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Theoretical aspects of Q-learning

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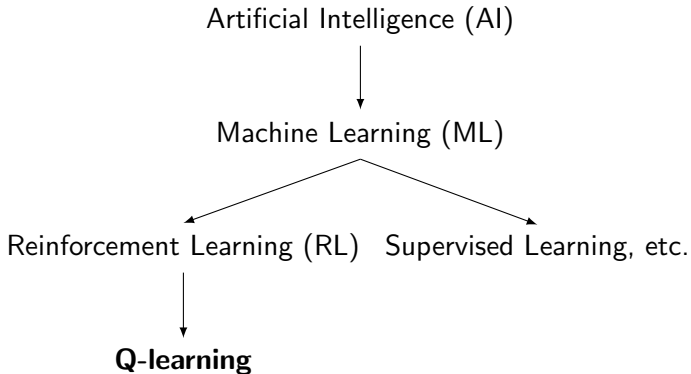
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Machine learning

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Machine Learning is “the study of computer algorithms that improve automatically through *experience*”.

- **Supervised learning**: Tasks are learned from data based on feedback from a *supervisor*. E.g. image classification.
- **Unsupervised learning**: Data is given without evaluatory feedback, general trends about the data are analysed. E.g. principal component analysis, and cluster analysis.
- \rightarrow^1 **Reinforcement learning**: Algorithms which learns through interactions with an *environment*.

¹ “ \rightarrow ”: Our main area of focus in this thesis.



Challenges in RL

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Challenges in Reinforcement Learning include:

- **Exploration-exploitation trade-off.** Training and performing occurs simultaneously so one optimizes the total reward on some time horizon. This is studied in e.g. the multi-armed bandit problem.
- → **Deriving optimal policies.** Training and performing is distinguished and emphasis is put on the expected performance of the final derived policy rather than rewards occurring during training.



The environment

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The **environment** in RL is often formalized as a **Markov decision process** (MDP), which consists of

- \mathcal{S} a measurable space of states.
- \mathcal{A} a measurable space of actions.
- $P : \mathcal{S} \times \mathcal{A} \rightsquigarrow \mathcal{S}$ a transition kernel².
- $R : \mathcal{S} \times \mathcal{A} \rightsquigarrow \mathbb{R}$ a reward kernel discounted by
- a discount factor $\gamma \in [0, 1)$.
- $\mathfrak{A}(s) \subseteq \mathcal{A}$ a set of admissible actions for each $s \in \mathcal{S}$.

²Here \rightsquigarrow denotes a *stochastic mapping* (to be defined soon).



Examples of MDPs

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Examples of Markov decision processes include

- Board games where one plays against a fixed opponent, e.g. *chess* where the set of states \mathcal{S} is the set of all obtainable chess-positions.
- Time-descretized physics simulations with action inputs and reward outputs, including most single player video games and the classic *cartpole* example (balancing a stick).



The probability kernels

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Probability kernel

A **probability kernel** (also called a *stochastic mapping*, *stochastic kernel* or *Markov kernel*) $\kappa : \mathcal{X} \rightsquigarrow \mathcal{Y}$ is a collection of probability measures $\kappa(\cdot \mid x)$, one for each $x \in \mathcal{X}$ such that for any measurable set $B \subseteq \mathcal{Y}$ the function $x \mapsto \kappa(B \mid x)$ is measurable.

The transition probability measure $P(\cdot \mid s, a)$ of the pair $(s, a) \in \mathcal{S} \times \mathcal{A}$ determines what states are likely to follow after *being* in state s and *choosing* action a . Similarly from the reward kernel R one obtains the measure $R(\cdot \mid s, a)$ determining the reward distribution following the timestep (s, a) .



Policies

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Given a Markov decision process one can define a **policy** π by sequence of probability kernels $\pi = (\pi_1, \pi_2, \dots)$ where $\pi_i : \mathcal{H}_i \rightsquigarrow \mathcal{A}$ and $\mathcal{H}_i = \mathcal{S} \times \mathcal{A} \times \dots \times \mathcal{S}$ is the *history space* at the i th timestep.



Stochastic processes

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An MDP $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$ together with a policy $\pi = (\pi_1, \pi_2, \dots)$ and a distribution μ on \mathcal{S} give rise to a stochastic process $(S_1, A_1, S_2, A_2, \dots) \sim \kappa_\pi \mu$ such that for any $i \in \mathbb{N}$ we have $(S_1, A_1, \dots, S_i) \sim P\pi_{i-1} \dots P\pi_1 \mu$ where $P\pi_{i-1} \dots P\pi_1$ denotes the *kernel-composition* of the probability kernels $P, \pi_1, \dots, \pi_{i-1}$. We denote by \mathbb{E}_s^π expectation over $\kappa_\pi \mu$ where $\mu = \delta_s$, that is, $S_1 = s$ a.s.



Policy evaluation

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For a policy π we can define the policy evaluation function:

Policy evaluation

Denote by $r(s, a) = \int x \, dR(x \mid s, a)$ the *expected reward function*.

We define the **policy evaluation function** by

$$V_{\pi}(s) = \mathbb{E}_s^{\pi} \sum_{i=1}^{\infty} \gamma^{i-1} r \circ \rho_i$$

where ρ_i is projection onto $(\mathcal{S}_i, \mathcal{A}_i)$.

This an example of a (state-) *value function*, as it assigns a real number to every state $s \in \mathcal{S}$.



Finite policy evaluation

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Similar to the infinite horizon policy evaluation we can also consider a finite horizon version:

Definition: Finite policy evaluation

We define the function $V_{n,\pi} : \mathcal{S} \rightarrow \mathbb{R}$ by

$$V_{n,\pi}(s) = \mathbb{E}_s^\pi \sum_{i=1}^n \gamma^{i-1} r \circ \rho_i$$

called the k th **finite policy evaluation**^a.

^aWhen $n = 0$ we say $V_{0,\pi} = V_0 := 0$ for any π .



Optimal value function

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Definition: Optimal value functions

$$V_n^*(s) := \sup_{\pi \in R\Pi} V_{n,\pi}(s) = \sup_{\pi \in R\Pi} \mathbb{E}_s^\pi \sum_{i=1}^n r_i$$

$$V^*(s) := \sup_{\pi \in R\Pi} V_\pi(s) = \sup_{\pi \in R\Pi} \mathbb{E}_s^\pi \sum_{i=1}^{\infty} r_i$$

This is called the **optimal value function** (and the n th optimal value function). A policy $\pi^* \in R\Pi$ for which $V_{\pi^*} = V^*$ is called an **optimal policy**. If $V_{n,\pi^*} = V_n^*$ then π^* is called n -optimal.

Provided such an optimal policy π^* exists, obtaining such a policy is the ultimate goal of Reinforcement Learning.



