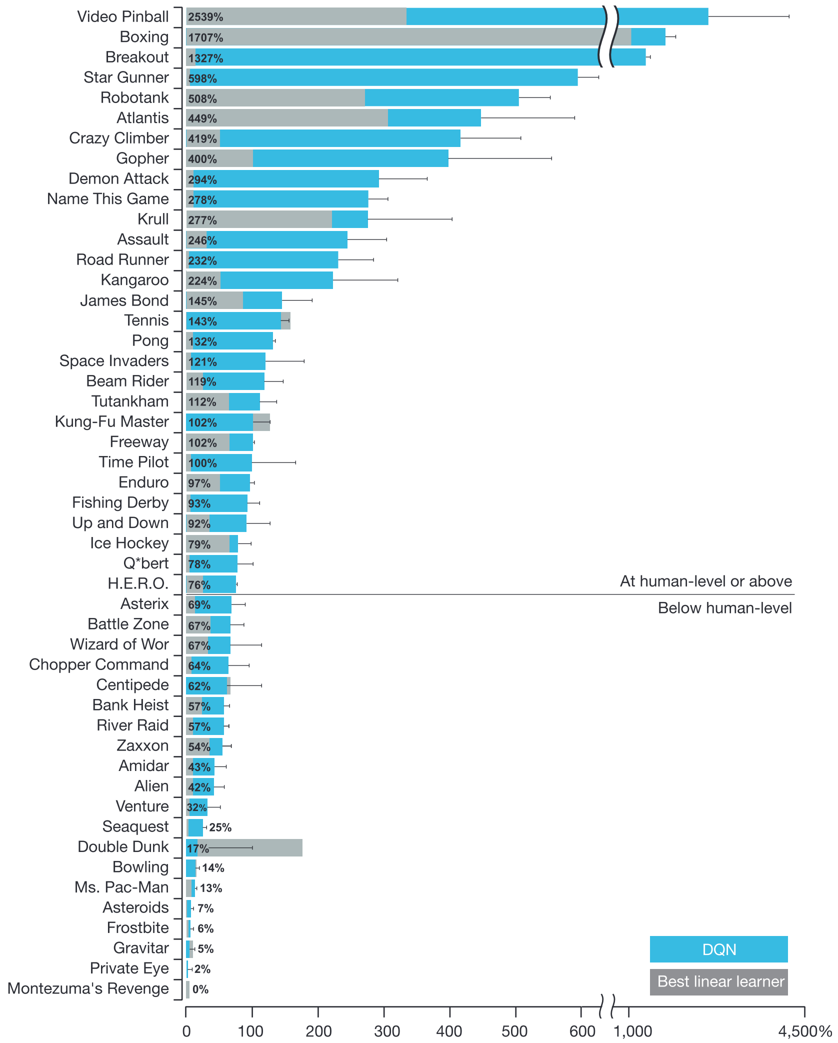
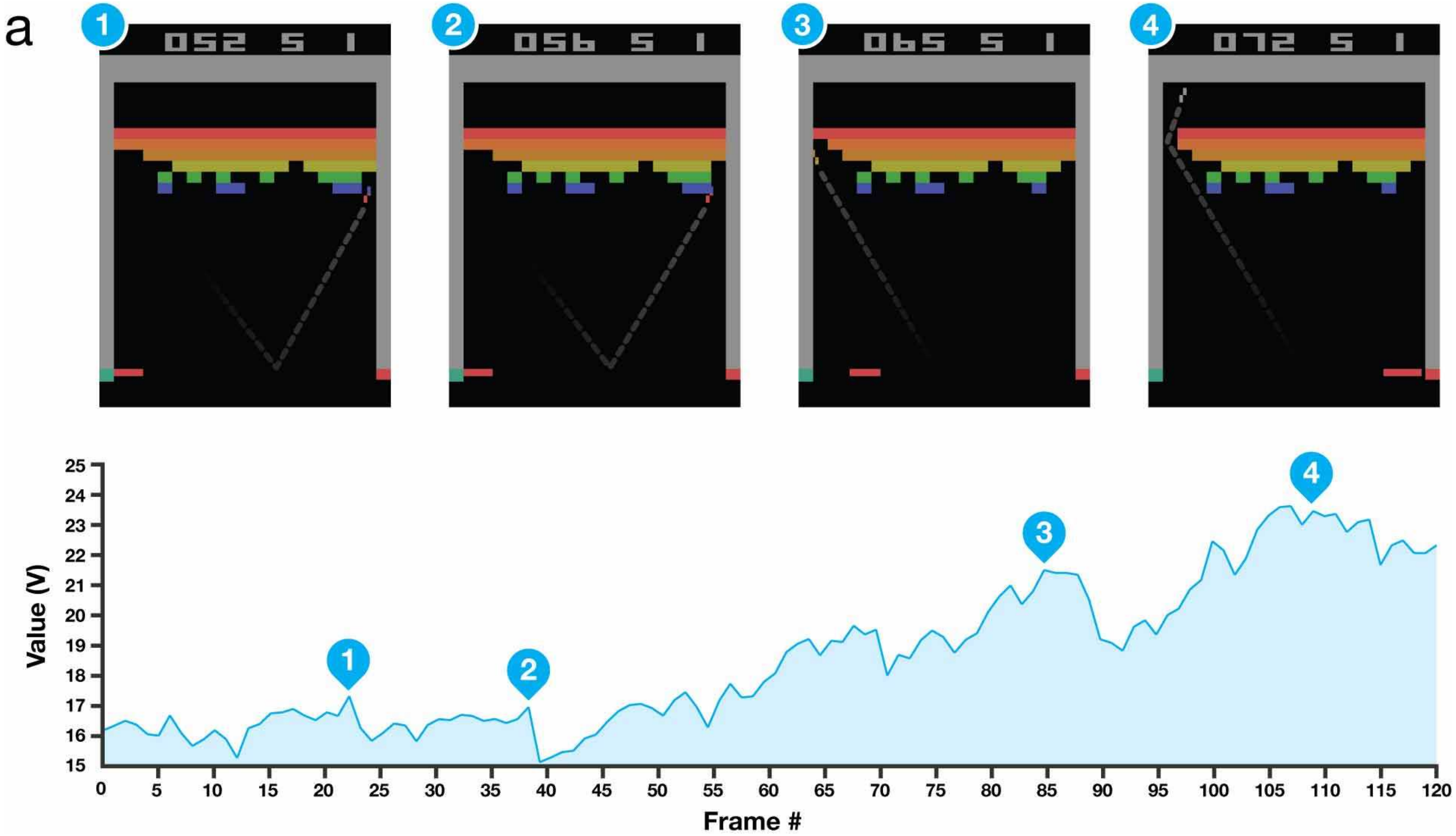


