Reinforcement Learning
Lecture 7: Function approximation [1]

Lecturer: Prof. Dr. Mathias Niepert

Institute for Parallel and Distributed Systems
Machine Learning and Simulation Lab

University of Stuttgart
Germany

imprs-is

June 15, 2023

[1] Many slides adapted from R. Sutton's course, D. Silver's course as well as previous RL courses given at U. of Stuttgart by J. Mainprice, D. Hennes, M. Toussaint, H. Ngo, and V. Ngo.

Outline

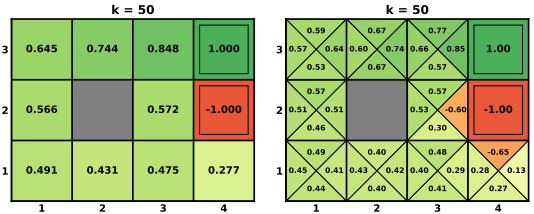
Introduction

Large state spaces

- Backgammon: 10^{20} states
- Go: 10^{170} states
- Continuous spaces:
  - inverted pendulum
  - mountain car
  - helicopter
  - ...

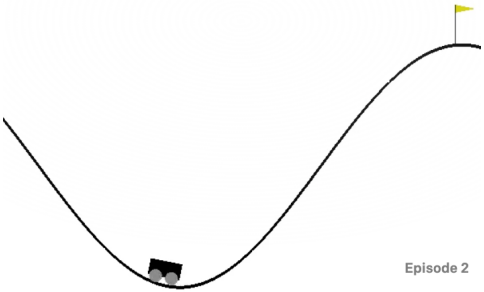
Small domains: tabular representation

- So far V and Q were just *lookup tables*:



- Problems with large MDPs:
  - too many states to store in memory
  - too slow to learn
- How can we scale the tabular solution methods to arbitrarily large state/action spaces?
  - *generalize* from previous encounters of similar states (or state–action pairs)
  - **function approximation** (supervised learning)

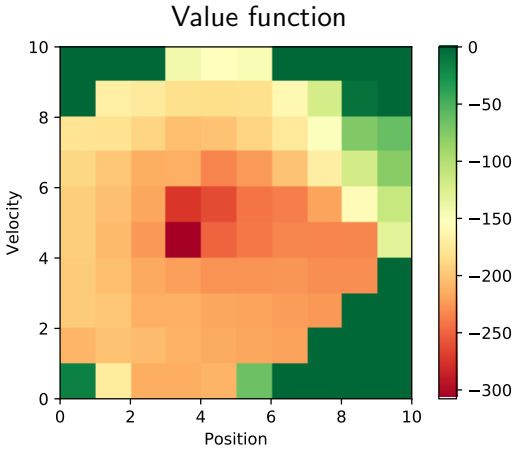
Example: mountain car

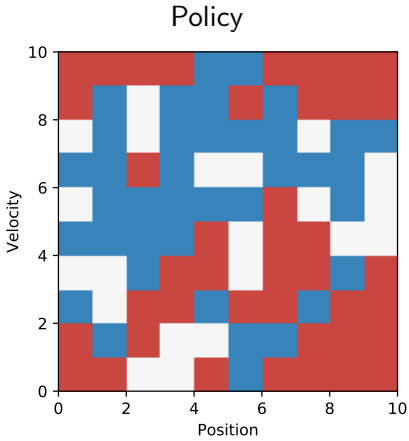


Dynamics : $\underbrace{\frac{\mathrm{d}^2 x}{\mathrm{d}t^2}}_{\text{acceleration}} = \underbrace{\cos(3x)}_{\text{gravity}} + \underbrace{u \cdot a}_{\text{force}}$

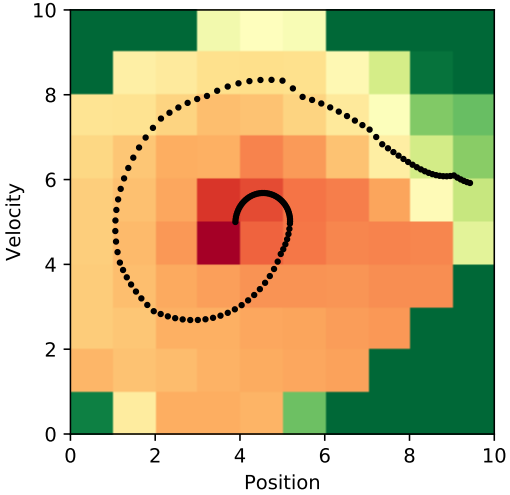
where $a \in \{-1, 0, 1\}$ is the action

