Reinforcement Learning Introduction

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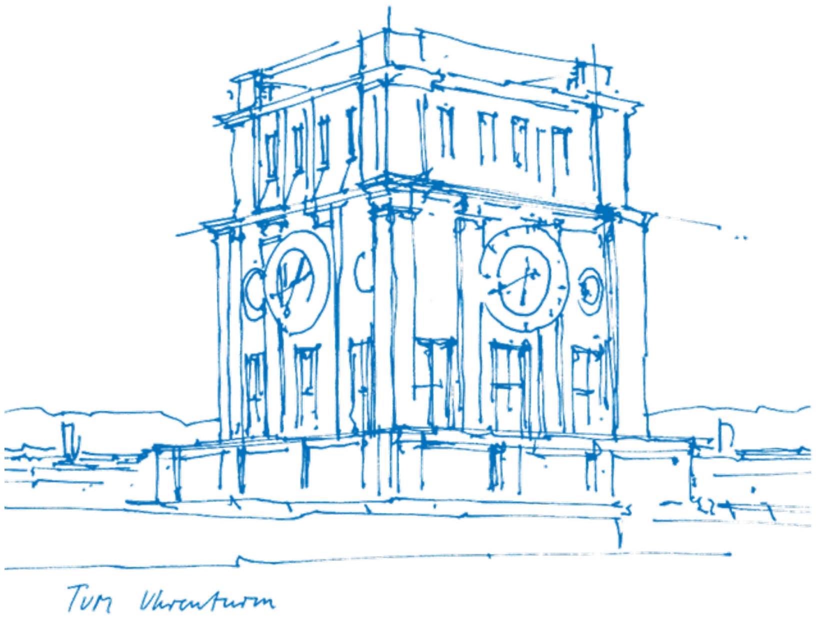
https://github.com/cmendl/reinforcement-learning-course



Outline

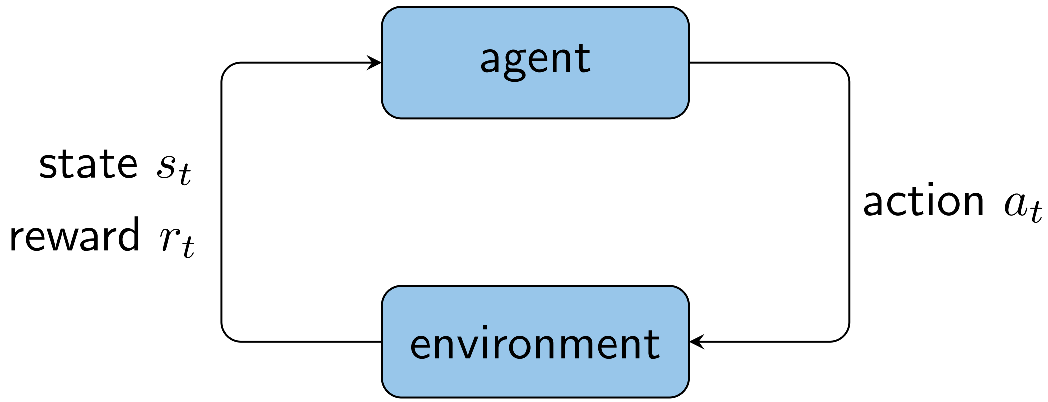
- Introduction and motivation
- Theoretical framework
  - Markov decision processes (MDPs)
  - Iterative “dynamic programming” algorithms
  - Deep reinforcement learning
  - Policy gradients
- Hands-on example: simplified Pac-Man

Introduction and motivation

Motivation

Goal-oriented behavior in a complex, non-deterministic environment

Example autonomous driving: steer vehicle safely from A to B, "environment" consists of other vehicles, bikes, pedestrians, street signs, . . .



