



Machine Learning in Accelerators Introduction to Reinforcement Learning

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Introduction RL in nature



Introduction *RL in the machine learning landscape*





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Introduction *RL: state-of-the-art*



DeepMind, 2016: AlphaGo



OpenAl, 2019: Hide and seek

DeepMind, 2022: AlphaTensor

- Improving computational efficiency of matrix multiplication
- RL agent discovered more efficient algorithms than previously known



DeepMind & SPC-EPFL, 2022: Tokamak control

- > Maintaining plasma within Tokamak
- Requires high-dimensional, high-frequency, closed-loop control
- > RL agent as magnetic controller



and more ...

UZH & Intel Labs, 2023: Drone racing

champions in real environment

residual models from real data

 \geq

 \geq

RL agent beats human drone racing

Training in simulations with mixed-in

Introduction RL in a nutshell

- Iterative, online, trial-and-error learning
 - At every time step t, agent observes environment state s_t,
 selects an action a_t, and collects reward r_{t+1}
 - > **Environment transitions** from s_t to s_{t+1} under action a_t
- Objective
 - Learn to act in a way that maximises cumulative reward over time (= return)
 - > In other words: learn an optimal policy (= agent's behaviour)



Example: Pac-man



Environment: everything you interact with & its dynamics *maze structure, Pac-man, ghosts, food, game rules, etc.* **Agent:** player (you!) **State:** where am I? Where are ghosts, snacks, cookies? **Actions:** \uparrow , \leftarrow , \downarrow , \rightarrow **Reward:** food (+), ghosts, time (-) **Return:** game score (food eaten, lives lost, time elapsed) **Policy:** given current state, should I go \uparrow , \leftarrow , \downarrow , \rightarrow ?

- **Objective:** navigate around a gridworld maximising return (= cumulative reward over time)
- Four discrete actions: \uparrow , \leftarrow , \downarrow , \rightarrow
- Reward model
 - Stepping into empty field costs -1, bumping into walls -5
 - Stepping through fire costs -10
 - Reaching destination gives +30
- Use RL to learn an optimal policy

"what's the best action to pick from any of the fields (= state)?"





(An) optimal policy

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- Introduction
- Formalism
- Algorithms
 - Value-based methods
 - Policy gradient method
 - Actor-critic scheme
- Challenges
- Summary

Introduction Lecture scope

• Formalism⁺

- > RL terminology
- Markov decision process

• Algorithms

- Value- and policy-based methods foundation for understanding many other RL algorithms
- > Q-learning and actor-critic scheme
- Discrete and continuous state-action spaces
- Challenges



RL is a broad and exciting topic! The goal is to give you an introductory perspective and hopefully spark your interest in exploring it further ③

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Formalism Overview







- Memoryless random process consisting of
 - \succ State space $\mathcal S$
 - discrete or continuous
 - > State transition probabilities $\mathcal{P}_{ss'}$
- States possess the Markov property (= memorylessness)
 - > The future evolution of the Markov chain depends only on the information contained in the present state s_t , but not on the history of past states s_{t-1} , s_{t-2} , ...
 - $\succ P(s_{t+1} \mid s_t) = P(s_{t+1} \mid s_t, s_{t-1}, \dots, s_0)$

Chess

Arrangement of pieces on the board fully defines current state.

There may be many ways to arrive at that particular state, but this is irrelevant for deciding the next move and the future progression of the game.