Operators on value functions

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Before defining value iteration we introduce some operators

The T -operators

For a stationary policy $\tau \in \mathcal{S}\Pi$ and a value function $V : \mathcal{S} \rightarrow \mathbb{R} \in \mathcal{L}_\infty(\mathcal{S})$ we define the operators

The policy evaluation operator:

$$T_\tau V := s \mapsto \int r(s, a) + \gamma V(s') \, d(P\tau)(a, s' \mid s)$$

The Bellman optimality operator:

$$TV := s \mapsto \sup_{a \in \mathcal{A}(s)} \left(r(s, a) + \gamma \int V(s') \, dP(s' \mid s, a) \right)$$



Value iteration

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Value iteration is the iterative application of the T -operator. The following theorem show why value iteration is a central idea Reinforcement Learning³.

Theorem (Existence optimal policies & convergence of value iteration)

Given a greedy MDP we have that

$$V_k^* = T^k V_0 = T_{\tau_{k-1}^*} \dots T_{\tau_0^*} V_0 = V_{k, (\tau_{k-1}^*, \dots, \tau_0^*)}$$

The policy $(\tau_{k-1}^*, \dots, \tau_0^*)$ is a deterministic k -optimal policy where $\tau_k^* = \tau_{T^k V_0}$ is any deterministic greedy policy for $T^k V_0$ for any $k \in \mathbb{N}$. Furthermore $V^* = \lim_{k \rightarrow \infty} T^k V_0^*$, the greedy policy $\tau^* = \tau_{V^*}$ exists and an optimal policy.

³Actually value iteration is inherited from dynamic programming.



Convergence rates

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We can also show that the optimal value function V^* is a fixed point of the Bellman optimality operator T .

$$TV^* = V^*$$

This is often called *Bellman's optimality equation*.

Recalling that T is γ -contractive, by Banach's fixed point theorem we get exponential convergence rates for value iteration:

$$\|T^k V - V^*\| \leq \gamma^k \|V - V^*\|_\infty = \mathcal{O}(\gamma^k)$$



Example: Gridworld

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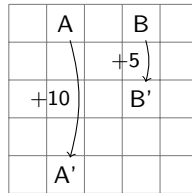
The *gridworld*

MDP consist of 25 states $\mathcal{S} = [5]^2$ and 4 actions $\mathcal{A} = \{U, D, L, R\}$

for *up*, *down*, *left* and *right*

and moves the agent 1 square up, down, left or right. A reward of 0 is given by default, except when

- *hitting the boundary* a reward of -1 is given
- when in $A = (2, 1)$ any action moves to $A' = (2, 5)$ and is rewarded 10.
- when in $B = (4, 1)$ any action moves to $B' = (4, 3)$ and is rewarded 5.



Finally $\gamma = 0.9$ is the standard value of the discount factor in this example.



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-0.50	10.00	-0.25	5.00	-0.50
-0.25	0.00	0.00	0.00	-0.25
-0.25	0.00	0.00	0.00	-0.25
-0.25	0.00	0.00	0.00	-0.25
-0.50	-0.25	-0.25	-0.25	-0.50

V_1, τ_r

3.31	8.79	4.43	5.32	1.49
1.52	2.99	2.25	1.91	0.55
0.05	0.74	0.67	0.36	-0.40
-0.97	-0.44	-0.35	-0.59	-1.18
-1.86	-1.35	-1.23	-1.42	-1.98

V_{400}, τ_r

Figure: Policy evaluations of the gridworld environment. Note that $V_{\max} \cdot \gamma^{400} = 100 \cdot (0.9)^{400} \approx 4.97 \cdot 10^{-17}$ so $V_{\tau_r, 400}$ are very close to the true infinite horizon value functions V_{τ_r} (providing numerical errors are insignificant).



Example: Gridworld

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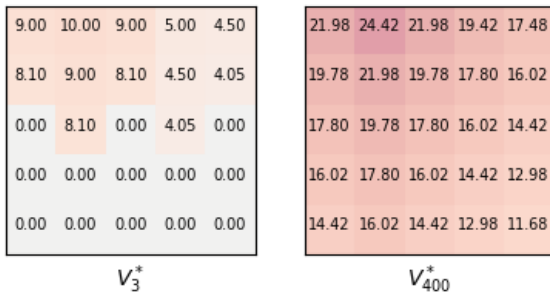


Figure: Optimal value functions of the gridworld environment. By the same upper bound as before we have $\|V^* - V_{400}^*\|_\infty < 4.97 \cdot 10^{-17}$.



Example: Gridworld

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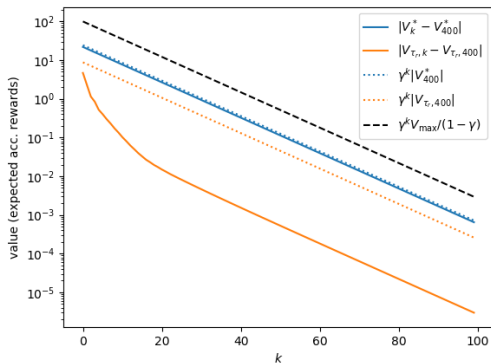
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Convergence of gridworld value functions compared with the theoretical bounds. The black dashed line is the general theoretical bound for both T and T_τ by Banachs fixed point theorem and the maximum value $V_{\max} = R_{\max}/(1 - \gamma)$. The dotted blue and orange uses $|V_k^*|$ and $|V_{\tau,k}|$ respectively, which might not be available. ($\gamma = 0.9$).



Q-functions

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A **Q-function** is simply any function assigning a real number to every state-action pair. They are also called (state-) *action value functions*.

A **Q-learning** algorithm is any algorithm which uses Q-functions to derive a policy for an environment⁴.

⁴Some authors refer to Q-learning as a specific variation of temporal difference learning, but this fails to capture many algorithms which are also referred to as *Q-learning algorithms*.



Motivation for Q-functions

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A clear advantage of working with Q-function $Q : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$ rather than a value function $V : \mathcal{S} \rightarrow \mathbb{R}$, is that finding the optimal action $a^* \in \mathcal{A}(s)$ at state s requires only a maximization over the Q-function itself:

$a^* = \operatorname{argmax}_{a \in \mathcal{A}(s)} Q(s, a)$. This should be compared to finding an optimal action according to a value function V :

$$a^* = \operatorname{argmax}_{a \in \mathcal{A}(s)} r(s, a) + \gamma \mathbb{E}_{P(\cdot|s,a)} V.$$



Q-function operators

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Moreover we define T -operators similar to ones for value functions

Operators for Q-functions

For any stationary policy $\tau \in \mathcal{S}\Pi$ and integrable Q-function

$Q : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R} \in \mathcal{L}_\infty(\mathcal{S} \times \mathcal{A})$ we define

Next-step operator:

$$P_\tau Q(s, a) = \int Q(s', a') \, d\tau P(s', a' \mid s, a)$$

Policy evaluation operator:

$$T_\tau Q(s, a) = r(s, a) + \gamma \int Q(s', a') \, d\tau P(s', a' \mid s, a)$$

Bellman optimality operator:

$$TQ(s, a) = r(s, a) + \gamma \int \max_{a' \in \mathcal{A}} Q(s', a') \, dP(s' \mid s, a)$$

where $T_a = T_{\delta_a}$.