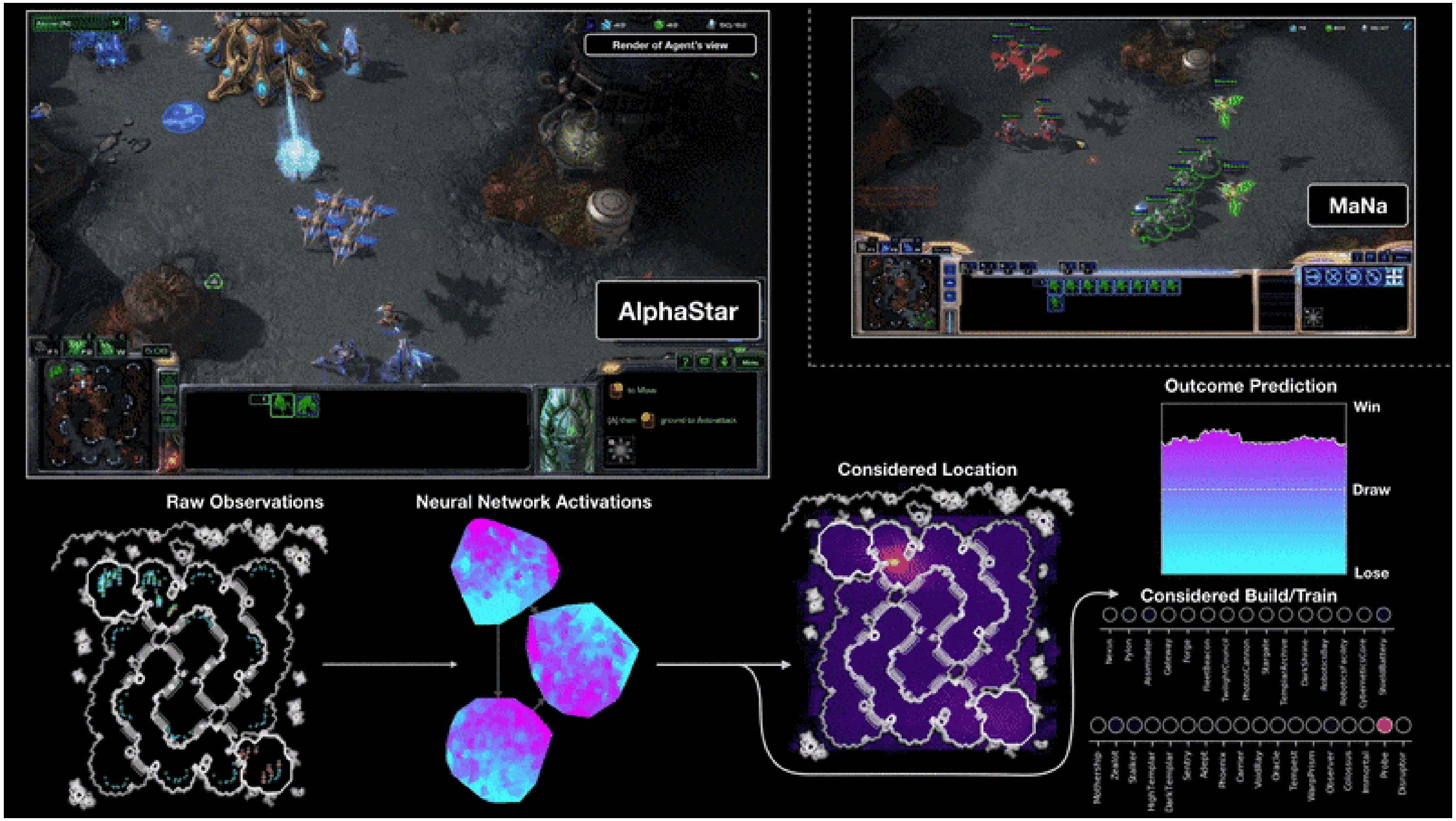
S. Russell and P. Norvig. *Artificial Intelligence: A Modern Approach (3rd edition).* Prentice Hall (2009)

R. S. Sutton and A. G. Barto. *Reinforcement Learning: An Introduction (2nd edition).* MIT Press (2018)

Deepmind's AlphaGo

Deepmind's Alphastar

Reinforcement learning to train an agent to play StarCraft II

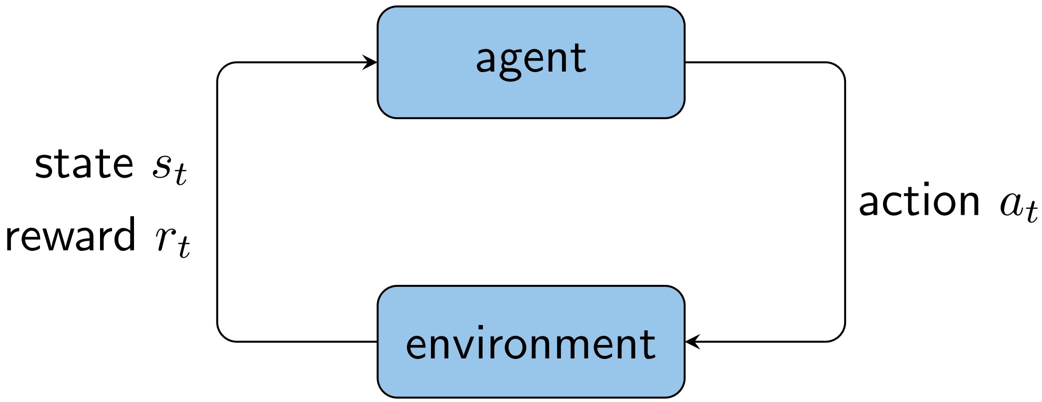


https://deepmind.com/blog/article/alphastar-mastering-real-time-strategy-game-starcraft-ii

Theoretical framework

MDPs: agent and environment

Formal description: an agent interacts with an environment



State of agent and environment at time points $t = 0, 1, 2, \ldots$ denoted $s_t \in S$

