Machine Learning techniques for numerical solvers

Day 4: Reinforcement Learning

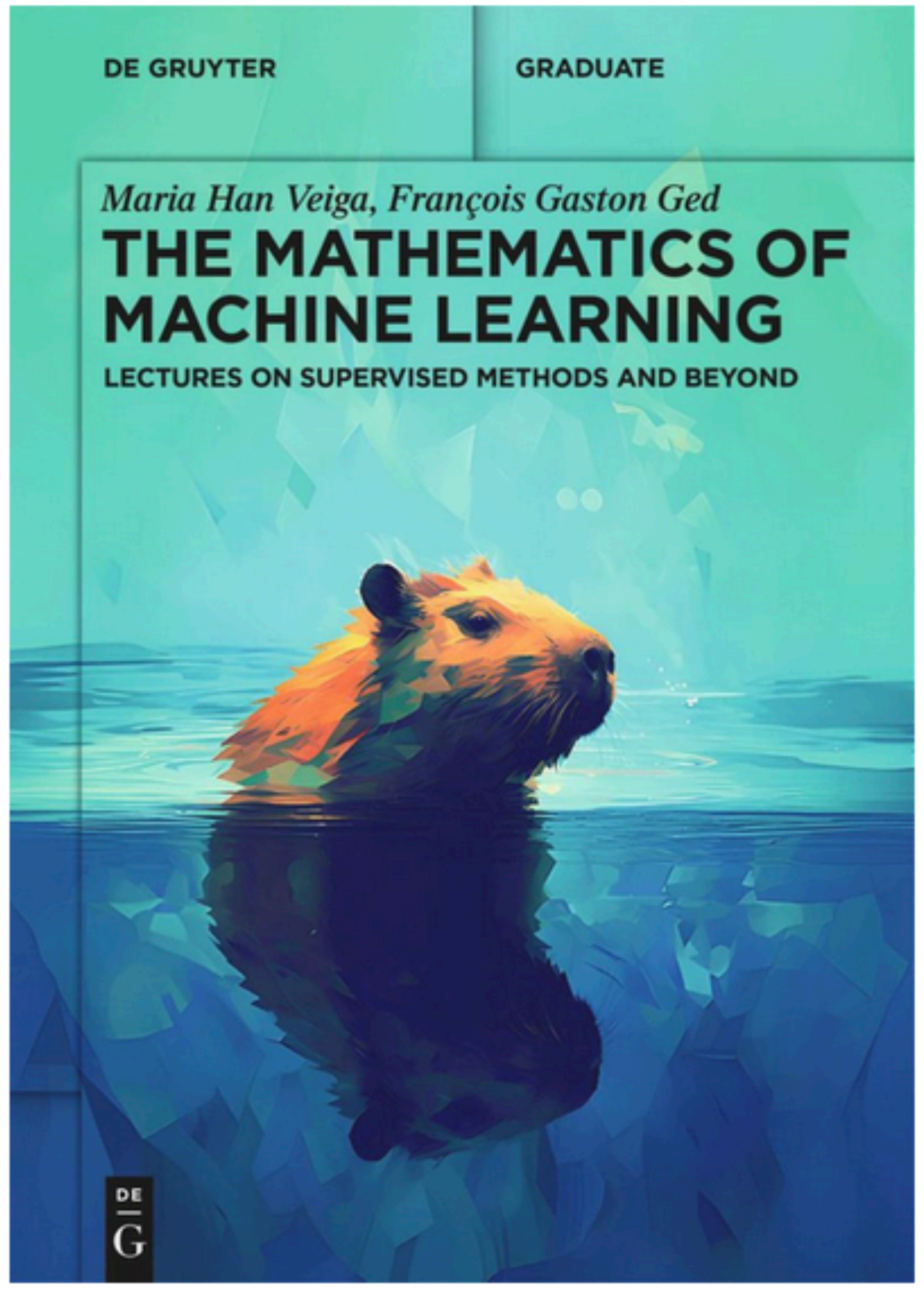
Maria Han Veiga
Mini-course SUSTech
11.03 - 14.03

THE OHIO STATE UNIVERSITY
COLLEGE OF ARTS AND SCIENCES

Schedule

- **Monday:** Introduction to Machine Learning (1h) 17:00-18:00
- **Tuesday:** Computational Framework + Supervised learning: integrating data-driven methods within a numerical solver + Hands-on session (2h) 14:00-16:00
- **Wednesday:** Unsupervised learning: Physics informed neural networks (1h) 11:00-12:00
- **Thursday:** Reinforcement Learning (1h) 11:00-12:00

A quick advertisement



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The Mathematics of Machine Learning

Lectures on Supervised Methods and Beyond

Maria Han Veiga and François Gaston Ged

In the series De Gruyter Textbook

Day 4: Reinforcement learning

Outline

- Introduction to Reinforcement Learning (RL)
  - Markov Decision Process
  - Iterative methods
  - Policy gradient method
- RL in numerics

Reinforcement Learning

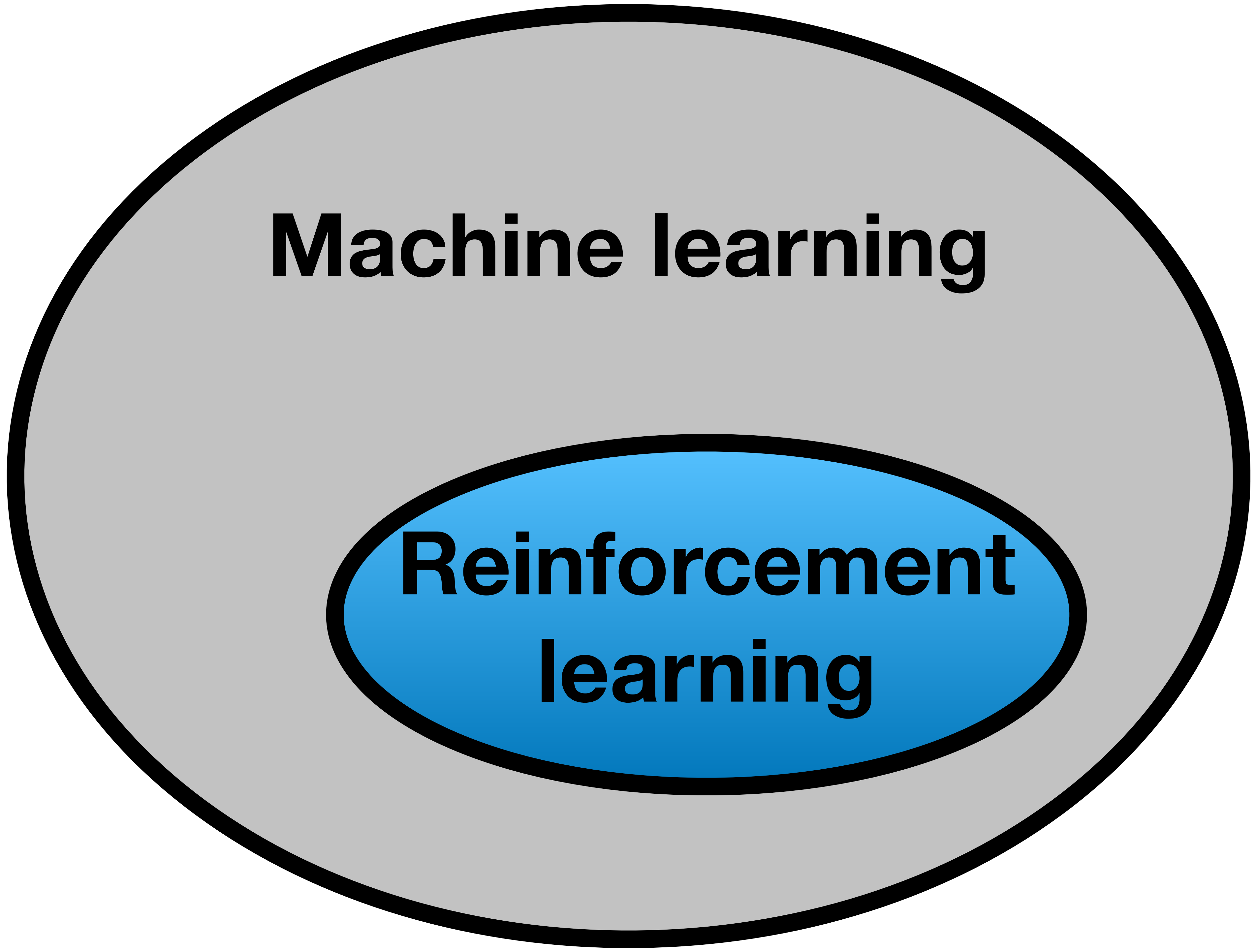
- **Task:** Consider a dynamical system that evolves over time. At a discrete time step n, the state of the system is describe by an element s_n at some state space.

