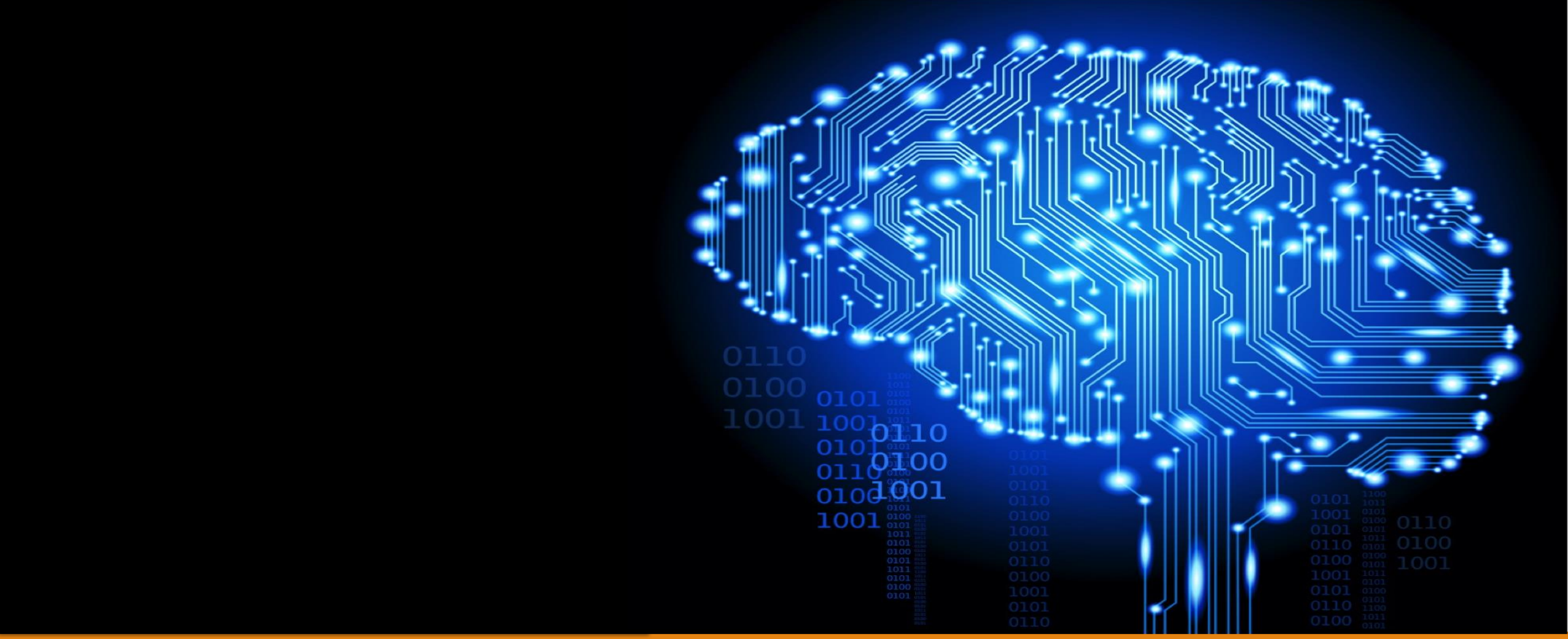
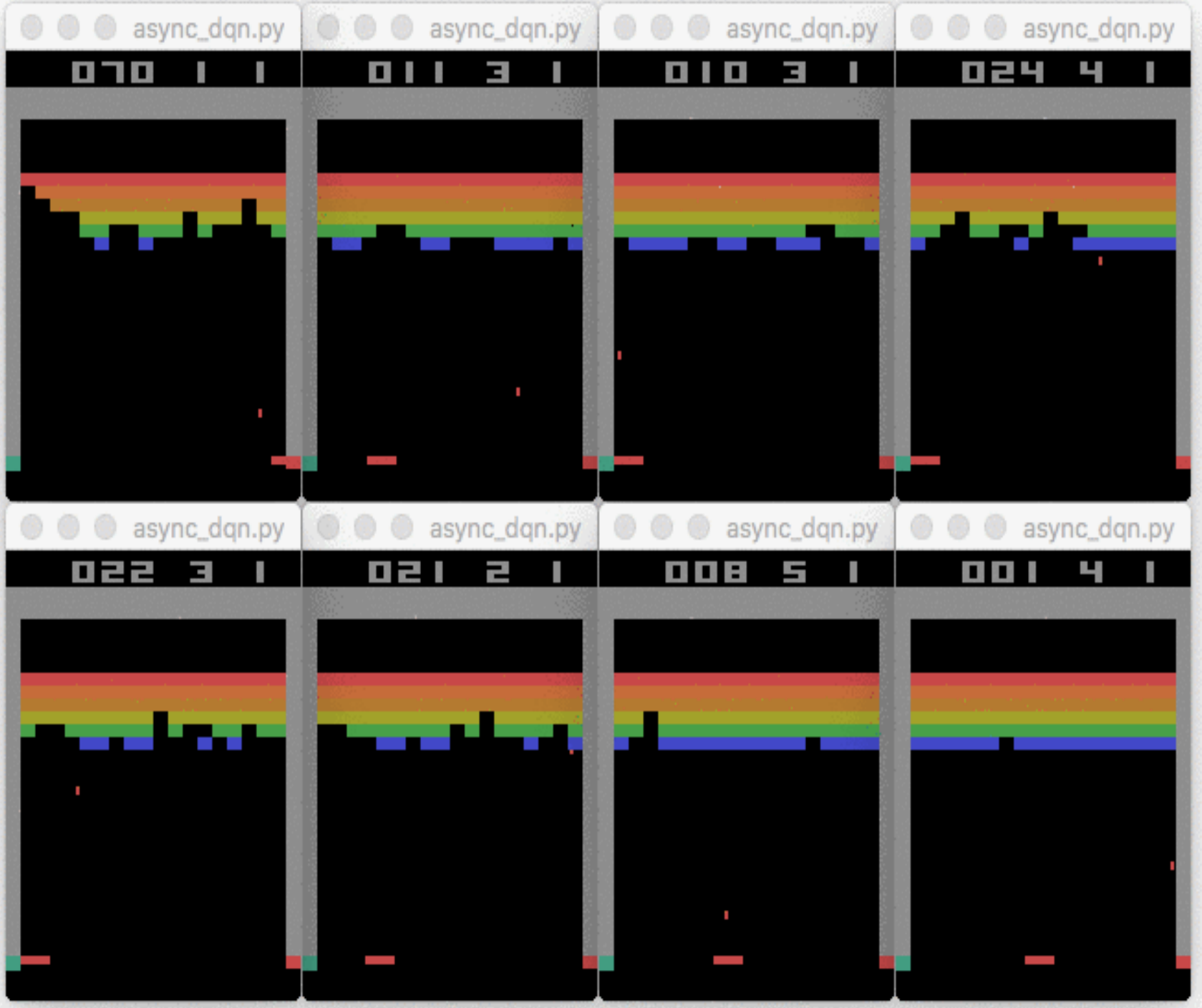