Agent chooses an **action** $a_t \in A \rightsquigarrow$ system transitions to next state $s_{t+1} \in S$ with transition probability

$$\mathbb{P}(s_{t+1} | s_t, a_t)$$

Markov property: probability does not explicitly depend on previous time points

MDPs: reward and return

At each time point the agent receives a **reward** (can be positive, zero or negative):

$$r_t = R(s_t)$$

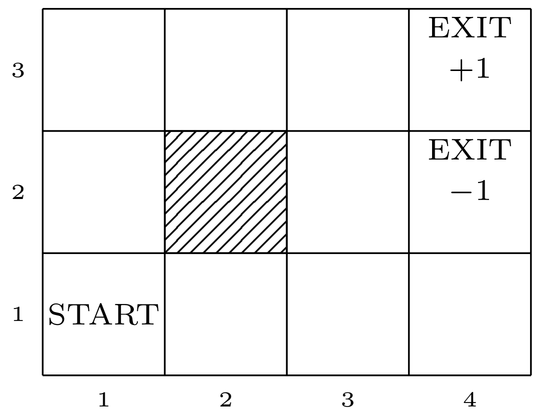
Goal: maximize **return**: cumulative discounted reward

$$\sum_{t=0}^{\infty} \gamma^t R(s_t), \quad 0 < \gamma \leq 1$$

with γ^t the discount factor

Model example: grid world

4×3 grid world with one player (hatched field $(2, 2)$ is inaccessible):



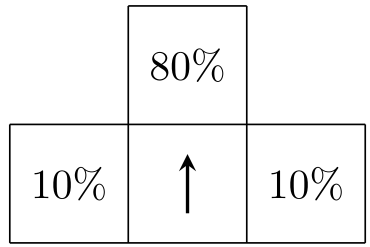
s_t: current actor (player) position

Possible actions: $\uparrow$, $\downarrow$, $\leftarrow$, $\rightarrow$: “try to move in corresponding direction by one field”

S. Russell and P. Norvig. *Artificial Intelligence: A Modern Approach (3rd ed).* (2009)

Model example: grid world, continued

Transition probability:



Formally:

$$
\begin{aligned}
\mathbb{P}\left(s_{t+1} = s_t + \left(\begin{smallmatrix}0\\1\end{smallmatrix}\right) \middle| s_t, a_t = \uparrow\right) &= 0.8,\\
\mathbb{P}\left(s_{t+1} = s_t + \left(\begin{smallmatrix}1\\0\end{smallmatrix}\right) \middle| s_t, a_t = \uparrow\right) &= 0.1,\\
\mathbb{P}\left(s_{t+1} = s_t + \left(\begin{smallmatrix}-1\\0\end{smallmatrix}\right) \middle| s_t, a_t = \uparrow\right) &= 0.1
\end{aligned}
$$

Analogously for $\downarrow$, $\leftarrow$, $\rightarrow$

Reward: $+1$ for exit field $(4, 3)$, -1 for exit field $(4, 2)$, -0.04 for any other field (agent wants to reach exit as fast as possible)

S. Russell and P. Norvig. *Artificial Intelligence: A Modern Approach (3rd ed).* (2009)

MDPs: policy function and utility

How do we specify possible solutions?

Actions of agent specified by **policy** $\pi : \mathrm{S} \to \mathrm{A}$:

$$a_t = \pi(s_t)$$

Due to Markov property: only dependency on s_t required (instead of full history $s_0, s_1, \ldots, s_t$)

MDPs: policy function and utility

How do we specify possible solutions?

Actions of agent specified by **policy** $\pi : S \to A$:

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"Quality" of π quantified by *expected return*, denoted **utility** or **value function**:

$$U^\pi(s_0) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t) \middle| \pi\right],$$

$s_1, s_2, \dots$ now regarded as random variables

Notation $\mathbb{E}[\dots|\pi]$: use policy π for choosing actions a_t

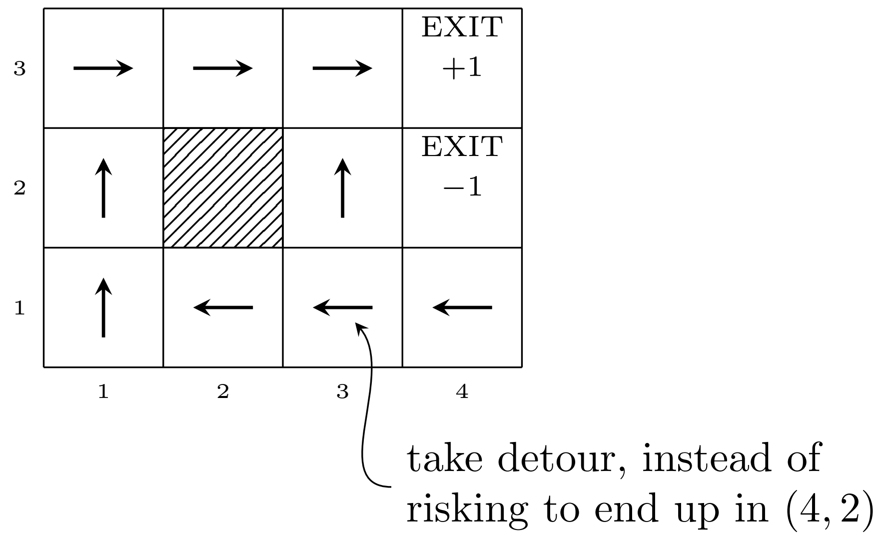
Optimal policy and utility

$$\pi^* = \underset{\pi}{\operatorname{argmax}}\, U^\pi(s_0)$$

π^* does not depend on s_0! Justification: self-similar form:

$$\mathbb{E}\left[\sum_{t'=t}^{\infty} \gamma^{t'} R(s_{t'}) \middle| \pi, s_t = \tilde{s}_0\right] = \gamma^t\, \mathbb{E}\left[\sum_{\Delta t=0}^{\infty} \gamma^{\Delta t} R(s_{t+\Delta t}) \middle| \pi, s_t = \tilde{s}_0\right] = \gamma^t\, U^\pi(\tilde{s}_0).$$

Example (for $\gamma = 1$):



Optimal policy and utility, continued

Corresponding value function for optimal policy: $U = U^{\pi^*}$ (omit superscript π^*)

3	0.812	0.868	0.918	EXIT +1
2	0.762		0.660	EXIT −1
1	0.705	0.655	0.611	0.388
	1	2	3	4

Conversely, can obtain π^* from U:

$$\pi^*(s) = \underset{a \in A}{\operatorname{argmax}} \sum_{s'} \mathbb{P}(s'|s,a) U(s')$$

"Choose action which maximizes the expected return."

Bellman equation for U, value iteration algorithm

Intuition: expected utility of a state s is equal to the instantaneous reward and the expected utility of the next state, assuming optimal behavior of the agent.

$\rightsquigarrow$ *Bellman equation* for the value function:

$$U(s) = R(s) + \gamma \max_{a \in \mathrm{A}} \sum_{s' \in \mathrm{S}} \mathbb{P}(s'|s,a) U(s') \quad \forall s \in \mathrm{S}$$

(uniquely solvable for $\gamma < 1$)

Corresponding **value iteration algorithm**:

$$U_{i+1}(s) = R(s) + \gamma \max_{a \in \mathrm{A}} \sum_{s' \in \mathrm{S}} \mathbb{P}(s'|s,a) U_i(s') \quad \forall s \in \mathrm{S}, \quad i = 0, 1, \dots$$

Policy iteration algorithm

Idea: "best" policy according to U_i, i.e.,

$$\pi_i(s) = \operatorname*{argmax}_{a \in \mathsf{A}} \sum_{s'} \mathbb{P}(s'|s,a) U_i(s'),$$

might already agree with optimal policy π^*, even if U_i still deviates from U^{π^*}

$\rightsquigarrow$ **policy iteration algorithm**:

Require: initial policy π_0 (e.g., randomly selected)

for $i \leftarrow 0, 1, 2, \dots$ **do**

(a) policy evaluation: compute expected utility, if agent follows policy π_i:

$$U_i(s) = U^{\pi_i}(s) \quad \forall s \in \mathsf{S}$$

by solving linear system

$$U_i(s) = R(s) + \gamma \sum_{s'} \mathbb{P}(s'|s,\pi_i(s)) U_i(s')$$

(b) policy improvement: use U_i to derive a new policy π_{i+1}:

$$\pi_{i+1}(s) = \operatorname*{argmax}_{a \in \mathsf{A}} \sum_{s'} \mathbb{P}(s'|s,a) U_i(s') \quad \forall s \in \mathsf{S}$$

Stop if optimal policy has been found, i.e., if $\pi_{i+1} = \pi_i$ or (equivalently) $U_{i+1} = U_i$ (in this case U_i is unique fixed point of value iteration)

Q-value function

So far: value function $U^\pi(s)$ for state s

Q-value function: evaluate state-action tuple (s, a):

$$Q^\pi(s, a) := \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t) \middle| s_0 = s, a_0 = a, \pi\right]$$

"expected utility, if agent in state s chooses action a and then follows policy π"

Optimal Q-value function for optimal policy:

$$Q^*(s, a) = \max_\pi Q^\pi(s, a)$$

Advantage: optimal value function U and optimal policy π^* can be directly obtained from Q^*:

$$U(s) = \max_a Q^*(s, a),$$
$$\pi^*(s) = \operatorname{argmax}_a Q^*(s, a)$$

No knowledge of transition probability $\mathbb{P}(s'|s, a)$ required, "**model free**"

Bellman equation for Q-value function, iteration

Similar to Bellman equation for U:

$$\begin{aligned} Q^*(s,a) &= R(s) + \gamma \sum_{s' \in \mathrm{S}} \mathbb{P}(s'|s,a) \max_{a' \in \mathrm{A}} Q^*(s',a') \\ &= \mathbb{E}_{s'}\left[R(s) + \gamma \max_{a' \in \mathrm{A}} Q^*(s',a') \middle| s,a \right], \end{aligned}$$

with $\mathbb{E}_{s'}[\dots|s,a]$ the expectation value with respect to random variable $s' \sim \mathbb{P}(\cdot|s,a)$