- A control u_n is applied and the system then moves to a new state, $s_{n+1} = f(n, s_n, u_n)$ for some transition map f.

- For a given sequence of states and controls (trajectory) of length N, the performance on this task is measured using a performance criterion $J((s_n, u_n)_{n \leq N})$.

Reinforcement Learning

- Reinforcement Learning (RL) is an approach to solve such problems through trials and errors:
    - a learner (agent) samples a trajectory, collects rewards (based on performance J) and reinforces positively or negatively the chosen actions (control).



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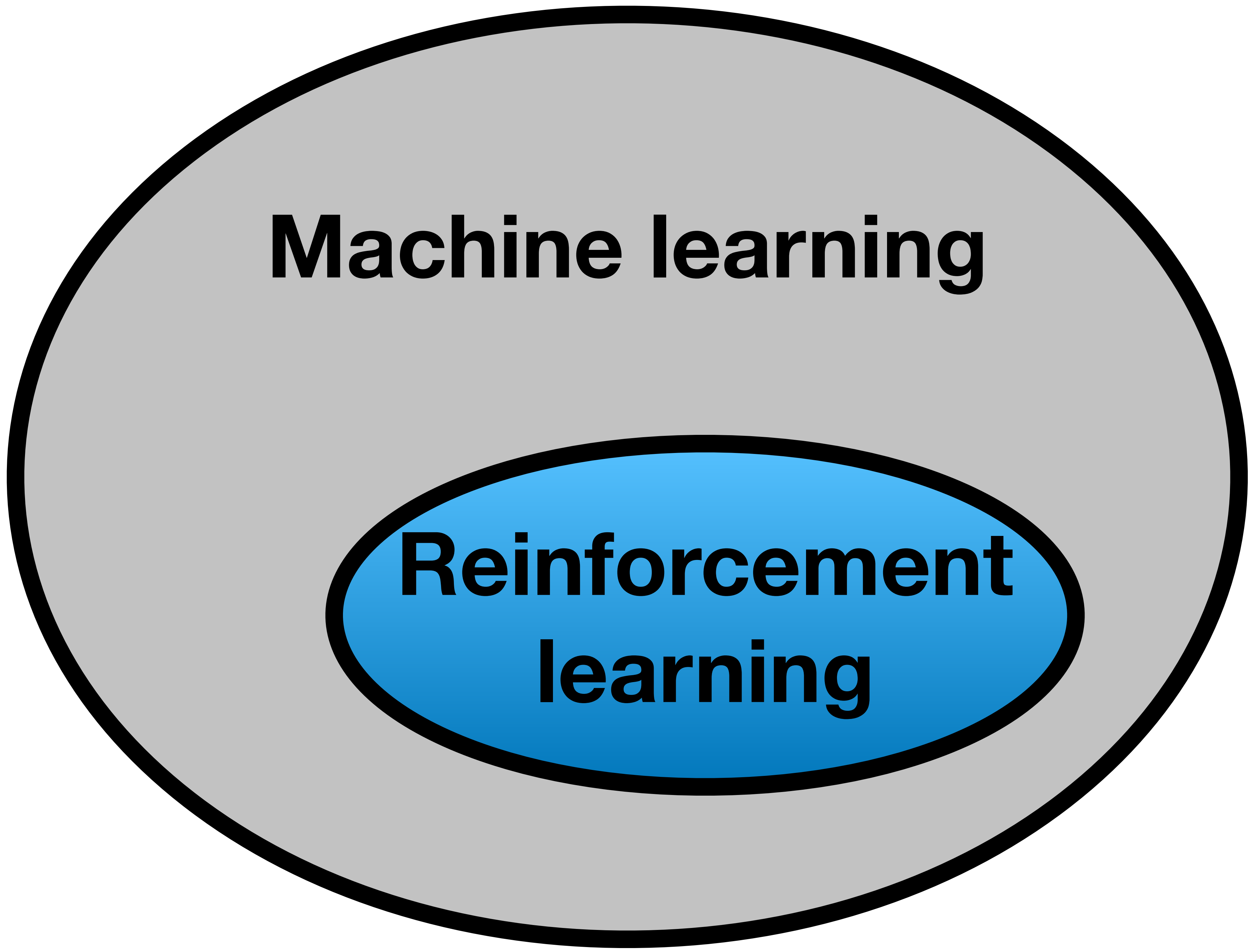

- **Example:** Playing a chess game. At the end of the game (a sequence of moves), we get a reward, e.g. +1 for winning, -1 for losing or 0 for drawing.

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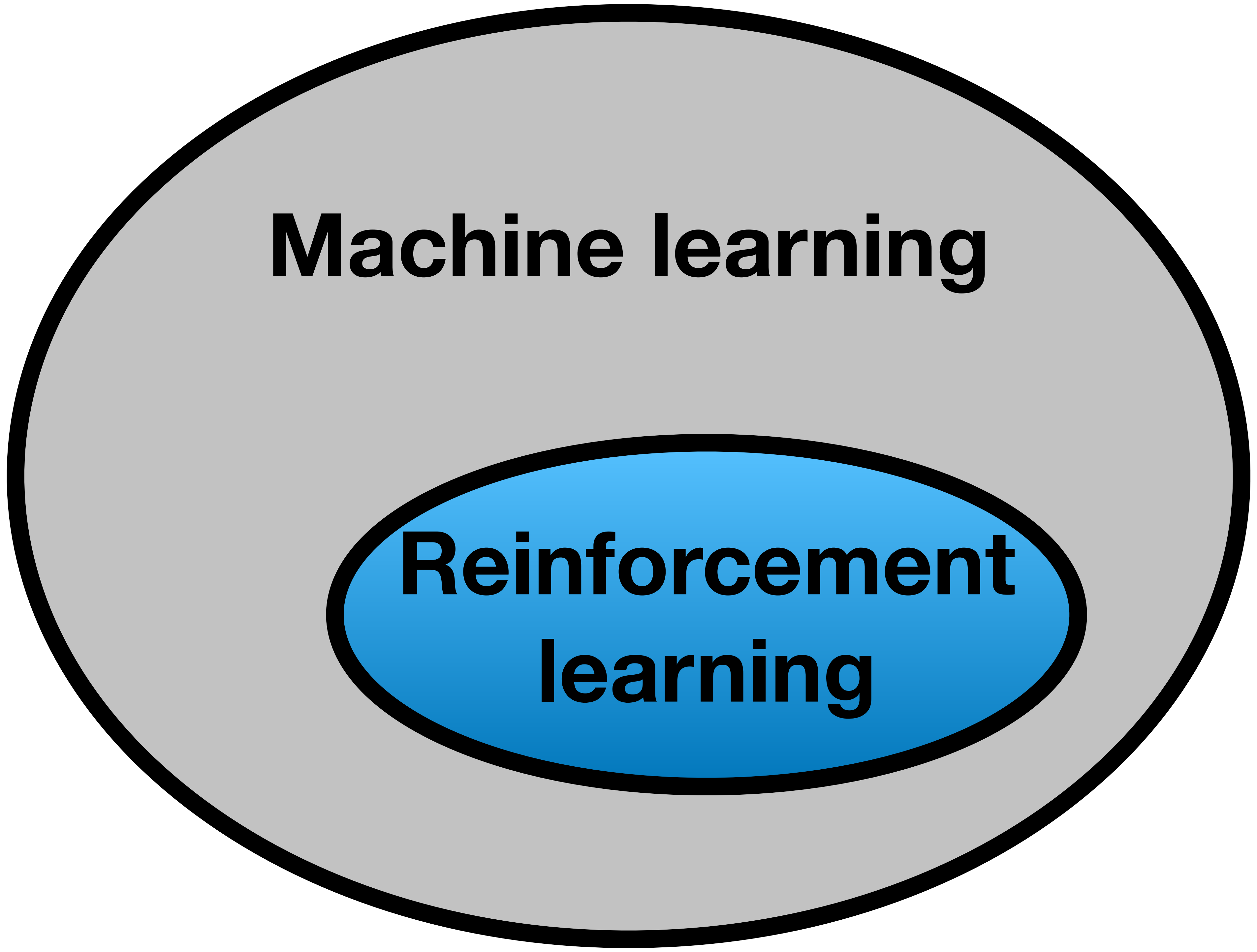