State aggregation in mountain car





State aggregation in mountain car

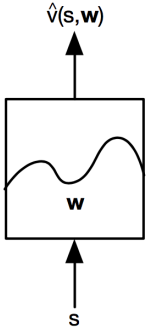


Value function approximation

Idea of value function approximation

- Parameterized functional form, with weights $\boldsymbol{w} \in \mathbb{R}^d$:

$$\hat{v}_\pi(s, \boldsymbol{w}) \approx v_\pi(s)$$

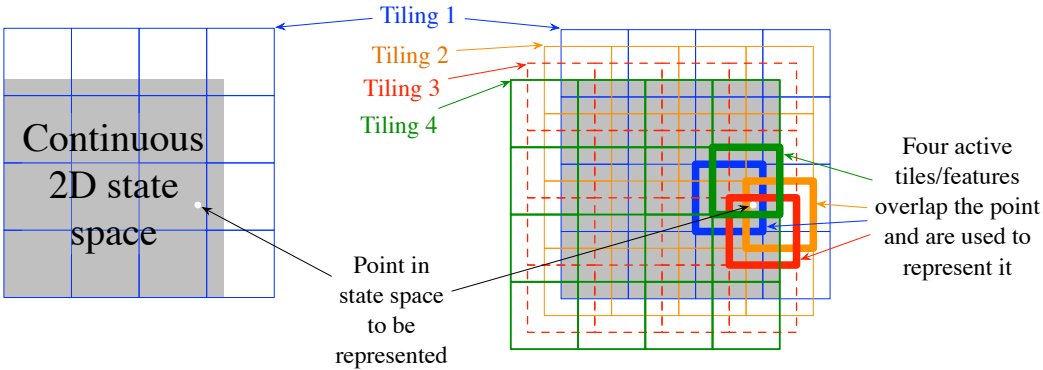


- Generally, much less weights than states $d \ll |\mathcal{S}|$
  - obvious for continuous state spaces
  - changing single weight, changes value estimate of many states
  - when one state is updated, change *generalizes* to many states
- Update $\boldsymbol{w}$ with MC or TD learning

Function approximators

- Linear combinations of features
  - **state aggregation**
  - **tile coding**
  - polynomials
  - radial basis functions (RBFs)
  - Fourier bases
  - ...
- Neural networks
- Decision trees
- Non-parametric approaches

Tile coding


Tiling 1
Tiling 2
Tiling 3
Tiling 4
Continuous 2D state space
Point in state space to be represented
Four active tiles/features overlap the point and are used to represent it

Function approximators for RL

- Differentiable function approximators, e.g.:
  - Linear combination of features
  - Neural networks
- RL specific problems:
  - non-stationary
  - non-iid data
  - bootstrapping
  - delayed targets

Random variables are *independent and identically distributed* (iid) if they each have the same probability distribution and are mutually independent

Stochastic Gradient Descent (SGD)

- Approximate value function $\hat{v}(s, \boldsymbol{w})$
  - differentiable for all $s \in \mathcal{S}$
- Weight vector $\boldsymbol{w} = (w_1, w_2, \ldots, w_d)^\top$
  - $\boldsymbol{w}_t$ weight vector at time $t = 0, 1, 2, \ldots$
- *Gradient* of $f(\boldsymbol{w})$: $\nabla f(\boldsymbol{w}) = \left(\frac{\partial f(\boldsymbol{w})}{\partial w_1}, \frac{\partial f(\boldsymbol{w})}{\partial w_2}, \ldots, \frac{\partial f(\boldsymbol{w})}{\partial w_d} \right)^\top$
- Do gradient descent by sampling additive parts of the full gradient (i.e., each state consecutively)
- We can compute our update over smaller sets of inputs

Stochastic Gradient Descent (SGD) (part 2)

- When we **approximate** the gradient
- For example

$$\mathcal{L}(\boldsymbol{w}) = \sum_{n=1}^{N} \mathcal{L}_n(\boldsymbol{w})$$

where $\boldsymbol{w}$ are weights.