Relation between value- and Q-functions

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Theorem (Relations between Q- and value functions)

Let $\pi = (\tau_1, \tau_2, \dots) \in M\Pi$ be a Markov policy and $\tau \in S\Pi$ stationary.
Then

- Policy evaluations are related by $\mathbb{E}_{\tau}(\cdot|s)Q_{k,\pi} = V_{k+1,(\tau,\pi)}(s)$.
- T_{τ} -operators are related by $T_{\tau}Q_{k,\pi}(s, a) = r + \gamma\mathbb{E}_{P(\cdot|s,a)}T_{\tau}V_{k,\pi}$.
- τ is greedy for $Q_{k,\pi}$ if and only if τ is greedy for $V_{k,\pi}$ and
 τ is greedy for Q_{π} if and only if τ is greedy for V_{π} .
- Optimal policies are related by $\max_{a \in \mathcal{A}(s)} Q^*(s, a) = V^*(s)$ and
 $Q_k^*(s, a) = r(s, a) + \gamma\mathbb{E}_{P(\cdot|s,a)}V_k^*, \quad Q^*(s, a) = r(s, a) + \gamma\mathbb{E}_{P(\cdot|s,a)}V^*$



Q-iteration

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Q-iteration is the analogue of value-iteration for Q-function. It can be stated in the form of an algorithm as follows:

Algorithm (Q-iteration)

Data: MDP $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$, number of iterations K

Initialize expected reward function $r \leftarrow \int x \, dR(x \mid \cdot)$ and $\tilde{Q}_0 \leftarrow r$.

for $k = 0, 1, \dots, K - 1$ **do**

$\tilde{Q}_{k+1} \leftarrow T\tilde{Q}_k$

end

Output: \tilde{Q}_K

In the context of a greedy MDP we immediately have that the output of the Q-iteration algorithm $\tilde{Q}_K = Q_K^*$ is K -optimal.



Value iteration with Q-functions

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Conclusion

Similar to value-iteration we can use Banach fixed point theorem with the contractive properties of the T -operator for Q-functions to obtain exponential convergence of Q-iteration:

Proposition (Convergence of Q-iteration)

Suppose the Q-iteration algorithm is run with a greedy MDP. Then the output $\tilde{Q}_K = Q_K^*$ satisfy

$$\|Q^* - Q_K^*\|_\infty \leq \gamma^K V_{\max}$$



What have we done so far?

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For greedy MDPs we have proved

- Existence of optimal policies.
- Exponential convergence of Q-iteration to the optimal policy.



Are we not done?

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We have exponential convergence for the broad class of problems expressible as a greedy MDP. This class includes highly difficult environments such as control problems in time-descretized simulation environments such as computer games, including the game of *chess*. Are we then done?



Problems of Q-iteration

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Model-dependency: It is assumed that we know how to integrate over P and R .

- The distributions of P and R might be impractical to work with in a computer.
- It is common in RL to assume that P and R are unknown, thus including a variety of environments, which we have not yet considered.

Representation infeasibility: It is assumed that we know how to represent Q functions in a feasible way in a computer.

- Representing the functions arising from use of the T -operator may be difficult as these functions are defined by successive integration over potentially complex transition kernels.
- Even in the finite case where Q can be represented as a table, this table may be excessively large.



Example: Chess

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The state space of chess is very large (roughly $|\mathcal{S}_{\text{chess}}| \geq 10^{43}$). This means that if we were to use Q-iteration naively (with finite implementation as in the gridworld example) then we would have to store a vector of roughly $N \cdot 10^{43}$ real numbers for each Q-function we define, where N is the average number of admissible actions at each state $\mathcal{A}(s)$, $s \in \mathcal{S}$ which has been estimated to around $N \approx 35$ for chess. This requires roughly $1.4 \cdot 10^{45}$ bytes, if each number is stored as a single precision floating point number (4 bytes). For comparison the entire digital data capacity in the world is estimated less than 10^{23} bytes as of 2020. Needless to say this is beyond any practical relevance.



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To deal with the problem of representation infeasibility we will investigate what happens when using approximations of TQ in the Q-iteration algorithm. The hope is then that we can choose an class of approximation-functions

$$\mathcal{F} \subseteq \mathcal{Q} = \{Q : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}\}$$

that is both *representable* (in a computer) and *dense* (to some degree) in $T\mathcal{F} = \{TQ \mid Q \in \mathcal{Q}\}$.



Approximation and algorithmic errors

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Suppose we have a sequence of Q-functions satisfying

$$\left\| T\tilde{Q}_{k-1} - \tilde{Q}_k \right\| \leq \varepsilon_k, \forall k \in \mathbb{N}$$

Observe that

$$\begin{aligned} \left\| T^k \tilde{Q}_0 - \tilde{Q}_k \right\| &\leq \left\| T^k \tilde{Q}_0 - T\tilde{Q}_{k-1} \right\| + \left\| T\tilde{Q}_{k-1} - \tilde{Q}_k \right\| \\ &\leq \gamma \left\| T^{k-1} \tilde{Q}_0 - \tilde{Q}_{k-1} \right\| + \left\| T\tilde{Q}_{k-1} - \tilde{Q}_k \right\| \end{aligned}$$

Using this iteratively we get

$$\left\| T^k \tilde{Q}_0 - \tilde{Q}_k \right\| \leq \sum_{i=1}^k \gamma^{k-i} \varepsilon_i$$

Using this we can bound ...



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$$\begin{aligned}\|Q^* - \tilde{Q}_k\| &\leq \|Q^* - T^k \tilde{Q}_0\| + \|T^k \tilde{Q}_0 - \tilde{Q}_k\| \\ &\leq \gamma^k \|Q^* - \tilde{Q}_0\| + \sum_{i=1}^k \gamma^{k-i} \varepsilon_i\end{aligned}$$

- The first term is called the **algorithmic error** and decreases exponentially with k , so we will be content with this.
- The second term $\sum_{i=1}^k \gamma^{k-i} \varepsilon_i$ is where the trouble from our approximative strategy arises and is therefore called the **approximation error**. We denote it $\varepsilon_{\text{approx}}(k)$. It is this the approximation error which we will now struggle to bound.



Theoretical approximation errors

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We here give a few examples of how the approximation error behave in relation to the step-wise errors ε_i .