- **Example:** Playing a chess game. At the end of the game (a sequence of moves), we get a reward, e.g. +1 for winning, -1 for losing or 0 for drawing.
  - **Reward does not have to be differentiable!**

Reinforcement Learning

- Reinforcement Learning (RL) is an approach to solve such problems through trials and errors:
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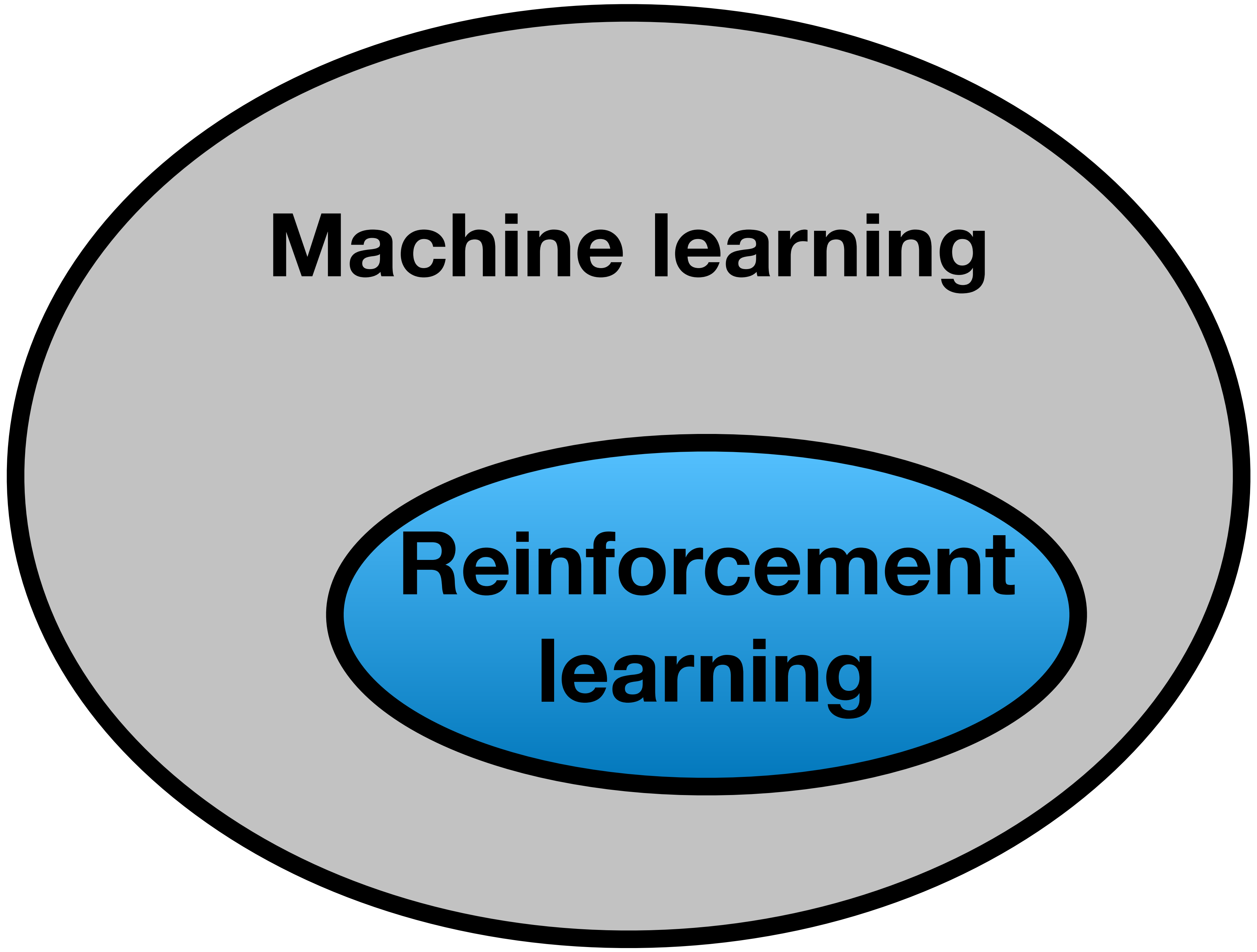
- Frame numerical analysis problems as RL tasks: limiting a numerical solution [1], solving PDEs [2], etc.

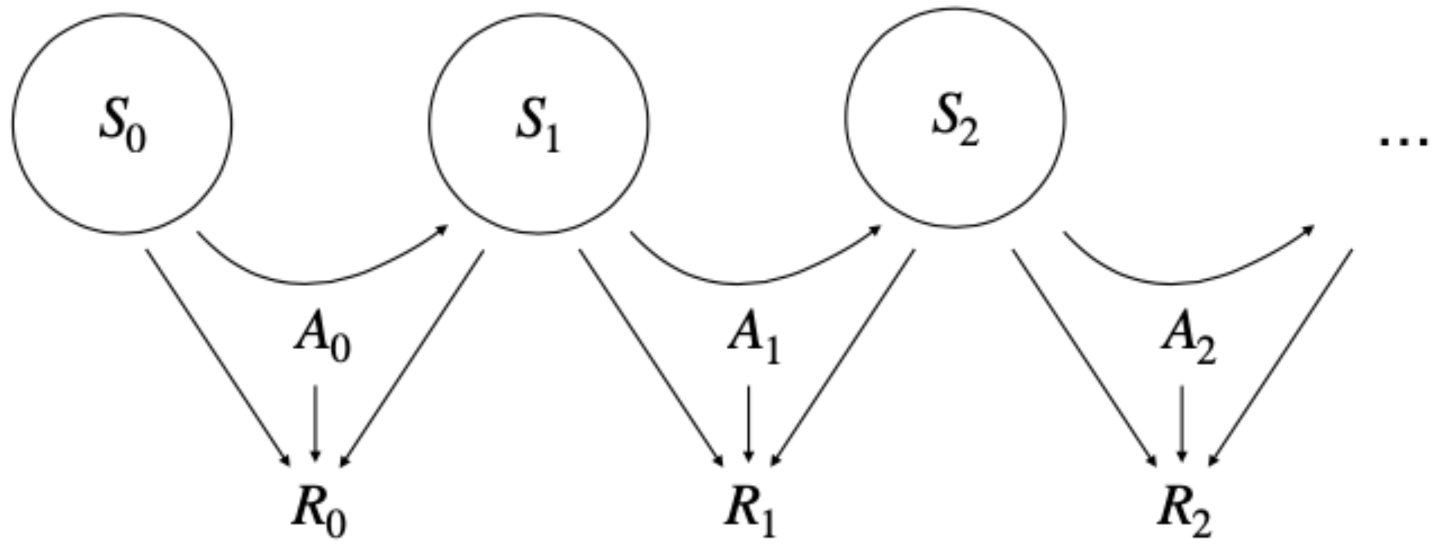


[1] "*A Reinforcement Learning Based Slope Limiter for Second-Order Finite Volume Schemes*", Schwarz et al., PAMM, 2023