Flight trajectory of a cannonball

State given by its current position and velocity $s_t = (\vec{x}_t, \vec{v}_t)$ provides enough information to predict the future (in an ideal world ...) *N.B.*: $s_t = (\vec{x}_t)$ or $s_t = (\vec{v}_t)$ do not fulfil the Markov property



State given by single video frame is not Markov, but a sequence of frames is *E.g.: need to know what direction the ball is moving to forecast future progression of the game and be able to take an optimal decision*



50 m/s 40 m/s 30 m/s 45° $|-R = 91.8 \text{ m} \rightarrow|$ $|-R = 163 \text{ m} \rightarrow|$ $|-R = 255 \text{ m} \rightarrow|$



Formalism *Markov Process: example*



- $S = \{$ Class 1, Class 2, Class 3, Facebook, Pub, Pass, Sleep $\}$
- N.B.: "Sleep" is also called a terminal state, because once in it we will never leave it

Formalism Markov Reward Process

- A Markov Process that has in addition a
 - > **Reward function** $r_{t+1} = R(s_t, s_{t+1})$
 - ▶ **Discount factor** $\gamma \in [0, 1]$
- Return

 $G_t = \sum_{k=0} \gamma^k r_{k+t+1}$

sum of discounted future rewards

- The **discount factor** γ controls the relative importance of immediate vs future rewards
 - > $\gamma \rightarrow 0$: only care about immediate rewards
 - $\succ \gamma \rightarrow 1$: care about long-term rewards
- Can be better to give up immediate rewards to collect higher rewards in the long run ... *Example: sacrificing a piece in chess to eventually win the game*



Class 1 \rightarrow Class 2 \rightarrow Class 3 \rightarrow Pass \rightarrow Sleep $G_0 = (-2) + 0.5^1 \cdot (-2) + 0.5^2 \cdot (-2) + 0.5^3 \cdot (+10) = -2.25$ $\gamma = 0.5$

Formalism Markov Decision Process (MDP)



- Extend Markov Reward Process by adding **decision making mechanism**
 - Action space A
 discrete or continuous
 - > A decision maker (= agent) acts on the environment following a policy π
 - > Stochastic state transitions are still allowed
- We define a trajectory τ as a sequence of states, actions, and rewards over time

 $\tau = (s_0, a_0, r_1, s_1, a_1, r_2, \dots, r_T, s_T)$

MDPs form the foundation of RL

Formalism *RL objective & policy*

- The **policy** π encodes an agent's decision making or **behaviour**
- Two formulations are common
 - > **Stochastic policy:** *assigns probabilities to state-action pairs* (*s*, *a*)

$$\pi: S \times \mathcal{A} \to [0, 1]$$

$$\pi(a \mid s) = P(A_t = a \mid S_t = s) \text{ with } \sum_a \pi(a \mid s) = 1$$

> **Deterministic policy:** outputs specific action a_t for given state s_t

$$\pi: S \to \mathcal{A}$$
$$a_t = \pi(s_t)$$

- We will also distinguish between
 - > Behaviour policy π_b : policy guiding the agent's actions during exploration and data collection
 - > Target policy π_t : policy we aim for the agent to learn and optimise towards

Example: random policy

$$\pi(\uparrow \mid s) = 0.25$$

$$\pi(\downarrow \mid s) = 0.25$$

$$\pi(\leftarrow \mid s) = 0.25$$

$$\pi(\leftarrow \mid s) = 0.25$$

$$\pi(\rightarrow \mid s) = 0.25$$



Formalism *RL objective*

- RL objective
 - Learn optimal behaviour in an environment: trained agent should select best sequence of actions from any state
 - \succ Also known as the **optimal policy** π^*
 - "Best sequence of actions" means "the one maximising return"
- RL is based on the **reward hypothesis**

"Any goal can be formalised as the outcome of maximising a scalar, cumulative reward"

Interesting thoughts by Sutton and Barto: <u>http://incompleteideas.net/rlai.cs.ualberta.ca/RLAI/rewardhypothesis.html</u>

- Finite MDP: sets of possible states, actions, and rewards are finite
- Stochastic vs deterministic MDP
 - Stochastic: outcomes of taking a specific action not deterministic, i.e. starting from state s_t and taking action a_t might not always bring us to the same state s_{t+1}
 - > **Deterministic:** outcome of an action is fully predictable
- Episodic MDP
 - > Each episode ends in a terminal state (or is truncated)
 - Return is the sum of discounted rewards from time t till end of episode
 - Episodes are independent of each other
- **Continuous** (= infinite horizon) **MDP**
 - Runs indefinitely with no terminal states
 - > Discount factor $\gamma < 1$ is key to avoid infinite returns
- Partially vs fully observable MDPs
 - > Agent might not see the true, full environment state s_t but only be able to make a partial observation
 - Real-world environments are very often only partially observable