- If $\varepsilon_i(k) = \varepsilon$ for some $\varepsilon > 0$ we easily get the bound

$$\varepsilon_{\text{approx}}(k) = \varepsilon \frac{1 - \gamma^k}{1 - \gamma} \leq \frac{\varepsilon}{1 - \gamma}$$

- If $\varepsilon_i \leq c\gamma^i$ we get

$$\varepsilon_{\text{approx}}(k) \leq ck\gamma^k \rightarrow 0$$

as $k \rightarrow \infty$.

- Generally we have $\sum_{i=1}^k \gamma^{k-i} \varepsilon_i \rightarrow 0$ whenever $\varepsilon_k \rightarrow 0$ as $k \rightarrow \infty$.



Artificial Neural Networks

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We will now consider the approach of (model-dependent) Q-iteration using artificial neural networks (ANNs) as function approximators.

Definition: Artificial neural network

An **artificial neural network** (ANN) with $L \in \mathbb{N}_0$ hidden layers, structure $(d_i)_{i=0}^{L+1} \subseteq \mathbb{N}$, activation functions $(\sigma_i)_{i=1}^L$, weights $(W_i)_{i=1}^{L+1} \in M^{d_i \times d_{i-1}}$ and biases $(v_i)_{i=1}^{L+1} \in \mathbb{R}^{d_i}$ is the function $f : \mathbb{R}^{d_0} \rightarrow \mathbb{R}^{d_{L+1}}$ defined by

$$f = w_{L+1} \circ \sigma_L \circ w_L \circ \sigma_{L-1} \circ \cdots \circ \sigma_1 \circ w_1$$

where w_i is the affine function $x \mapsto W_i x + v_i$, and $\sigma_i : \mathbb{R}^{d_i} \rightarrow \mathbb{R}^{d_i}$ is coordinate-wise application of components $\sigma_{ij} : \mathbb{R} \rightarrow \mathbb{R}$. We denote the class of these networks (or functions)

$$\mathcal{DN} \left((\sigma_i)_{i=1}^L, (d_i)_{i=0}^{L+1} \right)$$

An ANN is called *deep* if there are two or more hidden layers.



ANNs as graphs

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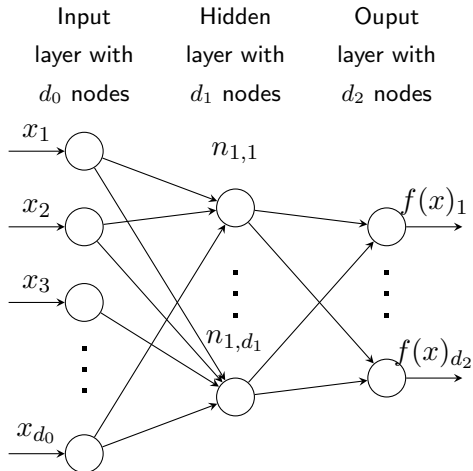


Figure: An ANN with one hidden layer ($L = 1$). Notice that there is no edge from $n_{0,3}$ to $n_{1,1}$ which means that $W_1(1,3) = 0$.



Universal approximation theorem for ANNs

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Theorem (Universal approximation theorem for ANNs)

Let $\sigma : \mathbb{R} \rightarrow \mathbb{R}$ be non-constant, bounded and continuous activation function. Let $\varepsilon > 0$ and $f \in C([0, 1]^w)$. Then there exists an $N \in \mathbb{N}$ and a network $F \in \mathcal{DN}(\sigma, (w, N, 1))$ with one hidden layer, unbiased final layer (that is $v_2 = 0$) and activation function σ such that

$$\|F - f\|_{\infty} < \varepsilon$$

In other words $\bigcup_{N \in \mathbb{N}} \mathcal{DN}(\sigma, (w, N, 1))$ is dense in $C([0, 1]^w)$.



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Rectified linear unit (ReLU) activation function:

$$\sigma_r(x) = \max(0, x)$$

Class of *ReLU networks*:

$$\mathcal{RN} \left((d_i)_{i=0}^{L+1} \right) := \mathcal{DN} \left(\sigma_r, (d_i)_{i=0}^{L+1} \right)$$

Setting: Greedy MDP with state-space $\mathcal{S} = [0, 1]^w \subseteq \mathbb{R}^w$ inside the unit (hyper-) cube, finite action space $|\mathcal{A}| < \infty$ and expected reward function r being (fully) *continuous*.



Q-iteration with ANN-approximation - bound

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Theorem

Let $\varepsilon > 0$. Assume that one of the following two conditions hold:

1. P is deterministic with $P(\cdot \mid s, a) = \delta_{p(s,a)}$. For some continuous $p : \mathcal{S} \times \mathcal{A} \rightarrow \mathcal{S}$.
2. $P(\cdot \mid s, a)$ is absolutely continuous with respect to the same measure ν on \mathcal{S} for all $(s, a) \in \mathcal{S} \times \mathcal{A}$ with density $p(\cdot \mid s, a)$ which is continuous in s .

Then for every $k \in \mathbb{N}$ there exists a $N \in \mathbb{N}$ and a sequence of Q-networks $(\tilde{Q}_i)_{i=1}^k \subseteq \mathcal{RN}(w|\mathcal{A}|, N, 1)$ such that

$$\varepsilon_{\text{approx}}(i) = \left\| T\tilde{Q}_{i-1} - \tilde{Q}_i \right\|_{\infty} < \varepsilon$$

for all $i \in [k]$. In particular

$$\left| Q^* - \tilde{Q}_k \right| < \gamma^k V_{\max} + \varepsilon/(1 - \gamma)$$



Q-iteration with ANN: conclusion

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What we have accomplished: Arbitrarily precise approximation of Q^* using a concrete class of approximators, namely ANNs.

What is still missing:

- How large must the network width N be? This requires going through a constructive proof of the universal approximation theorem, which is available in literature.
- How to obtain the each approximator \tilde{Q}_i ? Optimization using ANNs are extensively studied, so this might be answered in literature.