- In machine learning

$$\mathcal{L}(\boldsymbol{w}) = -\sum_{n=1}^{N} \log p(y_n \mid \boldsymbol{x}_n, \boldsymbol{w})$$

where $\boldsymbol{x}_n \in \mathbb{R}^D$ are training *inputs* and y_n are the training *targets*

- The corresponding update

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t - \alpha_t \sum_{n=1}^{N} (\boldsymbol{\nabla} \mathcal{L}_n)(\boldsymbol{w}_t)$$

- Often the gradient is too difficult to compute (CPU/GPU expensive)
- **Mini-batch**: random subset
  a. Large: accurate but costly
  b. Small: noisy but cheep

Stochastic Gradient Descent (SGD) (part 3)

- *Mean squared Value Error*: $\mathcal{L}(\boldsymbol{w}) = \sum_{s \in S} \mu(s) \left[v_\pi(s) - \hat{v}(s, \boldsymbol{w}) \right]^2$
- Adjust $\boldsymbol{w}$ to reduce the error on sample $S_t \mapsto v_\pi(S_t)$:

$$
\begin{aligned}
\boldsymbol{w}_{t+1} &= \boldsymbol{w}_t - \frac{1}{2} \alpha_t (\boldsymbol{\nabla} \mathcal{L}_t)(\boldsymbol{w}_t) \\
&= \boldsymbol{w}_t - \frac{1}{2} \alpha_t \boldsymbol{\nabla} \underbrace{\left[v_\pi(S_t) - \hat{v}(S_t, \boldsymbol{w}_t) \right]^2}_{\textbf{squared sample error}} \\
&= \boldsymbol{w}_t + \alpha_t [v_\pi(S_t) - \hat{v}(S_t, \boldsymbol{w}_t)] \nabla \hat{v}(S_t, \boldsymbol{w})
\end{aligned}
$$

- α_t is a step size parameter
- Why not use $\alpha = 1$, thus eliminating full error on sample?

Linear methods

- Special case where $\hat{v}(\cdot, \boldsymbol{w})$ is *linear* in the weights
- **Feature vector** $\boldsymbol{x}(s)$ represents state s:

$$\boldsymbol{x}(s) = \begin{bmatrix} x_1(s), & x_2(s), & \dots, & x_d(s) \end{bmatrix}^\top$$

- Each component of $\boldsymbol{x}$ is a feature, examples:
  - distance of robot to landmarks
  - piece on a specific location on a chess board
- Value function is represented as a linear combination of features $\boldsymbol{x}(s)$:

$$\hat{v}(s, \boldsymbol{w}) = \boldsymbol{w}^\top \boldsymbol{x}(s) = \sum_{i=1}^{d} w_i x_i(s)$$

- Gradient is simply $\nabla \hat{v}(s, \boldsymbol{w}) = \boldsymbol{x}(s)$

Prediction

Prediction with function approximation

- We assumed the true value function $v_\pi(S_t)$ is known
- Substitute target U_t for $v_\pi(s)$

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \alpha[U_t - \hat{v}(S_t, \boldsymbol{w}_t)]\nabla\hat{v}(S_t, \boldsymbol{w}_t)$$

- U_t might be a noisy or bootstrapped approximation of the true value
- **Monte Carlo:** $U_t = G_t$
- **TD(0):** $U_t = R_{t+1} + \gamma\hat{v}(S_{t+1}, \boldsymbol{w}_t)$
- **TD(λ):** $U_t = G_t^\lambda$

Monte–Carlo with function approximation

- Target is unbiased by definition:

$$\mathbb{E}[U_t|S_t = s] = \mathbb{E}[G_t|S_t = s] = v_\pi(S_t)$$

- Training data:

$$\mathcal{D} = \big\{(S_1, G_1),\ (S_2, G_2),\ \ldots,\ (S_{T-1}, G_{T-1}),\ (S_T, 0)\big\}$$