Corresponding Q-value iteration:

$$Q_{i+1}(s,a) = R(s) + \gamma \sum_{s' \in \mathrm{S}} \mathbb{P}(s'|s,a) \max_{a' \in \mathrm{A}} Q_i(s',a') \quad \forall s \in \mathrm{S}, a \in \mathrm{A}, \quad i = 0,1,\dots$$

Classical Q-learning algorithm

So far: iteration $Q_i \to Q_{i+1}$, but instead of (unknown) transition probability $\mathbb{P}(s'|s,a)$, use observed transition $s_t \to s_{t+1}$ based on simulation of environment

Update Q-value function at $(s,a) = (s_t, a_t)$ (otherwise unchanged):

$$Q_{i+1}(s_t, a_t) = (1 - \eta_i) Q_i(s_t, a_t) + \eta_i \left(R(s_t) + \gamma \max_{a'} Q_i(s_{t+1}, a') \right)$$

with learning rate η_i $(0 < \eta_i < 1)$

Watkins and Dayan prove convergence $Q_i \xrightarrow{i \to \infty} Q^*$ under mild assumptions, in the limit of infinite number of episodes, such that every tuple (s,a) appears infinitely often.

C. J. Watkins, P. Dayan (1992)

Reinforcement learning concepts

Instead of working with explicit transition probabilities, repeat many simulations of the systems; agent "learns" during the simulations

Trade-off between "**exploration**" and "**exploitation**": try action that hasn't been used or rarely used (even if not optimal) to gain experience, or choose action that is likely to maximize the benefit?

Concepts:

- **on-policy training**: the policy to be optimized is also used to select actions during simulations, i.e., to generate training samples
- **off-policy training**: the policy to be optimized is usually different from the policy used to select actions during the simulations

Opportunities for "exploration" in both cases:

- on-policy: use probability distribution, transition to deterministic action in the course of training (i.e., a single action has probability 1)
- off-policy: exploration using the policy for choosing actions during the simulation; often used: ε-**greedy** strategy (random action with probability ε)

Deep reinforcement learning overview

Issues of iterative “dynamic programming” algorithms considered so far:

1. Requires storing entries $U(s)$, $\pi(s)$ or $Q(s, a)$ for all possible state $s \in \mathrm{S}$ (and actions $a \in \mathrm{A}$), only feasible for relatively small state space
   Classical board games:
   $$|\mathrm{S}| \approx b^d,$$
   with
   b: mean number of allowed moves for a given board position
   d: depth, i.e., typical total number of moves per game
   - chess: $b \approx 35$, $d \approx 80$
   - Go: $b \approx 250$, $d \approx 150$

   $\rightsquigarrow$ cannot enumerate all possible board positions
2. Requires knowledge of transition probability $\mathbb{P}(s'|s, a)$, but in practice often unknown or hard to estimate (e.g., autonomous driving)
   Instead: conceptual goal of reinforcement learning: agent should choose sensible actions in (initially unknown) environment

Ansatz **deep reinforcement learning**: approximate U, π or Q by neuronal network; “deep” refers to network depth (number of layers)

Deep Q-learning (now mostly historical relevance)

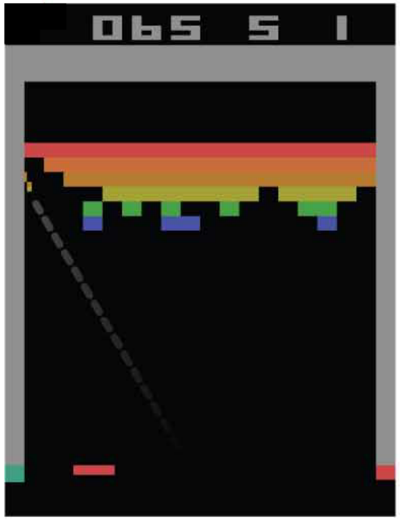
Goal: algorithms to (approximately) solve Bellmann equation

$$Q^*(s,a) = \mathbb{E}_{s'}\left[R(s) + \gamma \max_{a' \in A} Q^*(s',a') \middle| s,a\right]$$

Ansatz:

$$Q^*(s,a) \approx Q(s,a;\theta),$$

with $Q(s,a;\theta)$ a neural network (Q network) with parameters θ (weights and bias vectors); iterative optimization: $\theta_{i-1} \to \theta_i$, $i = 1, 2, \dots$



V. Mnih, K. Kavukcuoglu, D. Silver, ..., D. Hassabis. *Human-level control through deep reinforcement learning.* Nature (2015)

Policy gradient methods

Idea: compute optimal policy π^* : S $\to$ A *directly*, i.e., in general without computing value function $U(s)$ or Q-value function $Q(s, a)$ (model free, works for high-dimensional state spaces)

Ansatz for policy function: π_θ, with to-be optimized parameters $\theta \in \mathbb{R}^m$, e.g., weights and bias vectors of an ANN

Use (as before) the expected utility to evaluate a policy function, with a default initial state $\hat{s}_0$:

$$J(\theta) := U^{\pi_\theta}(\hat{s}_0) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t R(s_t) \middle| s_0 = \hat{s}_0, \pi_\theta\right]$$