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We now turn to a new approximation technique:

Definition: Bernstein polynomial

The (multivariate) Bernstein polynomial $B_{f,n}$ of degree $n = (n_1, \dots, n_w) \in \mathbb{N}^w$ approximating the function $f : [0, 1]^w \rightarrow \mathbb{R}$ is defined by

$$B_{f,n}(x_1, \dots, x_w) = \sum_{j=1}^w \sum_{k_j=0}^{n_j} f\left(\frac{k_1}{n_1}, \dots, \frac{k_w}{n_w}\right) \prod_{\ell=1}^w \binom{n_\ell}{k_\ell} x_\ell^{k_\ell} (1 - x_\ell)^{n_\ell - k_\ell}$$



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Theorem: Approximation properties of Bernstein polynomials

Let $f : [0, 1]^w \rightarrow \mathbb{R}$ be Lipschitz w.r.t. the standard euclidean 2-norm induced metrics on $[0, 1]^w$ and \mathbb{R} with constant L . Let $n = (n_1, \dots, n_w) \in \mathbb{N}^w$. The Bernstein polynomial

$B_{f,n} : [0, 1]^w \rightarrow \mathbb{R}$ satisfies

1. $\|f - B_{f,n}\|_\infty \leq \frac{L}{2} \sqrt{\sum_{j=1}^w \frac{1}{n_j}}$
2. $\|B_{f,n}\|_\infty \leq \|f\|_\infty$



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Proposition

Suppose we are given a greedy MDP with $\mathcal{S} = [0, 1]^w$ and finite action space. Assume that there exists a probability measure $\mu \in \mathcal{P}(\mathcal{S})$ such that $P(\cdot \mid s, a)$ has density $p(\cdot \mid s, a) : \mathcal{S} \rightarrow \mathbb{R}$ w.r.t μ for all $(s, a) \in \mathcal{S} \times \mathcal{A}$. Furthermore assume that $r(\cdot, a)$ and $p(s \mid \cdot, a)$ are $\|\cdot\|_2$ -Lipschitz with constants L_r, L_p for all $(s, a) \in \mathcal{S} \times \mathcal{A}$.

Using Bernstein polynomials of degree $n = (m, \dots, m) \in \mathbb{N}^w$ for $m \in \mathbb{N}$ we have the following bound

$$\left\| Q^* - \tilde{Q}_k \right\|_{\infty} \leq \gamma^k V_{\max} + \frac{L_r + \gamma V_{\max} L_p}{2(1 - \gamma)} \sqrt{w} \frac{1}{\sqrt{m}}$$

In particular $\left\| Q^* - \tilde{Q}_k \right\|_{\infty} = \mathcal{O}(\gamma^k + \frac{1}{\sqrt{m}})$ when using k iterations.



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What we have achieved: $\mathcal{O}(\gamma^k + 1/\sqrt{m})$ convergence bound for Q-iteration with (m, \dots, m) -degree Bernstein polynomial approximation. This solves two problems with approximation with ANNs of

1. the function class not being concrete
2. not knowing how to obtain each approximator \tilde{Q}_i

We mention two weak points

1. The restriction on P : For example we cannot use the bound on deterministic decision processes, since if P is deterministic then there are no measure $\mu \in \mathcal{P}(\mathcal{S})$ which allows for a density $p(\cdot \mid s, a)$ (i.e. $p \cdot \mu = P(\cdot \mid s, a)$), unless $P(\cdot \mid s, a) = \delta_{s'}$ for all $(s, a) \in \mathcal{S} \times \mathcal{A}$, which would lead to a quite boring environment. Generally the processes with fast convergence bounds must be quite stochastic.
2. We lack understanding of the computational complexity involved.



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We deal with the model-free algorithm of this thesis in two parts:

1. The first part (section 3.1 and 3.2) is a survey on various old and recent convergence bounds. Most bounds are either confined to finite processes (section 3.1) or not establishing concrete bounds (section 3.2).
2. The second section (section 3.3) is a detailed presentation of a preprint [Fan et al. (2020+)] proving convergence of a Q-learning algorithm in a continuous state-space setting.



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In model-free algorithms are based on *sampling* from the environment dynamics instead of using these distributions directly (e.g. by taking expectations).

This means that we cannot use any of the approaches so far considered without modification because taking expectations over the kernels P and R is no longer possible (directly).



Motivating model-free algorithms

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Why put the model-free restriction upon our algorithms?

- Big actors in both research and industry (such as *Google DeepMind*) favor model-free approaches. Thus much research goes in this direction.
- Some environments may be hard to model, but easy to sample from, such as the stock-market.
- *Works out of the box*: No need for adaptation to each model as only access to samples are required.
- Philosophical interest: Are humans model-free algorithms?
- Experience that Monte Carlo approaches can lead to faster computation.



The finite setting

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Finite action-uniform MDP

We consider a (discounted) MDP $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$ where $|\mathcal{S}| = s \in \mathbb{N}$ and $|\mathcal{A}| = a \in \mathbb{N}$ are finite. Also we assume unrestricted actions, i.e. that the set of admissible actions $\mathcal{A}(s) = \mathcal{A}$ is the same for all $s \in \mathcal{S}$

This setting is a special case of a greedy MDP, and thus we get existence of optimal value functions and convergence of $Q_k^* \rightarrow Q^*$.



TD-learning

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A popular way of dealing with the problems of naive model-free Q-iteration, is called *temporal difference learning* (TD-learning) and is based on the following *update-step*:

$$\tilde{Q}_{k+1}(s, a) \leftarrow (1 - \alpha_k) \tilde{Q}_k(s, a) + \alpha_k (r' + \gamma \cdot \max_{a' \in \mathcal{A}} \tilde{Q}_k(s', a'))$$

Where

- r' and s' are the reward and next-state drawn from the reward and transition kernels,
- $\alpha_k \in [0, 1]$ is called the **learning rate**,
- $r' + \gamma \max_{a' \in \mathcal{A}} \tilde{Q}_k(s', a')$ is called the **T-value**, due to its similarity to $T\tilde{Q}_k(s, a) = r(s, a) + \gamma \int \max_{a' \in \mathcal{A}} \tilde{Q}_k(s', a') dP(s' | s, a)$,
- the **temporal difference** term
 $\alpha_k (r' + \gamma \cdot \max_{a \in \mathcal{A}} \tilde{Q}_k(s', a') - \tilde{Q}_k(s, a))$.



Finite asynchronous Q-learning

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Algorithm: Finite asynchronous Q-learning

Input: Finite MDP $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$, number of iterations K ,
state-action pairs $(s_1, a_1, \dots, s_K, a_K)$, learning rates
 $(\alpha_1, \dots, \alpha_K)$, initial $\tilde{Q}_0 : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R}$

for $k = 1, 2, \dots, K$ **do**

 Sample $r' \sim R(\cdot \mid s_k, a_k)$, $s' \sim P(\cdot \mid s_k, a_k)$.