Quick recap



- The goal of RL is to **learn to make optimal decisions** (*take best actions*) in an environment based on some observables (*state*)
- The quality of a decision made is quantified by a scalar reward
- Through trial-and-error, the RL agent collects data samples $(s_t, a_t, r_{t+1}, s_{t+1})$ from which it learns optimal behaviour (optimal policy π^*)
- Formally, this is described by a Markov decision process (MDP)
- **Example RL tasks:** playing board or video games, humanoid robots learning to walk, control systems (e.g. tuning accelerator parameters), ...







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There are many ways to solve the RL problem and finding an optimal policy in an environment



Algorithms RL taxonomy

- Value-based methods
 - Agent learns a value function that estimates expected return
 - > Policy is indirectly obtained from value function
 - > E.g.: Deep Q-learning (DQN)
- Policy-based methods
 - Agent directly optimises parameters of a policy function
 - > E.g.: Proximal Policy Optimisation (PPO)
- Actor-critic scheme
 - Combines value-based and policy-based methods
- On- vs off-policy methods
- Model-free vs model-based algorithms



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Value-based methods Value functions



• Value functions estimate "how good it is" for the agent ...

"... to be in state s given that we follow policy π ?" State-value function

 $V^{\pi} \colon S \to \mathbb{R}$ $V^{\pi}(s) = \mathbb{E}_{\pi}[G_t \mid s_t = s]$

"... to take action a in state s given that we follow policy π ?"

State-action value function (= "Q-function") $Q^{\pi}: S \times A \rightarrow \mathbb{R}$ $Q^{\pi}(s, a) = \mathbb{E}_{\pi}[G_t \mid s_t = s, a_t = a]$

- "Goodness" is measured in terms of return expected following that policy
- The value functions associated with the (an) optimal policy π^* are denoted V^* and Q^* , respectively

$$V^*(s) = \max_{a'} Q^*(s, a')$$

State-action value function
(= "Q-function")

 $Q^{\pi}(s,a) = \mathbb{E}_{\pi}[G_t \mid s_t = s, a_t = a]$

Q-learning

The goal of Q-learning is to deduce the optimal policy by learning the optimal stateaction value function $Q^*(s, a)$ first

> Once $Q^*(s, a)$ is known, it is easy to read off the best policy (= greedy policy)

 $\pi^*(s) = \arg \max_{a'} Q^*(s, a')$

i.e.: "in a given state, what is the best action to take to maximise return?"

> How to learn $Q^*(s, a)$?

Bellman optimality equation

$$G_{t} = \sum_{k=0} \gamma^{k} r_{k+t+1} = r_{t+1} + \gamma \sum_{\substack{k=0 \\ k=0}} \gamma^{k} r_{k+t+2}$$

 $V^*(s') = \mathbb{E}_{\pi^*}[G_{t+1}]$ $V^*(s') = \max_{a'} Q^*(s', a')$

weighted sum over all possible next states s' under action a

assuming deterministic environment

> Bellman splits the trajectory into an "immediate part" and "whatever follows beyond"

Bellman optimality equation

> It allows us to apply the **Temporal Difference (TD) rule** when learning an **estimator** \hat{Q}^* of the optimal Q-function

$$Q^{*}(s, a) = \mathbb{E}_{\pi^{*}}[G_{t}]$$

$$S = S_{t}$$

$$a = a_{t}$$

$$s' = s_{t+1}$$

$$= \mathbb{E}_{\pi^{*}}[r_{t+1} + \gamma G_{t+1}]$$

$$= \mathbb{E}_{\pi^{*}}[r_{t+1} + \gamma \max_{a'} Q^{*}(s', a')]$$

$$= \sum_{s'} \mathcal{P}_{ss'}^{a}[R(s, s', a) + \gamma \max_{a'} Q^{*}(s', a')]$$