[2] "*Solving high-dimensional partial differential equations using deep learning*", Han et al., PNAS, 2018

Reinforcement Learning

- Formally, assume agent interacts with the environment with a sequence of discrete time steps $t = 0,1,2,...$, with a possibly random terminal time T, or continue indefinitely.
- At each time step t, agent has a representation of the environment's sate and its own internal state, $S_t \in \mathcal{S}$. Given that state, it selects an action $A_t \in \mathcal{A}$ and arrives at some other state S_{t+1}.
- In consequence of the tuple (S_t, A_t, S_{t+1}), the agent receives a reward $R_t \in \mathbb{R}$,



Yields a trajectory $S_0, A_0, R_0, S_1, A_1, R_1, \ldots$

Reinforcement Learning

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At each tilmestep t, we can define the *return at time* t as the sum of the current reward and all future rewards:

$$G_t := R_t + R_{t+1} + \ldots$$

$$G_t := R_t + \gamma R_{t+1} + \gamma^2 R_{t+2} + \ldots, \gamma \in (0,1)$$

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How to choose a good action?

Reinforcement Learning

Definition (Policy): A policy is a mapping $\pi : \mathcal{A} \times \mathcal{S} \to [0,1]$ such that

$$\pi(a \mid s) = P(A_t = a \mid S_t = s)$$

with the condition that $\sum_{a \in \mathcal{A}} \pi(a \mid s) = 1$ for all $s \in \mathcal{S}$.

Reinforcement Learning

Definition (Markov decision process): Let $(\mathcal{S}, \mathcal{A}, p, r)$ be given as:

- $\mathcal{S}$ is a finite set of states
- $\mathcal{A}$ is a finite set of actions
- p is the state transition kernel $p(s, a, s')$
- $r : \mathcal{S} \times \mathcal{A} \times \mathcal{S} \to \mathbb{R}$ is a reward function

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Given a policy π and an initial state distribution ν on $\mathcal{S}$, the MDP is constructed recursively as follows:

- At $t = 0$, the agent is located at $S_0 \sim \nu$
- At state S_t agent takes action $A_t \sim \pi(\,\cdot \mid S_t)$, transits to state $S_{t+1} \sim p(S_t, A_t, \cdot\,)$, collects reward $R_t = r(S_t, A_t, S_{t+1})$, <u>independently from all past random variables.</u>

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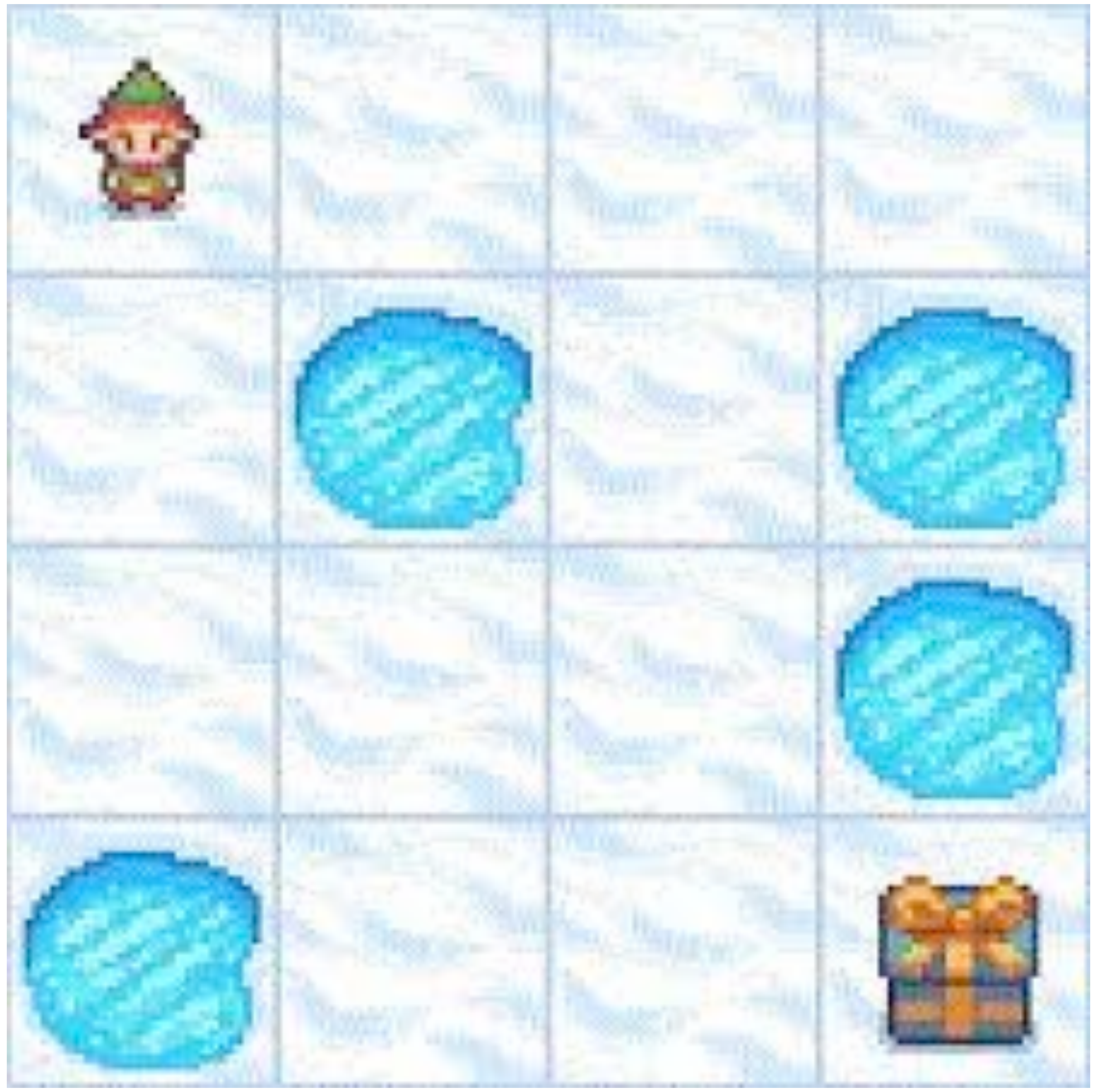
Example



Frozen lake game:

State space: {1,2,3,…,16}

Action space: {up, down, left, right}

Reward:

- Falling into hole: -1
- Finding treasure: 1

p(s,a,s’) deterministic or stochastic

Iterative methods

How to find a good policy?

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What is a *good* state or *good* action?

Iterative methods

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What is a *good* state or *good* action?