 Update action-value function: For all $(s, a) \in \mathcal{S} \times \mathcal{A}$ let

$$\tilde{Q}_k(s, a) \leftarrow \begin{cases} \tilde{Q}_{k-1}(s, a) & (s, a) \neq (s_k, a_k) \\ (1 - \alpha_k)\tilde{Q}_{k-1} + \alpha_k(r' + \gamma \max_{a' \in \mathcal{A}} \tilde{Q}_{k-1}(s', a')) & (s, a) = (s_k, a_k) \end{cases}$$

end

Define $\tilde{\pi}_K$ as the greedy policy w.r.t. \tilde{Q}_K

Output: An estimator \tilde{Q}_K of Q^* and policy $\tilde{\pi}_K$



Convergence result

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Theorem (Watkins, Dayan 1992): Convergence of asynchronous QL

Let $s_1, a_1, s_2, a_2, \dots \in \mathcal{S} \times \mathcal{A} \times \mathcal{S} \times \mathcal{A} \times \dots$ be random variables and $\alpha_1, \alpha_2, \dots \in [0, 1]$ be a sequence of learning rates. The output \tilde{Q}_K of the finite asynchronous Q-learning algorithm converges to Q^* provided that for all $(s, a) \in \mathcal{S} \times \mathcal{A}$ it holds that

- $\mathbb{P} \left(\sum_{i=1}^{\infty} \alpha_i [(s_i, a_i) = (s, a)] = \infty \right) = 1$ and
 $\mathbb{P} \left(\sum_{i=1}^{\infty} \alpha_i^2 [(s_i, a_i) = (s, a)] < \infty \right) = 1.$
- $\mathbb{V}(R(\cdot \mid s, a)) < \infty$ for all $(s, a) \in \mathcal{S} \times \mathcal{A}.$

Here $[(s_i, a_i) = (s, a)]$ is the Bernoulli random variable with $\mathbb{P}([(s_i, a_i) = (s, a)] = 1) = \mathbb{P}(s_i = s \text{ and } a_i = a).$



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Theorem (Szepesvári 1997)

Using the finite asynchronous algorithm let $K \in \mathbb{N}$ and $(s_1, a_1), (s_2, a_2) \dots, (s_K, a_K)$ be sampled i.i.d. from a distribution $p \in \mathcal{P}(\mathcal{S} \times \mathcal{A})$ with $\text{supp}(p) = \mathcal{S} \times \mathcal{A}$, i.e. all state-action pairs have non-zero probability of occurring. Set the learning rates such that $\alpha_k = |\{i \in [k] \mid (s_i, a_i) = (s_k, a_k)\}|^{-1}$, i.e. they are the reciprocal of the frequency of (s_k, a_k) at step k . Let $\beta = \max_{x \in \mathcal{S} \times \mathcal{A}} p(x) / \min_{x \in \mathcal{S} \times \mathcal{A}} p(x)$. Then for some $B > 0$ the following holds asymptotically almost surely

$$\left| \tilde{Q}_K - Q^* \right| \leq B \frac{1}{K^{\beta(1-\gamma)}} \quad (1)$$

and

$$\left| \tilde{Q}_K - Q^* \right| \leq B \sqrt{\frac{\log \log K}{K}} \quad (2)$$

For the output \tilde{Q}_K of the finite asynchronous Q-learning algorithm with K -steps.

Note that eq. (1) is tightest when $\gamma > 1 - \beta/2$ otherwise eq. (2) is tighter.



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Define $\mathcal{H}^* = \bigcup_{i \in \mathbb{N}} \mathcal{H}_i$ as the space of all *finite histories*. We will write (history-) tuples $h_k = (s_1, a_1, s_2, \dots, a_{k-1}, s_k) \in \mathcal{H}_k$ as strings $h_k = s_1 a_1 s_2 \dots a_{k-1} s_k$ for convenience.

- Transition dynamics are history dependent

$$P : \mathcal{H}^* \times \mathcal{A} \rightsquigarrow \mathcal{S}.$$

- Rewards are history dependent, deterministic

$r : \mathcal{H}^* \times \mathcal{A} \rightarrow \mathbb{R}$, and discounted by $\gamma \in [0, 1)$, that is

$r(h_n, a) \in [-\gamma^{n-2} R_{\max}, \gamma^{n-2} R_{\max}]$ for any $h_n \in \mathcal{H}_n$ and $a \in \mathcal{A}$.

- Actions are unrestricted, so that $\mathfrak{A}(s) = \mathcal{A}$ for all $s \in \mathcal{S}$.



Remark on existence of optimal value functions

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The finite history dependent setting can be analysed with theorems developed by [Schäl, 1974], which considers history dependent processes generalized to arbitrary standard Borel \mathcal{S} and \mathcal{A} . This implies by the existence of an optimal $\pi^* \in R\Pi$ and that $V_n^* \rightarrow V^*$ ⁵.

⁵These remarks was not discussed in the original article by Majeed and Hutter.



History dependent TD-learning

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Motivated by fact that the partial q -functions attains the (non-partial) optimum, we will use the asynchronous Q-learning algorithm with update step

$$q_{t+1}(x, a) = q_t(x, a) + \alpha_t(x, a) \left(r' + \gamma \max_{a' \in \mathcal{A}} q_t(x', a') - q_t(x, a) \right),$$



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Theorem

Assume

1. State-uniformity.
2. Any state is reached eventually under any policy.
3. Learning rate satisfies

$$\sum_{t=0}^{\infty} \alpha_t(x, a) = \infty, \quad \sum_{t=0}^{\infty} \alpha_t(x, a)^2 < \infty$$

Then starting with any $q_0 : \mathcal{X} \times \mathcal{A} \rightarrow \mathbb{R}$ the asynchronous Q-learning algorithm yields a sequence $(q_t)_{t \in \mathbb{N}}$ such that

$$q_t \rightarrow Q^*$$



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It seems relevant to ask how restrictive the state-uniformity assumption is. [Majeed, Hutter (2018)] answers this by an array of examples showing the following relations of the classes of decision processes:

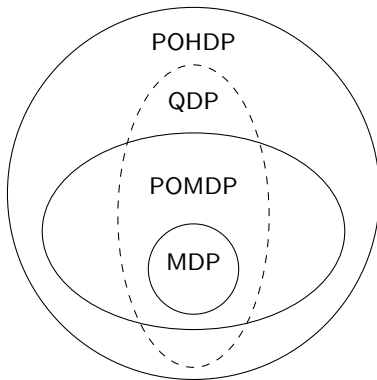


Figure: Classes of finite decision processes considered in [Majeed, Hutter (2018)].



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Q-functions approximation by a linear span from a set of basis functions.

Setting: Continuous state, finite action, discounted MDP

- An MDP $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$
- $\mathcal{S} \subseteq \mathbb{R}^w$ is a compact subset of a euclidean space.
- \mathcal{A} is finite and unrestricted, that is $\mathfrak{A}(s) = \mathcal{A}$ for all $s \in \mathcal{S}$.
- r_i is upper semicontinuous.



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$\{\xi_1, \dots, \xi_M\}$ - a finite set of linearly independent, measurable and bounded Q-functions.

$$\mathcal{F} = \text{span}\{\xi_i \mid i \in [M]\}$$

$$\theta_{k+1} = \theta_k + \alpha_k \xi(s_k, a_k) \left(r_k + \gamma \max_{b \in \mathcal{A}} Q_{\theta_k}(s_{k+1}, b) - Q_{\theta_k}(s_k, a_k) \right)$$

Theorem (Melo, Ribeiro 2007)

Convergence of $\theta_k \rightarrow \theta^*$ where $\theta^* = \rho_{\mathcal{F}} Q^*$.