Goal: $\theta^* = \operatorname{argmax}_\theta J(\theta)$

Policy gradient theorem

In the following: policy function specifies action probabilities: $\pi(a|s)$ (instead of $a = \pi(s)$)

$\rightsquigarrow$ **policy gradient theorem** (see supplementary slides for derivation):

$$\nabla J(\theta) = \mathbb{E}\left[\sum_{t=0}^{\infty}\left(\sum_{t'=t}^{\infty}\gamma^{t'}R(s_{t'})\right)\nabla_\theta \log \pi_\theta(a_t|s_t)\,\middle|\,\pi_\theta\right]$$

Interpretation: to optimize $J(\theta)$ via gradient descent: if remaining “cumulative discounted reward” $\sum_{t'=t}^{\infty}\gamma^{t'}R(s_{t'})$ starting from t is positive, then increase probability $\pi(a_t|s_t)$ of chosen actions

REINFORCE algorithm

Directly based on formula for $\nabla J(\theta)$: gradient descent with learning rate η

```
1: Chose initial parameters θ
2: for episode ← 0, 1, ... do
3:     Run simulation using policy π_θ, obtain trajectory (s_0, a_0, r_0, ..., s_T, a_T, r_T)
4:     for t ← 0, 1, ..., T do
5:         G_t ← Σ_{t'=t}^{T} γ^{t'-t} r_{t'}
6:         θ ← θ + η γ^t G_t ∇_θ log π_θ(a_t|s_t)                ▷ gradient step
```

1: Chose initial parameters θ
2: **for** episode $\leftarrow 0, 1, \dots$ **do**
3: Run simulation using policy π_θ, obtain trajectory $(s_0, a_0, r_0, \dots, s_T, a_T, r_T)$
4: **for** $t \leftarrow 0, 1, \dots, T$ **do**
5: $G_t \leftarrow \sum_{t'=t}^{T} \gamma^{t'-t} r_{t'}$
6: $\theta \leftarrow \theta + \eta\, \gamma^t G_t \nabla_\theta \log \pi_\theta(a_t|s_t)$ $\triangleright$ gradient step

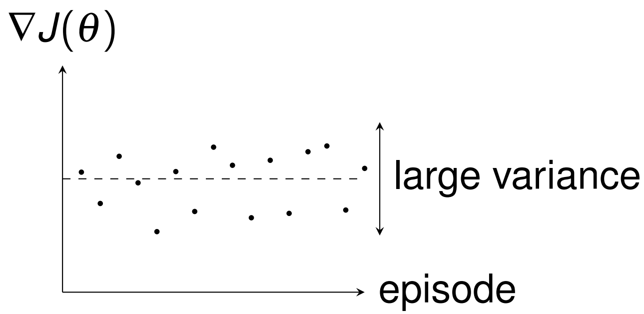
Remarks:

- Variants of the algorithm without factor γ^t in line 6
- Can apply gradient only “a posteriori”, i.e., after completing a game

R. J. Williams. *Simple statistical gradient-following algorithms for connectionist reinforcement learning* (1992)

Actor critic method

Motivation: reduce variance when estimating $\nabla J(\theta)$ via sampling



Idea: in derivation of the policy gradient theorem:

$$\nabla J(\theta) = \sum_{t=0}^{\infty} \sum_{s \in S} \mathbb{P}_\theta(\hat{s}_0 \to s \text{ in } t \text{ steps}) \gamma^t \sum_a Q^{\pi_\theta}(s,a) \nabla_\theta \pi_\theta(a|s) :$$

replace $\sum_a Q^{\pi_\theta}(s,a)\nabla_\theta \pi_\theta(a|s)$ by $\sum_a \left(Q^{\pi_\theta}(s,a) - b(s)\right) \nabla_\theta \pi_\theta(a|s)$ using an arbitrary "baseline"-function $b : S \to \mathbb{R}$: (only needs to be independent of parameters θ)

Overall value remains unchanged, since

$$\sum_a b(s) \nabla_\theta \pi_\theta(a|s) = b(s) \nabla_\theta \underbrace{\sum_a \pi_\theta(a|s)}_{=1} = 0$$

Actor critic method, continued

Leads to generalized formula for $\nabla J(\theta)$:

$$\nabla J(\theta) = \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \left(\left(\sum_{t'=t}^{\infty} \gamma^{t'-t} R(s_{t'})\right) - b(s_t)\right) \nabla_\theta \log \pi_\theta(a_t|s_t) \middle| \pi_\theta\right]$$

$$= \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \Big(Q^{\pi_\theta}(s_t, a_t) - b(s_t)\Big) \nabla_\theta \log \pi_\theta(a_t|s_t) \middle| \pi_\theta\right]$$

$\sum_{t'=t}^{\infty} \gamma^{t'-t} R(s_{t'}) - b(s_t)$: deviation of observed "cumulative reward" from baseline $\rightsquigarrow$ within gradient step: increase or decrease probability of chosen action depending on whether *deviation* positive or negative

