# (more on) Reinforcement Learning

#### Winter School on Quantitative Systems Biology

19<sup>th</sup> November 2018

David Hofmann david.hofmann@emory.edu



## Complex Environment



S - Set of states

 $\mathcal{A}$  - Set of actions

p(S'|S,A) - Transition probability

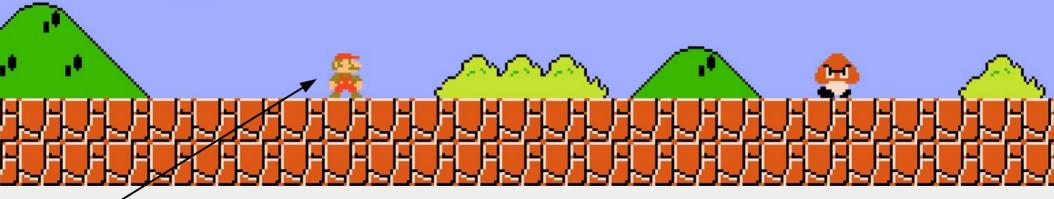
p(R|S,S') = Reward probability





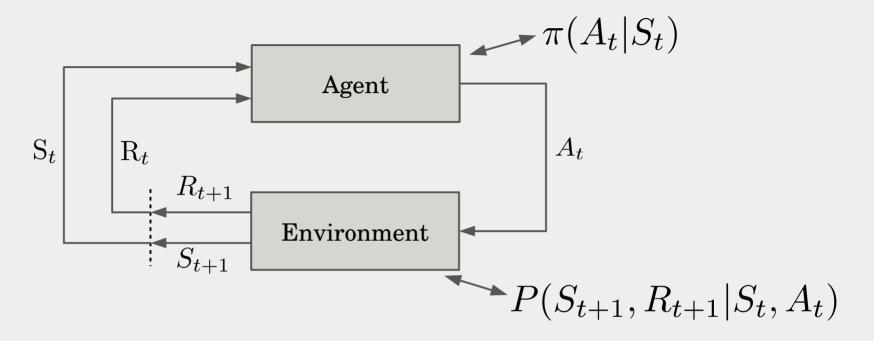






$$\pi(A|S)$$
 - Policy

#### Markov Decision Processes (MDP)



- An MDP is a tuple  $\mathcal{M} = (\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathcal{P})$
- Actions lead to state transitions
- Rewards are released on state transitions

## The simple RL problems

No actions:

No states:

• Classical conditioning (Markov Reward Process)

• Bandits!

- Multiple actions  $a \in \mathcal{A}$
- Each action a leads to a reward r with probability  $P(R_t|A_t)$ 
  - → Arguably simplest RL problem (it is state-less)



One-armed bandit: 1899 "Liberty Bell" machine [Wikimedia Commons]

#### **Action Selection**

#### Which of the *k* arms should I play?

Compute value of arms:

• Simplest algorithm: "Averaging"

$$Q_t(a) = \frac{R_1^a + \ldots + R_{N_t(a)-1}^a}{N_t(a) - 1}$$

• Iterative algorithm:

$$Q_{t+1}(a) = Q_t(a) + \frac{1}{N_t(a)} [R_{N_t(a)}^a - Q_t(a)]$$

Select an action:

- Greedy:  $a_t = \operatorname{argmax}_a Q_t(a)$
- Purely exploitative, no exploration

## Exploration vs. Exploitation

Epsilon greedy

$$a_t = \begin{cases} \operatorname{argmax}_a Q_t(a), & \text{with probability } 1 - \epsilon \\ \operatorname{random} a, & \text{with probability } \epsilon \end{cases}$$

- Usually the greedy action is chosen
- But with probability  $\epsilon$  choose a random action
- → Stochastic exploration

## Exploration vs. Exploitation

Upper Confidence Bound

$$a_t = \operatorname{argmax}_a \left( Q_t(a) + c \sqrt{\frac{\ln(t)}{N_t(a)}} \right)$$