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Question: How far is Q_{θ^*} from Q^* ?



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Fitted Q-Iteration Algorithm

Input: MDP $(\mathcal{S}, \mathcal{A}, P, R, \gamma)$, function class \mathcal{F} , sampling distribution $\nu \in \mathcal{P}(\mathcal{S} \times \mathcal{A})$, number of iterations K , batch-size n , initial estimator \tilde{Q}_0

for $k = 0, 1, 2, \dots, K - 1$ **do**

 Sample n times independently from the distribution ν to get the batch $(S_i, A_i)_{i \in [n]}$.

 For each $i \in [n]$ sample a reward $R_i \sim R(S_i, A_i)$ and a next-state $S'_i \sim P(S_i, A_i)$.

 From this define the T-values $Y_i \leftarrow R_i + \gamma \cdot \max_{a \in \mathcal{A}} \tilde{Q}_k(S'_i, a)$

 Update action-value function by solving the least squares optimization problem $\tilde{Q}_{k+1} \leftarrow \operatorname{argmin}_{f \in \mathcal{F}} \sum_{i=1}^n (Y_i - f(S_i, A_i))^2$ over the function class \mathcal{F} .

end

Define $\tilde{\tau}_K$ as the greedy policy w.r.t. \tilde{Q}_K

Output: An estimator \tilde{Q}_K of the optimal value function Q^* and an estimator of the optimal policy $\tilde{\tau}_K$



Function class

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Definition: Sparse ReLU networks

For $s, V \in \mathbb{R}$ the ReLU network f is called (s, V) -sparse if

- $\max_{\ell \in [L+1]} \|\widetilde{W}_\ell\|_\infty \leq 1$
- $\sum_{\ell=1}^{L+1} \|\widetilde{W}_\ell\|_0 \leq s$
- $\max_{j \in [d_{L+1}]} \|f_j\|_\infty \leq V$

The set of them we denote $\mathcal{SRN}(s, V, (d_i)_{i=0}^{L+1}, L)$ and by $\mathcal{SRN}(s, V)$ we mean the set of (s, V) -sparse ReLU networks with any (finite) structure. We may leave out L when clear from the structure writing $\mathcal{SRN}(s, V, (d_i)_{i=0}^{L+1})$.



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A **deep fitted Q-iteration** (DQI) algorithm, is the fitted Q-iteration algorithm when applied with a function class of sparse ReLU networks \mathcal{SRN} .



Definition: Hölder smooth functions

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Hölder smoothness

Define the **Hölder smooth norm** of f by

$$\|f\|_{C_w} := \sum_{|\alpha| < \beta} \|\partial^\alpha f\|_\infty + \sum_{\|\alpha\|_1 = \lfloor \beta \rfloor} \sup_{\substack{x \neq y \\ x, y \in \mathcal{S}^\circ}} \frac{|\partial^\alpha (f(x) - f(y))|}{\|x - y\|_\infty^{\beta - \lfloor \beta \rfloor}}$$

If $\|f\|_{C_w} < \infty$ then f is **Hölder smooth**. The space of Hölder smooth functions on $\mathcal{D} \subseteq \mathbb{R}^w$:

$$C_w(\mathcal{D}, \beta, H) := \left\{ f : \mathcal{D} \rightarrow \mathbb{R} \mid \|f\|_{C_w} \leq H \right\}$$

Hölder smooth compositions

For any $j \in [q]$ let $t_j, p_j \in \mathbb{N}$, $t_j \leq p_j$ and $H_j, \beta_j > 0$. We say that $f : [a_1, b_1]^{p_1} \rightarrow \mathbb{R}$ is a **composition of Hölder smooth functions** when

$$f = g_q \circ \dots \circ g_1$$

for some functions $g_j : [a_j, b_j]^{p_j} \rightarrow [a_{j+1}, b_{j+1}]^{p_{j+1}}$ (where $p_{q+1} = 1$) that only depend on t_j of their inputs for each of their components $g_{jk} : [a_j, b_j]^{p_j} \rightarrow [a_{j+1}, b_{j+1}]$, and satisfies $g_{jk} \in C_{t_j}([a_j, b_j]^{t_j}, \beta_j, H_j)$, i.e. they are Hölder smooth. We denote the class of these functions

$$\mathcal{G}(\{p_j, t_j, \beta_j, H_j\}_{j \in [q]})$$



Assumption 1: Hölder smoothness

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Definition

Define

$$\mathcal{F}_0 = \left\{ f : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R} \mid \forall a \in \mathcal{A} : f(\cdot, a) \in \mathcal{SRN} \left(s, V_{\max}, (d_i)_{i=0}^{L+1} \right) \right\}$$

and

$$\mathcal{G}_0 = \left\{ f : \mathcal{S} \times \mathcal{A} \rightarrow \mathbb{R} \mid \forall a \in \mathcal{A} : f(\cdot, a) = \mathcal{G} \left(\{p_j, t_j, \beta_t, H_j\}_{j \in [q]} \right) \right\}$$

It is assumed $T\mathcal{F}_0 \subseteq \mathcal{G}_0$.



Assumption 2: Concentration coefficients

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Concentration coefficients

Let $\nu_1, \nu_2 \in \mathcal{P}(\mathcal{S} \times \mathcal{A})$ be probability measures, absolutely continuous w.r.t. $\lambda^w \otimes \mu_{\mathcal{A}}$ (the product of the w -dimensional Lebesgue measure and the counting measure on \mathcal{A}). Define

$$\kappa(m, \nu_1, \nu_2) = \sup_{\pi_1, \dots, \pi_m \in S\Pi} \left[\mathbb{E}_{\nu_2} \left(\frac{d((P\pi_m) \circ \dots \circ (P\pi_1)\nu_1)}{d\nu_2} \right)^2 \right]^{1/2}$$

where $\frac{d\mu_1}{d\mu_2}$ are the Radon-Nikodym derivative

Assumption 2

For two probability measure $\nu, \mu \in \mathcal{P}(\mathcal{S} \times \mathcal{A})$ on $\mathcal{S} \times \mathcal{A}$ it is assumed that there exists a finite constant $\phi_{\mu, \nu} > 0$ such that

$$\phi_{\mu, \nu} := (1 - \gamma)^2 \sum_{m \geq 1} \gamma^{m-1} m \kappa(m, \mu, \nu) < \infty$$



The theorem

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Theorem (Fan et al. 2020)

Let $\nu, \mu \in \mathcal{P}(\mathcal{S} \times \mathcal{A})$ satisfy assumption 2 with $\phi_{\mu, \nu} > 0$. Let $n \in \mathbb{N}$ be a sufficiently large *batch size*.