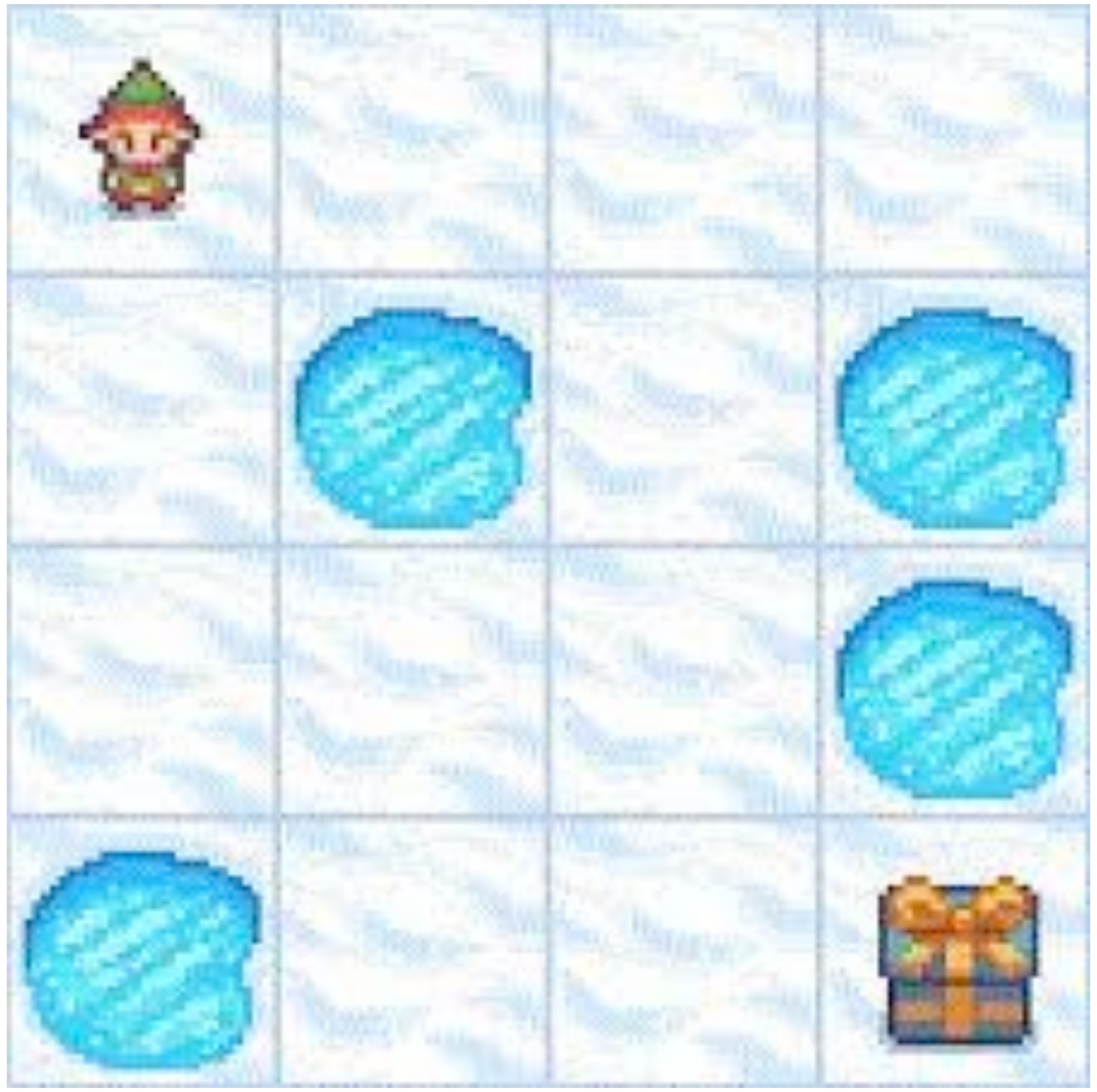
Value function: $v_\pi(s) := \mathbb{E}(G_t \mid S_t = s)$

Expected return of starting at state s and following policy π.

State-action value function: $q_\pi(s, a) := \mathbb{E}(G_t \mid S_t = s, A_t = a)$

Expected return of starting at state s and taking action a, then following policy π.

Example



Frozen lake game:

Policy: always going down

$$v(1) = \gamma^2(-1)$$

$$v(2) = (-1)$$

$$v(3) = 0$$

$$q(1,\text{'right'}) = \gamma(-1)$$

Iterative methods

One class of methods is to estimate v_π and q_π — q-learning, iterative methods.

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Theorem (Consistency condition for v_π). For any policy π and any state s, the following consistency condition holds between value function at s and the value of its possible successor states s'.

$$v_\pi(s) = \sum_{a \in \mathcal{A}} \pi(a \mid s) \left(r(a, s) + \gamma \sum_{s' \in \mathcal{S}} p(s, a, s') v_\pi(s') \right), \quad \forall s \in \mathcal{S} .$$

Iterative methods

- Suppose probability kernel $p(s, a, s')$ and reward r are known
- State space $\mathcal{S} = \{s_1, \ldots, s_n\}$ is finite
- Then, we can write:

$$\vec{v}_\pi = \overrightarrow{R} + \gamma P \vec{v}_\pi,$$

where $\vec{v}_\pi = (v_\pi(s_1), \ldots, v_\pi(s_n))$, $\overrightarrow{R}_i = \sum_{a \in \mathcal{A}} \pi(a \mid s_i) r(a, s_i)$, $P_{i,j} = \sum_{a \in \mathcal{A}} \pi(a \mid s_i) p(s_i, a, s_j)$.

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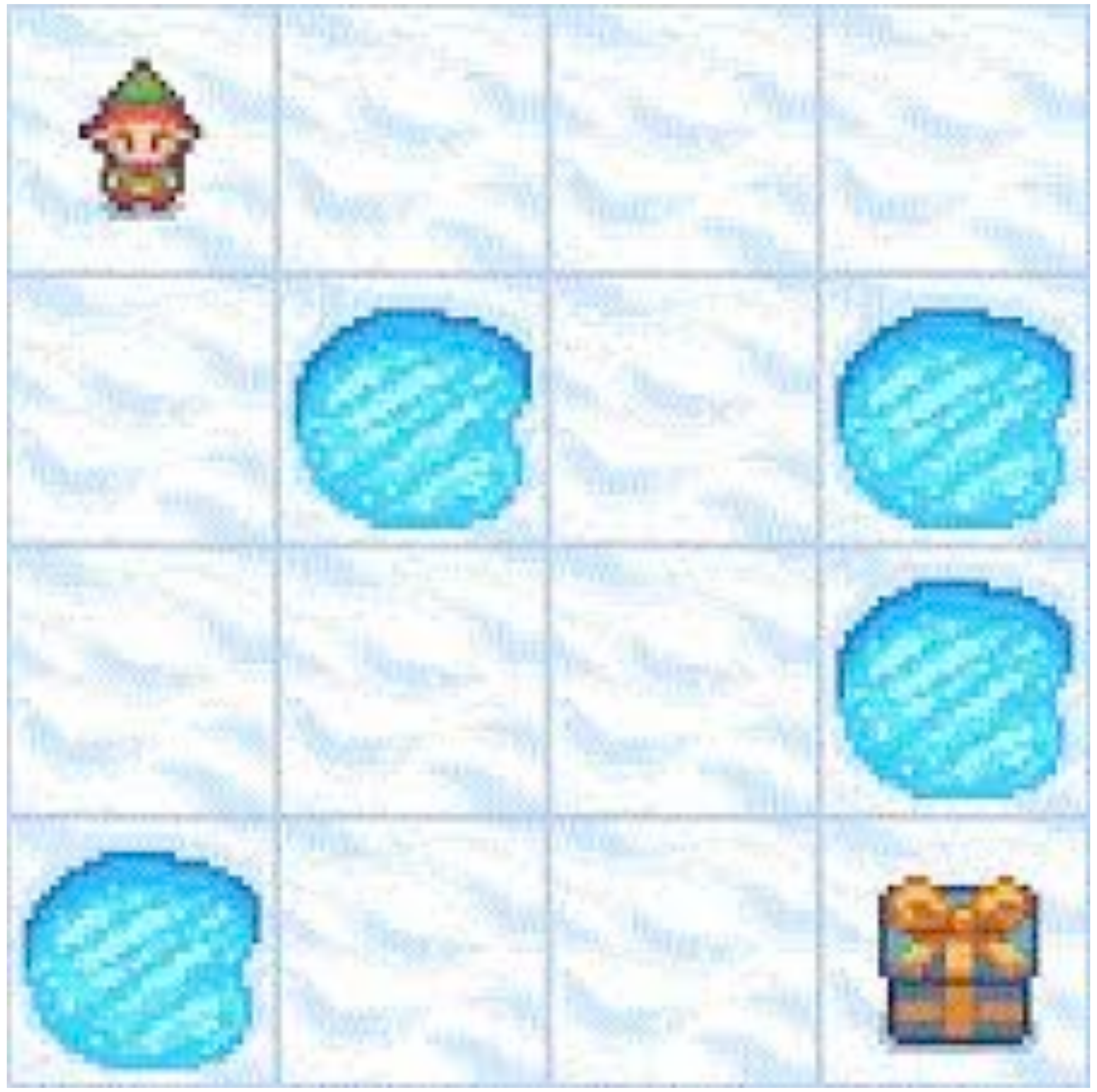
- Solve this system iteratively: $\vec{v}_\pi^{(k+1)} = \overrightarrow{R} + \gamma P \vec{v}_\pi^{(k)}$
- Using Banach's fixed point theorem, the iteration converges to v_π.