- Using SGD, $\boldsymbol{w}$ is guaranteed to converge to a *local optimum*
- MC prediction exhibits local convergence with linear and non-linear function approximation
- SGD update for sample $S_t \mapsto G_t$:

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

Gradient Monte Carlo Algorithm

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, $t = 0, 1, \ldots, T-1$:
    $\mathbf{w} \leftarrow \mathbf{w} + \alpha\big[G_t - \hat{v}(S_t,\mathbf{w})\big]\nabla\hat{v}(S_t,\mathbf{w})$

TD with function approximation

- TD-target $U_t = R_{t+1} + \gamma \hat{v}(S_{t+1}, \boldsymbol{w})$ is *biased* sample of the true value $v_\pi(S_t)$
- Training data:

$$\mathcal{D} = \big\{(S_1, R_2 + \gamma \hat{v}(S_2, \boldsymbol{w})),\ (S_2, R_3 + \gamma \hat{v}(S_3, \boldsymbol{w})),\ \ldots, (S_{T-1}, R_T)\big\}$$

- SGD update for sample $S_t \mapsto G_t$:

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \alpha[R_{t+1} + \gamma \hat{v}(S_{t+1}, \boldsymbol{w}) - \hat{v}(S_t, \boldsymbol{w})] \nabla \hat{v}(S_t, \boldsymbol{w})$$

- Linear TD(0):

$$\boldsymbol{w} \leftarrow \boldsymbol{w} + \alpha[\underbrace{R_{t+1} + \gamma \boldsymbol{w}^T \boldsymbol{x}(S_{t+1})}_{U_t\text{:TD-Target}} - \underbrace{\boldsymbol{w}^T \boldsymbol{x}(S_t)}_{\hat{v}\text{:value function}}] \boldsymbol{x}(S_t)$$

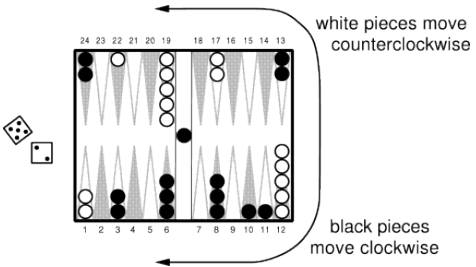
Semi-Gradient TD(0) Algorithm

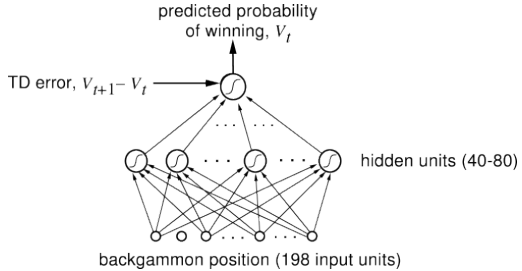
Semi-gradient TD(0) for estimating $\hat{v} \approx v_\pi$

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

Example: TD-Gammon

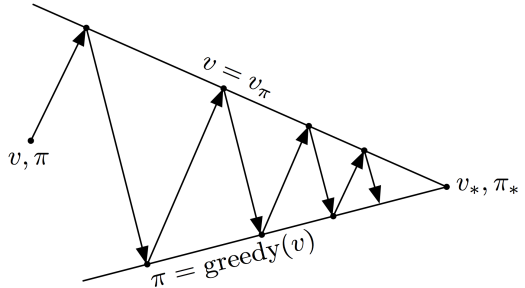




- by Gerald Tesauro (1992) - Multi-layer perceptron (neural network) represents value function - Only reward given at the end of game $(1, 0.5, 0)$ - **Self-play:** use the current policy to sample moves on both sides! - Same ideas used in recent work on Go, Chess, Shogi: - Alpha Go Zero (2015) - Alpha Zero (2017)