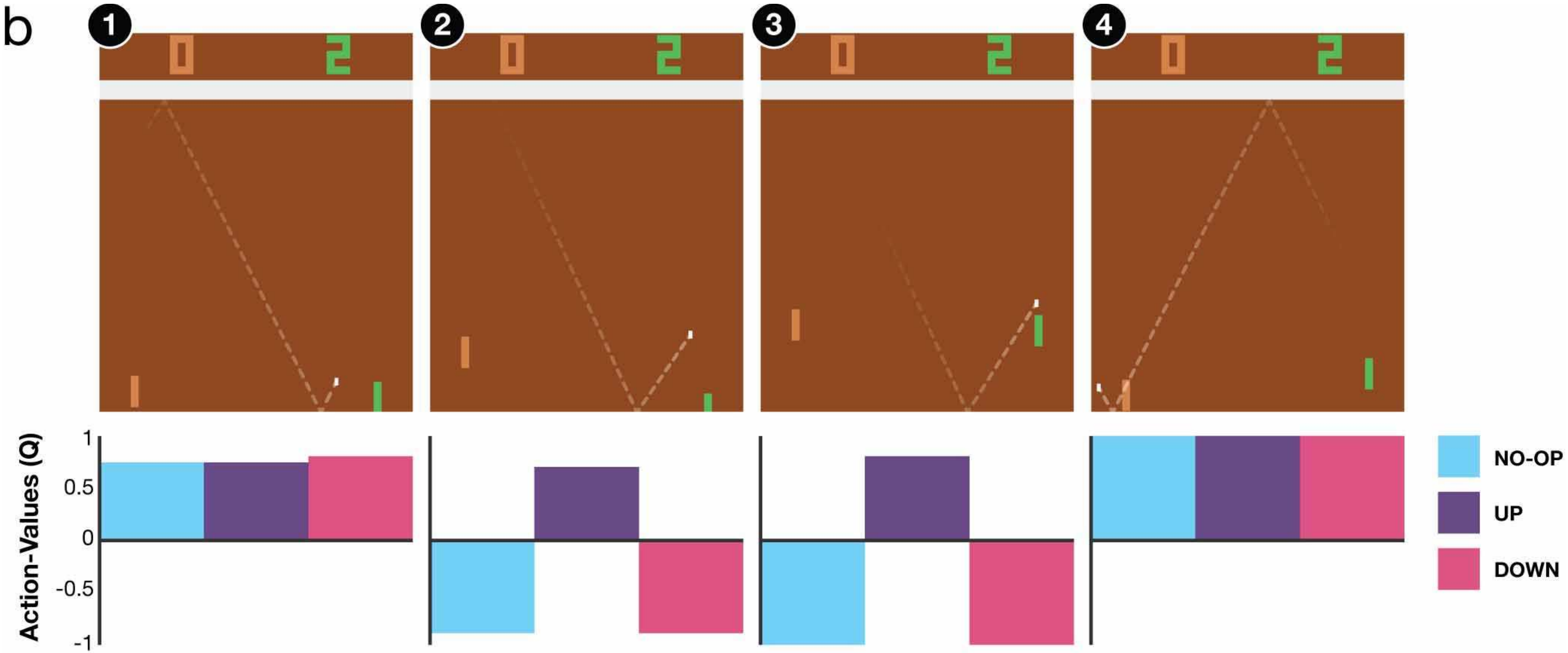
Figure 3 of the paper "Human-level control through deep reinforcement learning" by Volodymyr Mnih et al.

Deep Q Network



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

Deep Q Network



Extended Data Figure 2b of the paper "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^{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,
  - 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:

$$\mathcal{L} \stackrel{\text{def}}{=} \mathbb{E}_{(s,a,r,s')\sim data}\left[\left(r + [s' \text{ not terminal}] \cdot \gamma \max_{a'} Q(s', a'; \bar\theta) - Q(s, a; \theta)\right)^2\right].$$

- An ε-greedy behavior policy is utilized.

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;
- separate target network $\bar\theta$: 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;
- reward clipping: because rewards have wildly different scale in different games, all positive rewards are replaced by $+1$ and negative by -1
  - furthermore, $(r + [s' \text{ not terminal}] \cdot \gamma \max_{a'} Q(s', a'; \bar\theta) - Q(s, a; \theta))$ is also clipped to $[-1, 1]$ (i.e., a smooth_{L_1} loss or Huber loss).

Deep Q Networks

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 $\left(y_j - Q(\phi_j, a_j; \theta)\right)^2$ 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.

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 ε, final ε (linear decay) and frame of final ε	1.0, 0.1, 1M
replay start size	50k
no-op max	30