- On top of quality of action uncertainty is also
- → Deterministic exploration

## Exploration vs. Exploitation

• Bayesian approach

$$p_{\text{posterior}} = \frac{p_{\text{likelihood}}}{p_{\text{evidence}}} p_{\text{prior}}$$

$$p_t(Q(a)|\mathcal{D}_t) = \frac{p(r_t|Q(a))}{p(r_t)} p_t(Q(a)|\mathcal{D}_{t^-})$$

• Thompson Sampling: Sample from the posterior distribution.

$$Q_t(a) \sim p(Q(a)|\mathcal{D}_t)$$
$$a_t = \operatorname{argmax}_a Q_t(a)$$

•  $\rightarrow$  Stochastic exploration

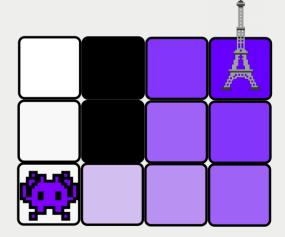
## **Bellman Equation**

- Extend to discrete, finite state space
- Table values of state action pairs

$$Q_{\pi}(s, a) = \mathcal{E}_{\pi} \left( \sum_{t=0}^{\infty} \gamma^{t} R_{t+1} | S_{0} = s, A_{0} = a \right)$$

$$= \sum_{\{a_{t+1}, s_{t+1}, r_{t+1}\}} p(\{R_{t+1}, S_{t+1}, A_{t+1}\} | S_{0} = s, A_{0} = a) \sum_{t=0}^{\infty} \gamma^{t} R_{t+1}$$

$$Q_{\pi}(s, a) = E_{\pi} (R_1 | S_0 = s, A_0 = a) + E_{\pi} \left( \sum_{t=1}^{\infty} \gamma^t R_{t+1} | S_1 = s', A_1 = a' \right)$$

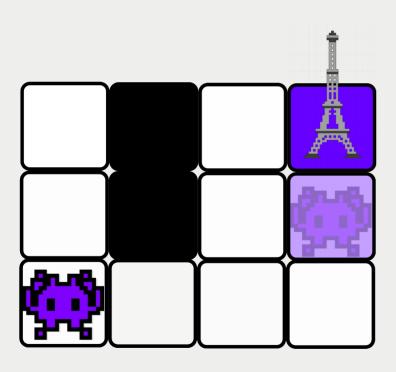


$$Q_{\pi}(s, a) = E_{\pi}(R_1|S_0 = s, A_0 = a) + \gamma E_{\pi}Q_{\pi}(s', a')$$

## On-policy and Off-policy learning

$$Q_{t+1}(s, a) = Q_t(s, a) + \alpha_t \delta_{t+1}(Q_t) \mathbb{I}_{\{S_t = s, A_t = a\}}$$

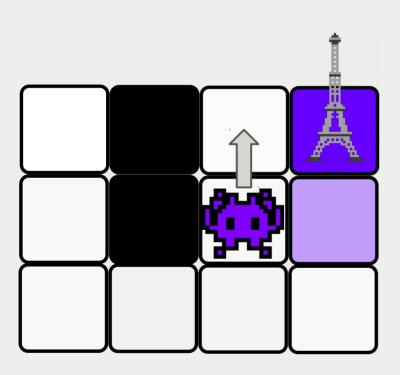
**SARSA:** 
$$\delta_{t+1} = R_{t+1} + \gamma Q(S_{t+1}, A_{t+1}) - Q(S_t, A_t)$$



## On-policy and Off-policy learning

$$Q_{t+1}(s, a) = Q_t(s, a) + \alpha_t \delta_{t+1}(Q_t) \mathbb{I}_{\{S_t = s, A_t = a\}}$$

**Q-learning:** 
$$\delta_{t+1} = R_{t+1} + \gamma \max_{a' \in A} Q(S'_{t+1}, a') - Q(S_t, A_t)$$



#### On-policy and Off-policy learning

$$Q_{t+1}(s, a) = Q_t(s, a) + \alpha_t \delta_{t+1}(Q_t) \mathbb{I}_{\{S_t = s, A_t = a\}}$$