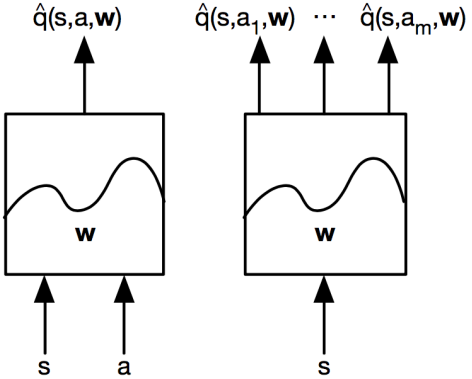
Control

Control with function approximation



- Control via generalized policy iteration (GPI):
  - *policy evaluation:* **approximate** policy evaluation: $\hat{q}(\cdot, \cdot, \boldsymbol{w}) \approx q_\pi$
  - *policy improvement:* ϵ-greedy policy improvement

Types of action–value function approximation



- Action as input: $\hat{q}(s, a, \boldsymbol{w}) \approx q_\pi(s, a)$
- Multiple action–value outputs: $\hat{\boldsymbol{q}}_a(s, \boldsymbol{w}) \approx q_\pi(s, a)$

Action-value function approximation

- Approximate action-value function $\hat{q}(s, a, \boldsymbol{w}) \approx q_\pi(s, a)$
- Linear case:

$$\hat{q}(s, a, \boldsymbol{w}) = \boldsymbol{w}^T \boldsymbol{x}(s, a) = \sum_{i=1}^{d} w_i x_i(s, a)$$

$$\nabla \hat{q}(s, a, \boldsymbol{w}) = \boldsymbol{x}(s, a)$$

- Minimize squared error on samples $S_t, A_t \mapsto q_\pi$: $\left[q_\pi - \hat{q}(S_t, A_t, \boldsymbol{w})\right]^2$
- Use SGD to find local minimum:

$$\begin{aligned} \boldsymbol{w}_{t+1} &= \boldsymbol{w}_t - \frac{1}{2}\alpha \nabla [q_\pi(S_t, A_t) - \hat{q}(S_t, A_t, \boldsymbol{w}_t)]^2 \\ &= \boldsymbol{w}_t + \alpha [q_\pi(S_t, A_t) - \hat{q}(S_t, A_t, \boldsymbol{w}_t)] \nabla \hat{q}(S_t, A_t, \boldsymbol{w}) \end{aligned}$$

Control with function approximation

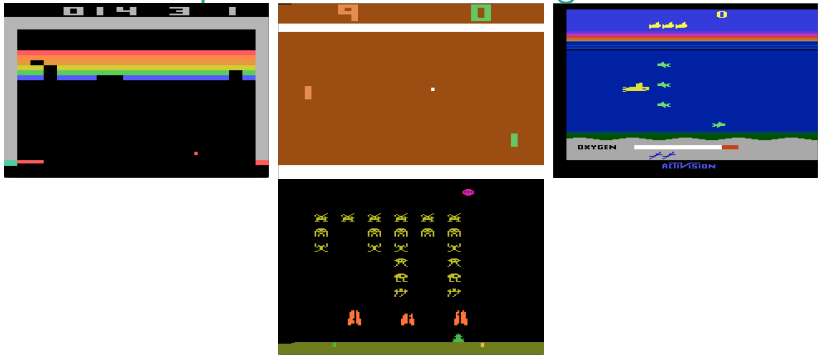
- Again, we must substitute target U_t for true action-value $q_\pi(s, a)$:

$$\boldsymbol{w}_{t+1} = \boldsymbol{w}_t + \alpha[U_t - \hat{q}(S_t, A_t, \boldsymbol{w}_t)]\nabla\hat{q}(S_t, A_t, \boldsymbol{w})$$

- **Monte Carlo:** $U_t = G_t$
- **One-step Sarsa:** $U_t = R_{t+1} + \gamma\hat{q}(S_{t+1}, A_{t+1}, \boldsymbol{w})$

Deep Reinforcement Learning

Recent successes of deep reinforcement learning



Deep (*supervised*) learning

- **Deep representation** is a composition of *many* functions

$$x \xrightarrow[\boldsymbol{w}_1]{} h_1 \xrightarrow[\boldsymbol{w}_2]{} h_2 \xrightarrow[\boldsymbol{w}_3]{} \dots \xrightarrow[\boldsymbol{w}_n]{} h_n \xrightarrow[\boldsymbol{w}_{n+1}]{} y$$