Iterative methods

- Suppose probability kernel $p(s, a, s')$ and reward r are known
- State space $\mathcal{S} = \{s_1, \ldots, s_n\}$ is finite
- Given a policy π, we can find v_π.
- To improve policy, select action a at state s, and then follow $v_\pi - q_\pi(s, a)$.
- If $q_\pi(s, a) > v_\pi(s)$ for some $a \in \mathcal{A}$, it means it's better to take action a when we are at state s, which yields a modified policy.

Example



Frozen lake game:

Policy: always going down

$v(15) = 0, \quad q(15,\text{'right'}) = 1$

Modify policy: in state 15, turn right.

Iterative methods

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Requires knowledge of transition probability kernel and reward function

Iterative method scales with $|\mathcal{S}|$

Policy gradient method

How to find a good policy when $\mathscr{A}$ and/or $\mathscr{S}$ are very large/infinite?

And we don't know the transition probability kernel and/or reward function?

Definition (Parametric policy): Let policy be a mapping $\pi_\theta : \mathscr{A} \times \mathscr{S} \to [0,1]$ parametrised by parameters $\theta \in \mathbb{R}^p$.

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Maximize the objective function:

$$J(\theta) = \sum_{s \in \mathscr{S}} v_{\pi_\theta}(s)\mu(s)$$

where μ is the initial state distribution.

Policy gradient method

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Write a gradient ascent on J:

$$\theta_{t+1} = \theta_t + \eta \nabla J(\theta).$$

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$$v_\pi(s) = \mathbb{E}_\pi(G_t \,|\, S_t = s) = \mathbb{E}_\pi \left(\sum_{k \geq 0} \gamma^k r(A_k, S_k) \,|\, S_t = s \right)$$

Policy gradient method

Theorem (Policy gradient theorem). The gradient of the objective $J(\theta)$ with respect to θ is:

$$\nabla J(\theta) = \sum_{s_0 \in \mathcal{S}} \mu(s_0) \sum_{s \in \mathcal{S}} \rho_{\pi_\theta}(s_0, s) \sum_{a \in \mathcal{A}} q_{\pi_\theta}(a, s) \nabla \pi_\theta(a \mid s)$$

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In practice, gradient is approximated using a Monte Carlo estimate of $q_\pi(s, a)$

Policy gradient method

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$$\nabla J(\theta) \propto \mathbb{E}_\pi \left(q_{\pi_\theta}(a, s) \nabla \log \pi_\theta(a \mid s) \right)$$

$$\nabla J(\theta) \propto \mathbb{E}_\pi \left(G_t \nabla \log \pi_\theta(A_t \mid S_t) \right)$$

Policy gradient method

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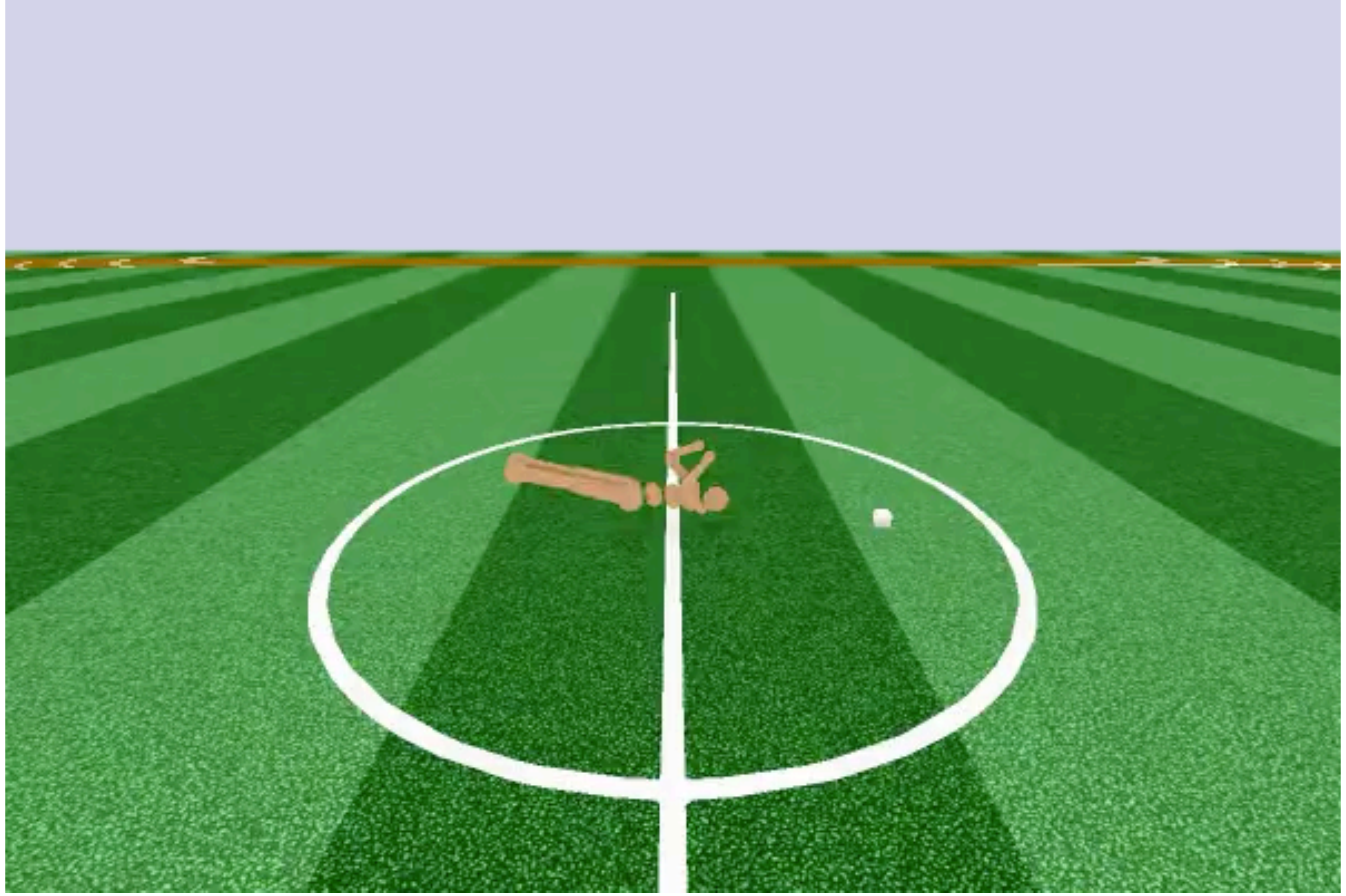
Take policy π, generate a trajectory $S_0, A_0, R_0, S_1, A_1, R_1, \ldots$