Typical choice of $b(s)$: value function $U_\phi(s)$ with parameters ϕ (independent of θ)

Deviation denoted **advantage**:

$$A_t = Q^{\pi_\theta}(s_t, a_t) - U_\phi(s_t)$$

Actor critic method, continued

$\rightsquigarrow$ **actor critic method**:

- actor: policy function π_θ
- critic: evaluation of chosen actions based on A_t

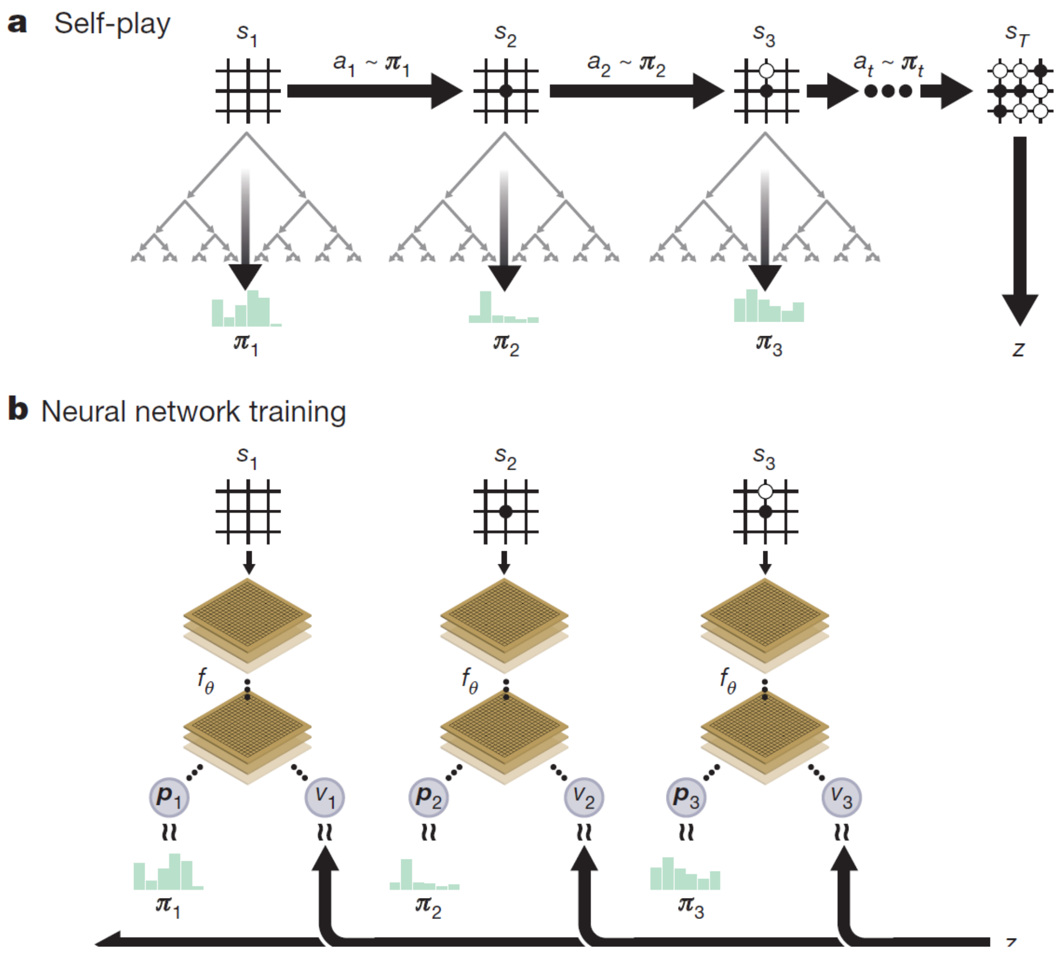
Parameters θ and ϕ are simultaneously optimized

Pseudo code (given learning rate η and $\tilde{\eta}$):

1: Chose initial parameters θ and ϕ
2: **for** episode $\leftarrow 0, 1, \dots$ **do**
3: Run simulation using policy π_θ, obtain trajectory $(s_0, a_0, r_0, \dots, s_T, a_T, r_T)$
4: **for** $t \leftarrow 0, 1, \dots, T$ **do**
5: $G_t \leftarrow \sum_{t'=t}^{T} \gamma^{t'-t} r_{t'}$
6: $A_t \leftarrow G_t - U_\phi(s_t)$
7: $\theta \leftarrow \theta + \eta\, \gamma^t A_t \nabla_\theta \log \pi_\theta(a_t|s_t)$ $\triangleright$ gradient step for θ
8: $\phi \leftarrow \phi + \tilde{\eta} A_t \nabla_\phi U_\phi(s_t)$ $\triangleright$ gradient step for ϕ

Remarks: typical asynchronous variants with multiple agents running in parallel cf. A3C (“asynchronous advantage actor critic”)