Assume assumption 1 holds with constants $q \in \mathbb{N}$ and $\{p_j, t_j, \beta_j, H_j\}_{j \in [q]}$ for \mathcal{F}_0 with any sparsity constant and structure.

Then there exists structure and sparsity constants (for \mathcal{F}_0) such that when running the FQI algorithm we have

$$\left\| Q^* - Q_{\pi_K} \right\|_{1, \mu} = \mathcal{O} \left(n^{-\varepsilon^*} \log(n)^{c^*} + \gamma^K \right)$$

For some $\varepsilon^*, c^* > 0$.



Mistake in proof

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f_1, \dots, f_N centers of a minimal $1/n$ -covering of \mathcal{F}_0 .

$$Z_j = \sum_{i=1}^n (Y_i - TQ(X_i)) \cdot (f_j(X_i) - TQ(X_i)) \left(\sum_{k=1}^n (f_j(X_k) - TQ(X_k))^2 \right)^{-1/2}$$

Lemma

Let X be a **centered** sub-exponential random variable. Then for t such that $|t| \leq c/\|X\|_{\psi_1}$ one has

$$\mathbb{E} \exp(tX) \leq \exp(Ct^2 \|X\|_{\psi_1}^2)$$

where $C, c > 0$ are absolute constants.

The mistake here is that while Z_j^2 is sub-exponential enough, it is not clear why it should be centered. Indeed as $Z_j^2 \geq 0$ a.s. it is centered if and only if it is equal to 0 a.s!



Correction of mistake

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We luckily end up with a very similar bound. Our argument is based on a lemma

Lemma (Vershynin)

$$\mathbb{E} \exp(cX^2/\|X\|_{\psi_2}^2) \leq \exp(1) = e$$

By this lemma we have

$$\mathbb{E} \exp\left(cZ_j^2/\|Z_j\|_{\psi_2}^2\right) \leq e$$

so

$$\begin{aligned}
\mathbb{E} \max_{j \in N_\delta} Z_j^2 &= \frac{\max_{j \in [N_\delta]} \|Z_j\|_{\psi_2}^2}{c} \mathbb{E} \left(\max_{j \in [N_\delta]} \frac{cZ_j^2}{\max_{k \in [N_\delta]} \|Z_k\|_{\psi_2}^2} \right) \\
&\leq \dots \\
&\leq \frac{4V_{\max}^2 C_1}{c} \log \left(\sum_{j \in [N_\delta]} \mathbb{E} \exp \left(\frac{cZ_j^2}{\|Z_j\|_{\psi_2}^2} \right) \right) \\
&\leq \frac{4V_{\max}^2 C_1}{c} \log(eN_\delta) \\
&\leq C_2^2 V_{\max}^2 \log(N_\delta)
\end{aligned}$$



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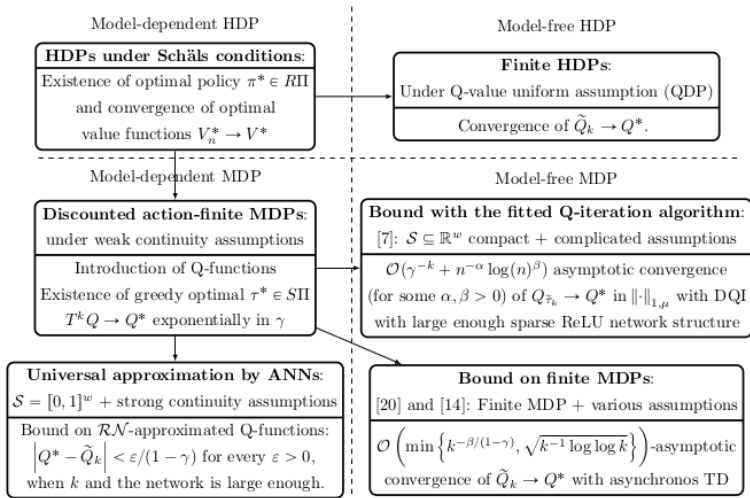
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Some of the convergence bound presented in this thesis. Arrows $A \rightarrow B$ implies that setting B is a special case of setting A .



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We have:

- Build up theory behind Q-learning: Decision models, optimality of policies, value functions and Q-iteration.
- Approximation with Q-iteration: Artificial neural networks, Bernstein polynomials.
- Survey of model-free algorithms.
- Proof of convergence bound of the fitted Q-iteration algorithm.

Are we closer to understanding the succes of DQN?

Yes: we have theoretical justification for convergence of related algorithms.

No: we still lack understanding of computational complexity aspects.



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Given more time it would have been interesting to go further into

- Exploring more concrete examples: Our only concrete example of a decision process is the finite gridworld environment.
- Use the results of Melo and Ribeiro (2007) on a concrete class of functions e.g. polynomials.
- Relations between $\|Q^* - Q_{\tilde{\pi}}\|_{\infty}$ and $\|Q^* - \tilde{Q}\|_{\infty}$.



Error corrections

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- p. 31 Continuous MDP should also be greedy (i.e. condition on P is missing).
- p. 33 Top: Discussion of proofs of theorem 2.77: "...to obtain a contradiction to the statement that $\bigcup_{N \in \mathbb{N}} \mathcal{DN}(\sigma, (w, N, 1))$ is **not** dense in $C([0, 1]^w)$ ".
- p. 33 Middle: the bound on $|Q^* - \tilde{Q}_k|$ should be $\leq \gamma^k V_{\max} + \varepsilon/(1 - \gamma)$ (and not $< \varepsilon/(1 - \gamma)$).
- p. 36 Corollary 2.84: $\|Q^* - \tilde{Q}_k\|_{\infty} \leq \gamma^k V_{\max} + \dots$
- p. 46 Top: "we may view FQI as a class of **algorithms**, because ...".



Algorithm reference error

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Due to an unexpected behavior of the \LaTeX -package *cleveref* when adding line numbers to algorithms, many references to 'algorithm n ' was accidentally changed to 'line k '.

p. 19 Replace 'line 3' with 'algorithm 1'.

p. 24 Replace 'line 3' with 'algorithm 2'.

p. 25 Top: "and therefore **algorithm 2** could be applied".

Middle: "To use **algorithm 1** and **algorithm 2**".

Bottom: "update step $\tilde{V}_{k+1} \leftarrow T_\tau \tilde{V}_k$ in **algorithm 2** becomes".

p. 26 "Similarly in **algorithm 2** the update step ...".

p. 29 "we thus have convergence of **algorithm 3**".

p. 30 Top: "which are used in **algorithm 3** are not [...] This means that if we were to use **algorithm 3** naively ...".

p. 37 "It is clear that in the model-free setting **algorithm 3** will not work ...".