$$= r_{t+1} + \gamma \max_{a'} Q^{*}(s_{t+1}, a')$$

Value-based methods *Q-learning algorithm*

Bellman optimality equation

 $Q^*(s_t, a_t) = r_{t+1} + \gamma \max_{a'} Q^*(s_{t+1}, a')$

- At t = 0: initialise $\hat{Q}^*(s, a)$, e.g. random, or all zeros
- At every time step
 - > Let agent interact with environment to collect $(s_t, a_t, r_{t+1}, s_{t+1})$ following some behaviour policy π_b Typically, " ε -greedy": select greedy action with probability 1- ε , random otherwise
 - > Update $\hat{Q}^*(s, a)$ based on TD rule using collected agent-environment interactions



• With enough iterations $\hat{Q}^*(s, a)$ will converge to the true $Q^*(s, a)$

Q-learning remarks

• Q-learning is an iterative process

- > Need a way to **track and update Q-values** for each state-action pair at every iteration
- For simple (small, discrete) state-action spaces, we can use a look-up table

• Q-learning uses **bootstrapping**

- > Update of $\hat{Q}^*(s, a)$ uses a **target** that is **itself based on an estimate** *"shooting at a moving target": training can be unstable as target also updates frequently*
- Typically solved using two separate Q-estimators: "target Q" and "online Q" with periodic synchronisation

• Q-learning is an off-policy method

> How agent chooses its actions (= behaviour policy π_b) to collect samples $(s_t, a_t, r_{t+1}, s_{t+1})$ does not necessarily match the policy, or associated value function, we are trying to learn (= target policy π_t)

Q-learning update rule

 $\hat{Q}^{*}(s_{t}, a_{t}) \leftarrow \hat{Q}^{*}(s_{t}, a_{t}) + \alpha \left[r_{t+1} + \gamma \max_{a'} \hat{Q}^{*}(s_{t+1}, a') - \hat{Q}^{*}(s_{t}, a_{t}) \right]$

target (new best guess)

- > Allows for experience replay (recycling previous samples), improving sample efficiency
- $\succ \quad More on that later <math>\textcircled{\odot} \dots$



old

prediction

Q-table example



Episode

 $\hat{Q}^{*}(s_{t}, a_{t}) \leftarrow \hat{Q}^{*}(s_{t}, a_{t}) + \alpha \left[r_{t+1} + \gamma \max_{a'} \hat{Q}^{*}(s_{t+1}, a') - \hat{Q}^{*}(s_{t}, a_{t}) \right]$



Deep Q-learning (DQN)

- Q-function of continuous or very large ${\mathcal S}$ can no longer be represented by a look-up table
- Replace table by neural net: deep Q-learning (DQN)
 - Universal function approximator and great interpolator (e.g. for unseen states)
 - Q-net is mapping from state to Q-values of all possible actions
 - Train network weights using Q-learning update rule
- Developed by DeepMind in 2013 and applied to playing Atari games – many at super-human level (DQN paper)
- **N.B.:** only for **discrete** A need one output node per action ...

Episode 2400				
s \ a +	up	down	left	right
(0, 0) (0, 1) (1, 0) (1, 1) (2, 0) (2, 1)	27.4 23.4 28.7 24.7 30.0 0.0	22.1 26.1 18.4 18.4 24.7 0.0	22.1 23.4 26.1 27.4 18.4 0.0	18.4 28.7 28.7 30.0 24.7 0.0



Value-based methods Example: DeepMind's RL for Atari games



Q-table vs DQN: pros, cons, limitations

Q-table

- Easy to understand and validate
- Discrete S, A spaces only
- Relatively small S, A spaces only

DQN

- Large, continuous *S* possible
- No need to visit all states during training: neural nets are great interpolators
- Discrete and relatively small \mathcal{A}
- Training may be unstable and hard to validate (incl. convergence)

- Many real-world problems require continuous S and continuous A
 ⇒ typically use policy gradient or actor-critic methods
- Other function approximators: (quantum) Boltzmann machines, ...