Example: AlphaGo Zero



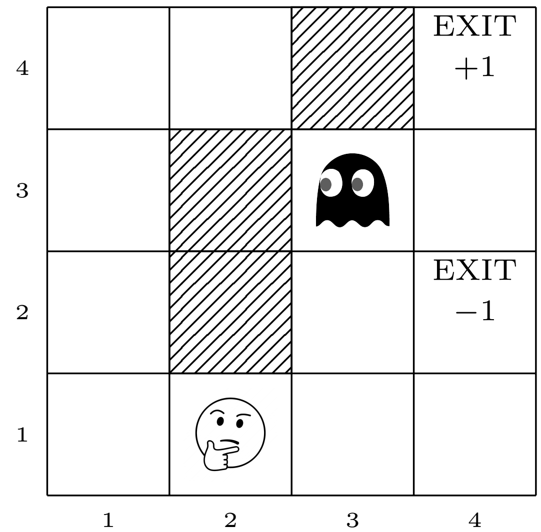
D. Silver, . . . , D. Hassabis. *Mastering the game of Go without human knowledge.* Nature (2017)

Hands-on example: simplified Pac-Man

https://github.com/cmendl/reinforcement-learning-course, subfolder *code/*

Code structure

https://github.com/cmendl/reinforcement-learning-course, subfolder *code/*



- Iterative "dynamic programming" algorithms in *mdp.py*
- Environment: plain maze or maze with ghost in *env.py*,
  geometry specified in text files (like *maze_geometry.txt*)
- Policy gradient algorithm in *pg.py*, corresponding (simple two-layer) network defined in *policy_net.py*
- Demos as Jupyter notebooks

References

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Supplementary slides

Derivation of the policy gradient theorem

Here generalization to probabilistic policy function: $\pi(a|s)$ (instead of $a = \pi(s)$)

Note that

$$U^\pi(s) = \sum_{a \in \mathrm{A}} \pi(a|s) Q^\pi(s,a) \quad \forall s \in \mathrm{S}$$

and

$$Q^\pi(s,a) = R(s) + \gamma \sum_{s'} \mathbb{P}(s'|s,a) U^\pi(s') \quad \forall s \in \mathrm{S}, a \in \mathrm{A}.$$

Therefore, combined with product rule:

$$\begin{aligned}
\nabla_\theta U^{\pi_\theta}(s) &= \sum_{a \in \mathrm{A}} \left(\nabla_\theta \pi_\theta(a|s) Q^{\pi_\theta}(s,a) + \pi_\theta(a|s) \nabla_\theta Q^{\pi_\theta}(s,a) \right) \\
&= \sum_a \nabla_\theta \pi_\theta(a|s) Q^{\pi_\theta}(s,a) + \gamma \sum_{s',a} \pi_\theta(a|s) \mathbb{P}(s'|s,a) \nabla_\theta U^{\pi_\theta}(s') \\
&= \sum_a \nabla_\theta \pi_\theta(a|s) Q^{\pi_\theta}(s,a) + \gamma \sum_{s'} \mathbb{P}_\theta(s'|s) \nabla_\theta U^{\pi_\theta}(s'),
\end{aligned}$$

with

$$\mathbb{P}_\theta(s'|s) = \sum_a \pi_\theta(a|s) \mathbb{P}(s'|s,a)$$

the transition probability $s \to s'$ following policy π_θ.

Derivation of the policy gradient theorem, continued

Equation for $\nabla_\theta U^{\pi_\theta}$ yields recursive relation; repeated application $\rightsquigarrow$

$$\nabla J(\theta) = \nabla_\theta U^{\pi_\theta}(\hat{s}_0) = \sum_{t=0}^{\infty} \sum_{s \in \mathrm{S}} \mathbb{P}_\theta(\hat{s}_0 \to s \text{ in } t \text{ steps}) \gamma^t \sum_a \nabla_\theta \pi_\theta(a|s) Q^{\pi_\theta}(s,a)$$

Rewrite last term:

$$\begin{aligned}
\gamma^t \sum_a \nabla_\theta \pi_\theta(a|s) Q^{\pi_\theta}(s,a) &= \gamma^t \sum_a \pi_\theta(a|s) Q^{\pi_\theta}(s,a) \nabla_\theta \log \pi_\theta(a|s) \\
&= \mathbb{E}_a\left[\gamma^t Q^{\pi_\theta}(s,a) \nabla_\theta \log \pi_\theta(a|s) \middle| \pi_\theta\right] \\
&= \mathbb{E}\left[\sum_{t'=t}^{\infty} \gamma^{t'} R(s_{t'}) \nabla_\theta \log \pi_\theta(a_t|s_t) \middle| s_t = s, \pi_\theta\right],
\end{aligned}$$

with the expectation value referring to trajectories $(s_t, a_t, s_{t+1}, a_{t+1}, \dots)$ starting from time t.

In summary:

$$\nabla J(\theta) = \mathbb{E}\left[\sum_{t=0}^{\infty} \left(\sum_{t'=t}^{\infty} \gamma^{t'} R(s_{t'})\right) \nabla_\theta \log \pi_\theta(a_t|s_t) \middle| \pi_\theta\right]$$