**SARSA:** 
$$\delta_{t+1} = R_{t+1} + \gamma Q(S_{t+1}, A_{t+1}) - Q(S_t, A_t)$$

**Q-learning:** 
$$\delta_{t+1} = R_{t+1} + \gamma \max_{a' \in \mathcal{A}} Q(S'_{t+1}, a') - Q(S_t, A_t)$$

#### SARSA (on-policy)

- Regular TD learning for actionvalue functions
- Policy iteration through sampling the quintuplet  $\{S_t, A_t, R_{t+1}, S_{t+1}, A_{t+1}\}$

#### **Q-learning (off-policy)**

- Q-learning is an instance of TD learning
- S' can be S but doesn't need to.
- Allows for sampling

#### Large or Continuous State Spaces

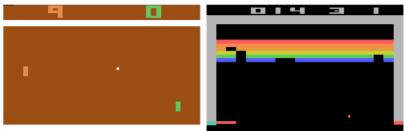
- So far we had discrete state space S. What if it is continuous?
- Common approach: "discretize"!

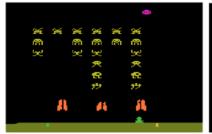
  By function approximation.

$$Q(s,a) = \sum_{i} \theta_{i} f_{i}(s,a)$$

$$f_i(s,a)$$
 ... basis functions  $\theta_i$  ... weights

## Deep Q-learning









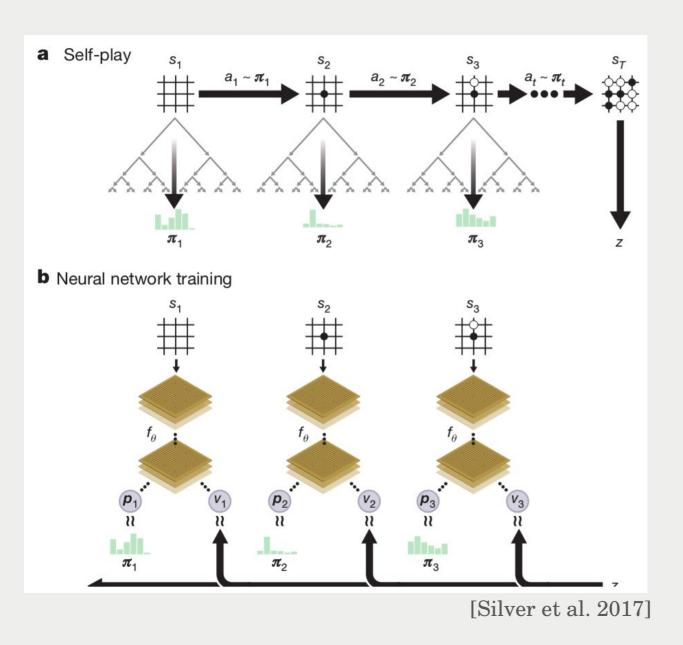
- Use DNNs to represent the value function
- "Experience replay" to make more efficient use of collected information
- (Explain SGD bit)

#### Advantages:

[Minh et al. 2013]

- Consecutive samples have strong correlations (little information)
- Not only one state update but propagating new information.
- Better convergence behavior when using function approximation (as DNN)
- When on-policy then training distribution depends on selected actions (can result in unwanted feedback loops)

## Alpha Go Zero



#### References

- Reinforcement Learning: An Introduction. **Sutton R. and Barto A.**, 2<sup>nd</sup> Edition, 2018
- Algorithms for Reinforcement Learning. Szepesvári C. 2012
- A Tutorial on Thompson Sampling. **Russo et al.** Foundations and Trends in Machine Learning 2018.
- Mastering the game of Go without human knowledge. **Silver et al.** *Nature* 2017
- Playing Atari with Deep Reinforcement Learning **Mnih et al.** arXiv:1312.5602 [cs] 2013