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Policy gradient methods In a nutshell

- Policy represented by **parameterised function** $\pi_{\theta}(a \mid s)$ θ : for example weights of a neural network
- Goal is to **directly optimise** θ s.t. π_{θ} **maximises expected return** over trajectories τ

$$J(\theta) = \mathbb{E}_{\tau \sim \pi_{\theta}}[G(\tau)]$$

> Perform gradient ascent for policy parameters θ

$$\theta \leftarrow \theta + \alpha \cdot \nabla_{\theta} J(\theta)$$

> Gradient can be calculated using the **policy gradient theorem**

$$\nabla_{\theta} J(\theta) = \mathbb{E}_{\tau \sim \pi_{\theta}} \left[\sum_{t=0}^{\infty} \Psi_t \nabla_{\theta} \log \pi_{\theta}(a_t \mid s_t) \right]$$

- **N.B.:** policy gradient algorithms typically differ in what they use for Ψ_t
 - > It can e.g. be the **return**, a so-called **advantage function**, a **baseline corrected return**, etc.
 - > More on that in the advanced lecture

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Algorithms Actor-critic scheme

- Introduce an actor (= policy) and a critic (= value function estimator) combining a value-based with a policy-gradient approach
- Typically, actor and critic are **represented by** (fairly small) **neural nets**, trained simultaneously
- Can solve the **continuous state** *and action* problem
- Various algorithms exist (DDPG, TD3, SAC, ...), e.g. handling exploration-exploitation differently, improving convergence behaviour, ...

Actor (policy net)

- > Represents the target policy π_t to be learned
- For each (continuous)
 state s, it proposes a
 (continuous) action a
- Its parameters χ are updated through the policy gradient



For given state s, how does the actor have to adjust its parameters χ to propose an action a that results in larger Q(s, a)?

Critic (*Q*-*net*)

- Learns Q-function and evaluates quality of the (s, a) pair proposed by actor net
- Parameters θ are updated using **TD rule** (like in Qlearning)
- Feeds back to the actor via policy gradient

Algorithms *On- vs off-policy methods*

- A priori, training an RL agent employs **two policies**
 - > Behaviour policy π_b : policy the agent follows to select action at every time step during data collection
 - > Target policy π_t : policy we aim for the agent to learn and optimise towards
- RL algorithms can be ...

On-policy

 $\succ \pi_t = \pi_b$

- Agent updates and learns the same policy (or value function) that it uses to interact with the environment
- > Example: **SARSA**

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha [r_{t+1} + \gamma Q(s_{t+1}, a_{t+1}) - Q(s_t, a_t)]$$

TD target based on action a_{t+1} that was selected by π_b and applied in the environment

 \blacksquare Learning Q-function **associated with** π_b

Off-policy

- $\succ \pi_t \neq \pi_b$
- Agent updates and learns a different policy (or value function) than it uses to interact with the environment
- > Example: **Q-learning**

$$Q(s_t, a_t) \leftarrow Q(s_t, a_t) + \alpha [r_{t+1} + \gamma \max_{a'} Q(s_{t+1}, a') - Q(s_t, a_t)]$$

TD target **always** based on current best guess of **greedy action**, **independent of action selected and applied** in the environment by π_b Learning Q-function **associated with a greedy policy** π_t

Algorithms Experience replay

- Off-policy algorithms boast improved sample efficiency
 - > They can learn from agent-environment interactions **collected according to** *any policy*
 - Experience replay
 - Keep buffer of past interactions and update value function on a batch of memories at every training step
 - Different sampling methods exist to select and learn from past experiences most efficiently
- **On-policy** algorithms can only learn "online"
 - > Learning step relies on **samples collected according to** *currently valid policy*
 - > We have to **discard past experiences** as they were **collected** according to a **different policy**
- **On-policy** methods typically feature **more stable training** than off-policy algorithms