For $t = 1,2,...,T$:

Estimate return $G_t := R_t + \gamma R_{t+1} + \ldots$

$\theta = \theta + \eta \gamma^t G_t \nabla \log \pi_\theta(A_t \mid S_t)$

Policy gradient method



Agent learns to get up and seek the pink ball, optimised using Proximal Policy Optimisation (PPO), a type of policy gradient method

Policy gradient method

- Suitable to deal with large state spaces $\mathcal{S}$
- Learns from trajectories
- Suitable for environments where we don't know transition probability kernel
- *Model-free* method (no model of environment)

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- *Model-free* method (no model of environment)

- Despite success, there is not much on the convergence of Policy Gradient methods
- Softmax policies of linear preferences:

$$\pi_\theta(a \,|\, s) = \frac{h_\theta(a, s)}{\sum_{a \in \mathcal{A}} \exp(h_\theta(a, s))}, \; h_\theta(a, s) = \theta \cdot \phi(a, s)$$

- $\nabla J(\theta)$ is L-Lipschitz
- Gradient descent converges to a critical point

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Can we say more about the critical point?

Advertisement II

Matryoshka Policy Gradient (MPG)

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Context:
- Fixed horizon problem
- Entropy regularised objective

Advertisement II

Matryoshka Policy Gradient (MPG)

Context:

- Fixed horizon problem
- Entropy regularised objective
- Proof of global convergence for softmax policies with linear features
- Optimal policy for infinite horizon problem can be approximated arbitrarily well by optimal policy for finite horizon
- Criterion for global optimality for neural networks

https://arxiv.org/abs/2303.12785

RL in numerics

Schwarz et al 2023 — Reinforcement learning based limiter

- State s_t is given by $(u^n_{i-1}, u^n_i, u^n_{i+1})$ (with some normalisation)

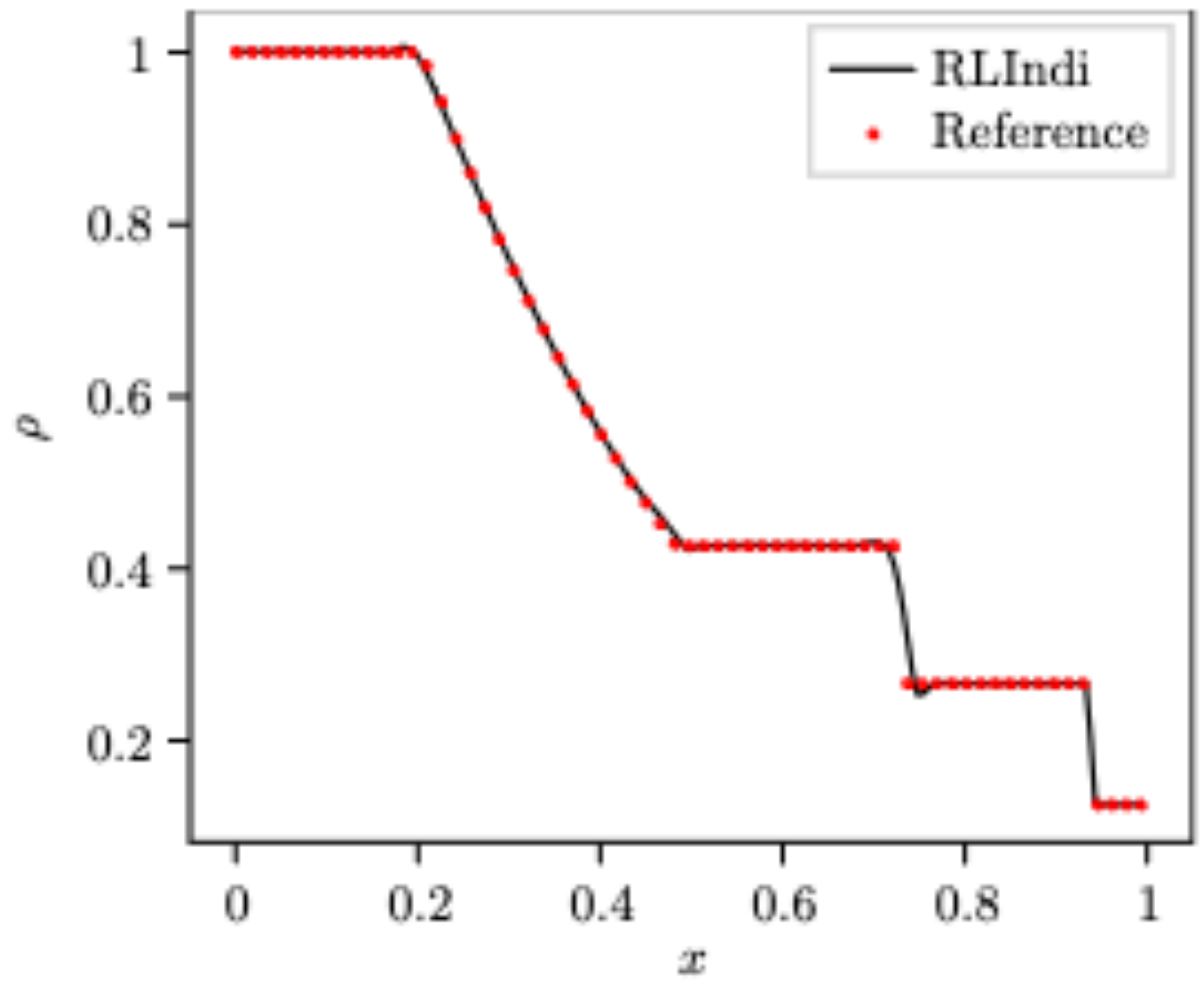
- Action computes the reconstruction slope:

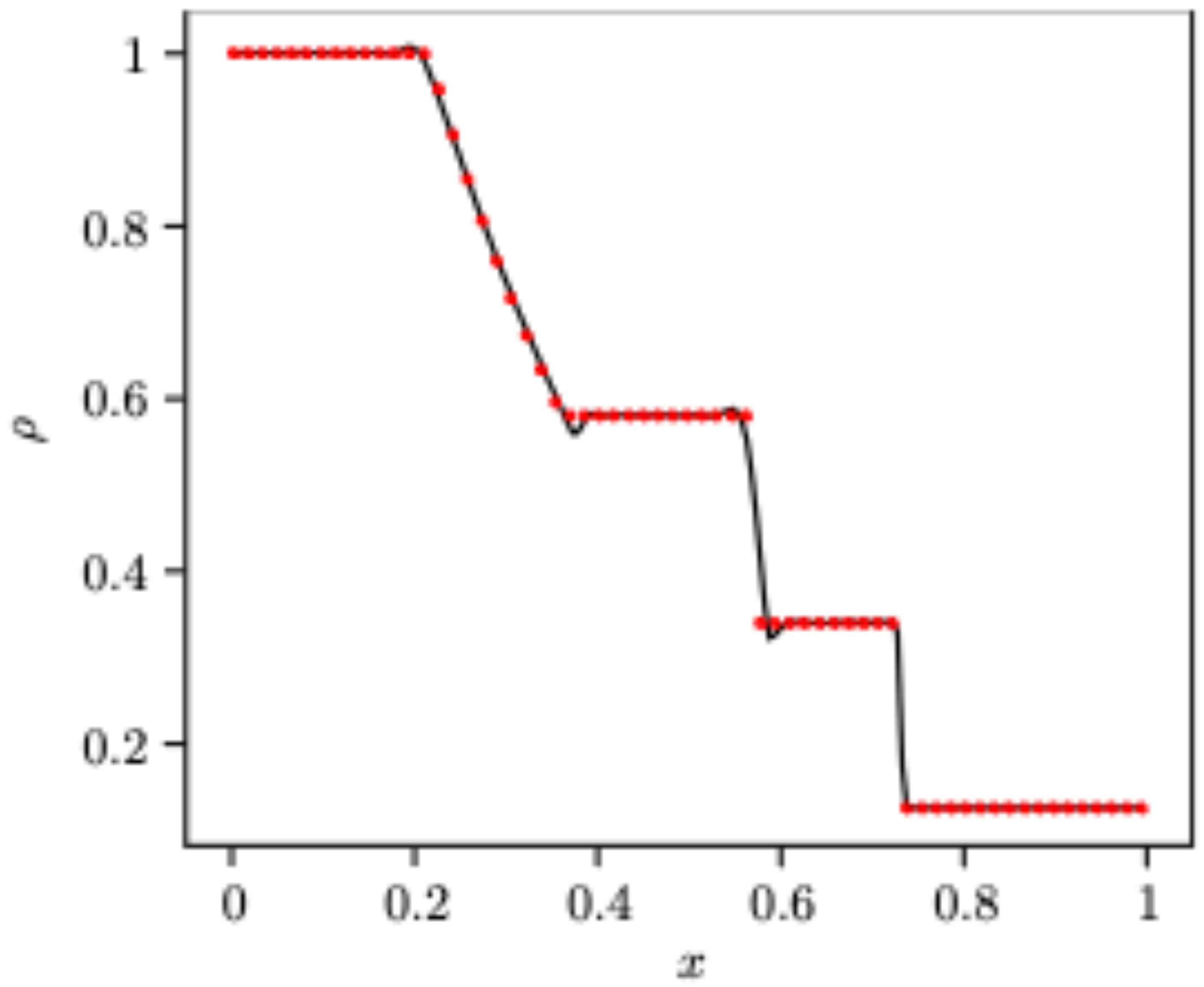
$$\delta u = 0.5(1 - a_i)(u_{i+1} - u_i) + (1 + a_i)(u_i + u_{i-1}), \quad a_i \in [-1,1]$$

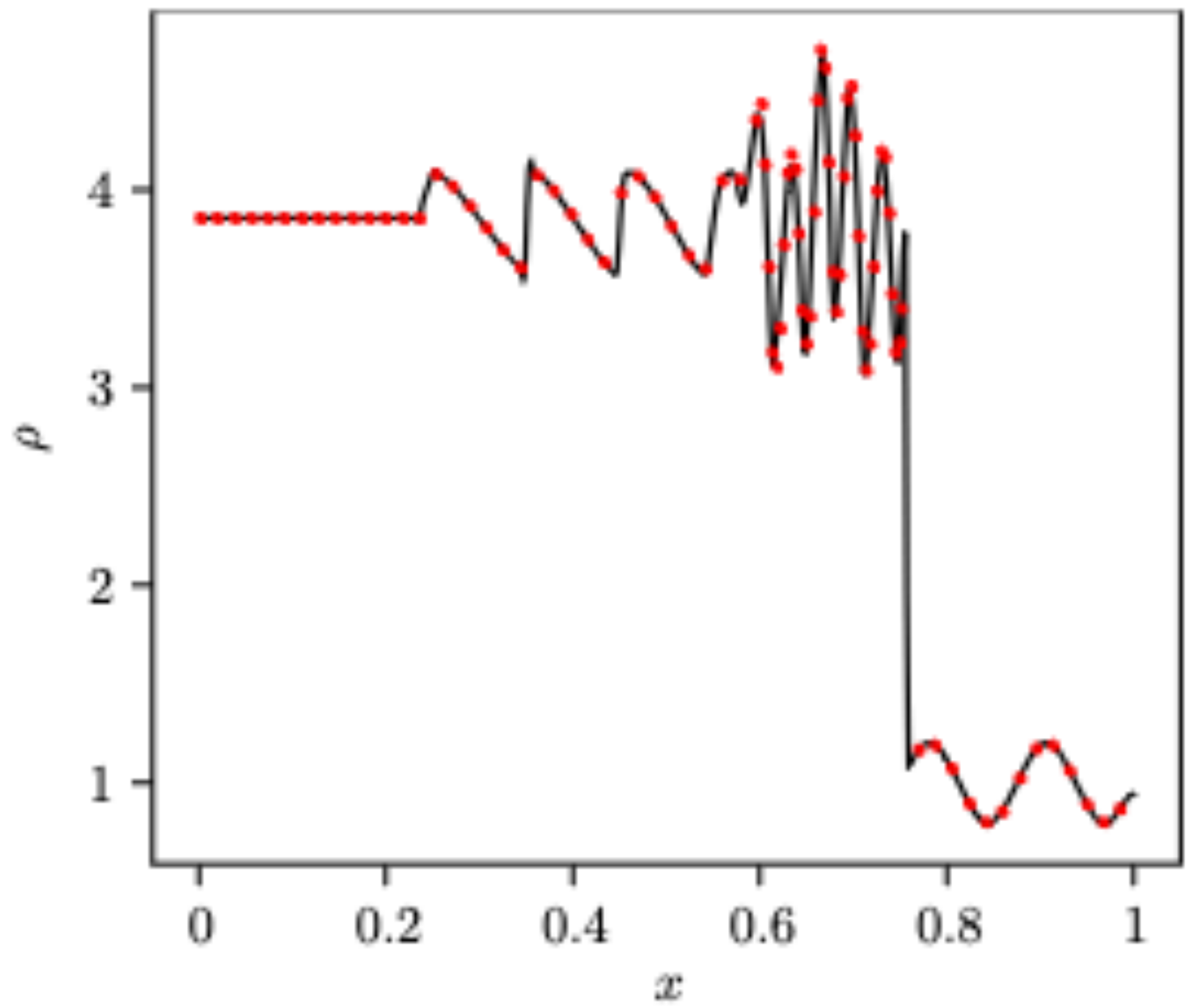
- Reward function $r(s_{t+1}, s_t, a_t)$ measures positivity and most accurate reconstruction before introducing oscillations (oscillator indicator)

- Training using Policy Gradient (Actor-critic)

RL in numerics







Reference N = 5000

RLIndi N = 500

RL in numerics

Kurz et al 2022, Beck et al 2023 — Discretisation-consistent Closure Schemes for Large Eddy Simulation using RL

https://arxiv.org/pdf/2309.06260.pdf

Speculative uses of RL

- Sequential decision making tasks
- Optimal experimental design
- Sequential sampling
- Control problems

DeepMind Alpha-Star plays Starcraft

That's all!

Congratulations, you survived.

Materials: https://github.com/hanveiga/sustech-ml-workshop

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