- Linear transformation and non-linear **activation functions** h_k
- Weight sharing
  - **Recurrent neural networks**: across time steps
  - **Convolutional neural networks**: across spatial (or temporal) regions
- Weights $\boldsymbol{w}$ optimized by stochastic gradient descent (SGD)
- Powerful **function approximation** and **representation learning**
  - finds compact low-dimensional representation (*features*)
- State-of-the-art for image, text and audio

Naive deep Q-learning

- Q-learning update rule:

$$Q(s,a) \leftarrow Q(s,a) + \alpha \left(r + \gamma \max_a Q(s',a) - Q(s,a) \right)$$

- Q is represented by a neural network with weights $\boldsymbol{w}$: $\hat{q}(s,a,\boldsymbol{w})$
- Loss is the mean-squared TD-error:

$$\mathcal{L}(\boldsymbol{w}) = \mathbb{E}\left[\left(r + \gamma \max_a \hat{q}(s',a,\boldsymbol{w}) - \hat{q}(s,a,\boldsymbol{w}]) \right)^2 \right]$$

- Minimize sample errors with SGD

Stability

Naive Q-learning with neural networks oscillates or diverges:

1. Data is non i.i.d!
   - trajectories
   - samples are correlated (generated by interaction)
2. Policy changes rapidly with slight changes to Q-values
   - policy may oscillate
3. Reward range is unknown
   - gradients can be large
   - instabilities during back-propagation
4. Maximization bias

Deep Q-networks (DQN)

Deep Q-networks (DQN) address instabilities through:

- **Experience replay**
  - store transitions (S_t, A_t, R_t, S_{t+1})
  - sample random mini-batches
  - removes correlation, restores i.i.d. property
- **Target network**
  - second q network (second set of parameters)
  - fixed parameters in target network
  - periodically update target network parameters
- **Reward clipping/normalization**
  - clip rewards to $r \in [-1, 1]$
  - batch normalization

DQN in Atari

"End-to-end" learning:

- *state:* stack of 4 frames, raw pixels
- *action:* joystick commands (18 discrete actions)
- *reward:* change in score

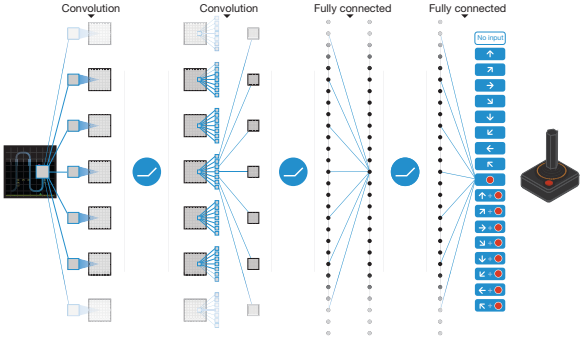


image from *Human-level control through deep reinforcement learning* (Google Deepmind / Nature)

DQN in Atari

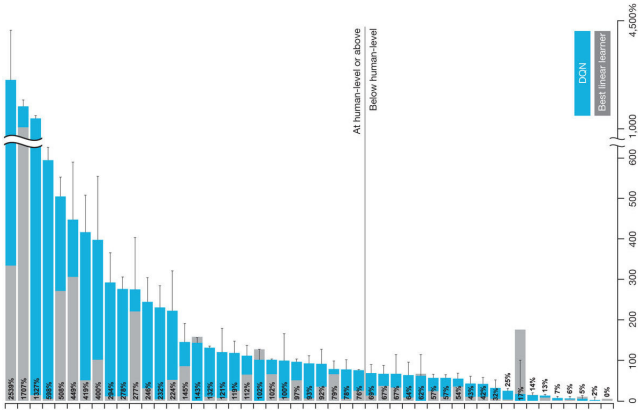


image from *Human-level control through deep reinforcement learning* (Google Deepmind / Nature)

Summary

- When state spaces are **too large** it is not possible to use tables
- Instead we can use **function approximation** to model v_π and q_π
- Many function models exist in the literature, the most popular and general are Neural Networks.
- Stochastic Gradient Descent (SGD) is used to optimize the **Value Function Error**
- Value function approximation is used for prediction
- ϵ-greedy or other covering policies can be used for improvement
- When using a deep-neural network it is important to train in batches using **experience replay** and other techniques to regularize the problem