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- Sample efficiency
 - > How many agent-environment interactions are required for training / convergence?
 - > Online training is not always possible: sim2real & sim2real gap
- Reward engineering
 - Alignment: getting the objective right
 Making sure the agent does what we want it to do ...
 - Credit assignment problem Which action contributed how to the reward?
- Exploitation vs exploration dilemma
- State definition
 - Markov property
 - Environments are sometimes only partially observable
- Non-stationarity
- Safety & validation
 - Particularly a concern during exploration
 - There are ways to add safety to RL agents





Computer Science > Artificial Intelligence (Submitted on 20 May 2022 (v1), last revised 20 Feb 2023 (this version, v4)) A Review of Safe Reinforcement Learning: Methods, Theory and Applications Shangding Gu, Long Yang, Yali Du, Guang Chen, Florian Walter, Jun Wang, Yaodong Yang, Alois Knoll Reinforcement learning (B1) has achieved tremendous success in many complex decision making tasks. When it comes to deploying B1 i https://grxiv.org/gbs/2205.10330

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$ar \times iv > cs > ar \times iv: 2205.10330$

Computer Science > Artificial Intelligence

[Submitted on 20 May 2022 (v1), last revised 20 Feb 2023 (this version, v4)]

A Review of Safe Reinforcement Learning: Methods, Theory and Applications

Shangding Gu, Long Yang, Yali Du, Guang Chen, Florian Walter, Jun Wang, Yaodong Yang, Alois Knoll

Reinforcement learning (RI) has achieved tremendous success in many complex decision making tasks. When it comes to deploying RI in

https://arxiv.org/abs/2205.10330

Challenges Sample efficiency

- How many agent-environment interactions are required for the value function / policy to converge?
- Depends heavily on choice of algorithm
 - Off- vs on-policy algorithms
 - > Online vs. offline RL
 - Model-free vs model-based RL
- Reliable simulations / surrogate models
 - Train RL agent on model, then deploy in real world (sim2real)
 - Model can be based on simulations, measurements, or both
 - sim2real gap can be a problem





Challenges *Exploration-exploitation dilemma*

- To learn the **best policy** in an efficient manner, algorithms need to have a good a **balance between**
 - exploration: trying out different actions to discover their effects and rewards
 - exploitation: picking *best-known* action to maximise return
- Why?
 - During training, best-known action is typically not yet the true best action
 - Keep some degree of exploration to potentially discover more rewarding actions and avoid settling for suboptimal policy
 - Too much exploration can slow down training progress
- Different algorithms use different techniques to balance out exploration and exploitation, e.g. ε-greedy with decay, entropy-based methods, ...



image by Berkeley AI course

Summary



- Reinforcement learning (RL) solves decision-making problems and optimises an agent for best behaviour (= optimal policy) in an environment, i.e. maximising expected return
- Formally, RL is based on Markov Decision Processes and the reward hypothesis
- RL algorithms employ different techniques
 - > Value-based methods: learn a value function that estimates expected return to deduce policy indirectly
 - > Policy-based methods: optimise parameters of a policy directly for highest expected return
 - > Actor-critic: combine learning policy and value functions

Functions to be learned are typically approximated by means of neural nets

- Some algorithms are **suitable only for discrete state-action spaces**
- We distinguish between **on- and off-policy algorithms:** behaviour vs target policy
- RL also faces many challenges
 - > Balancing exploration vs exploitation, sample efficiency, dealing with partially observable systems, etc.
 - > Some will be addressed in the **advanced RL lecture**

Further reading

- R.S. Sutton and A.G. Barto, <u>"Reinforcement learning an introduction"</u>, Book, 2nd edition, 2020.
- S. Levine, <u>Deep Reinforcement Learning</u>, Lecture, UC Berkeley, 2022.
- D. Silver, <u>Reinforcement learning</u>, Lecture, University College London (UCL), 2015.