Lecture 12: Deep Reinforcement Learning

Deep Learning @ UvA

Reinforcement Learning



What is Reinforcement Learning?

- General purpose framework for learning Artificial Intelligence models
- RL assumes that ***the agent*** (our model) can take ***actions***
- These actions affect ***the environment*** where ***the agent*** operates
  - more specifically ***the state*** of the environment and ***the state*** of the agent
- Given the state of the environment and the agent, an action taken from the agent causes a reward
  - can be positive or negative
- Goal: the goal of an RL agent is to learn how to take actions that maximize future rewards

Some examples of RL

Some examples of RL

- Controlling physical systems
  - Robot walking, jumping, driving
- Logistics
  - Scheduling, bandwidth allocation
- Games
  - Atari, Go, Chess, Pacman
- Learning sequential algorithms
  - Attention, memory

Reinforcement Learning: An abstraction

Dynamical System
("The World")

State
s_t

Reward
r_t

Observ
ation o_t

Action
a_t

Learning Agent
("Our Model")

State

- Experience is a series of observations, actions and rewards

$$o_1, r_1, a_1, o_2, r_2, a_2, \dots, o_t, r_t$$

- The state is the summary of experience so far

$$s_t = f(o_1, r_1, a_1, o_2, r_2, a_2, \dots, o_t, r_t)$$

- If we have fully observable environments, then

$$s_t = f(o_t)$$

Policy

- Policy is the agent's behavior function
- The policy function maps the state input s_t to an action output a_t
- Deterministic policy: $a_t = f(s_t)$
- Stochastic policy: $\pi(a_t|s_t) = \mathbb{P}(a_t|s_t)$

Value function

- A value function is the prediction of the future reward
  - Given the state s_t what will my reward be if I do action a_t

- The Q-value function gives the expected future reward

- Given state s_t, action a_t, a policy π the Q-value function is $Q^{\pi}(s_t, a_t)$

How do we decide about actions, states, rewards?

- We model the policy and the value function as machine learning functions that can be optimized by the data
- The ***policy function*** $\mathrm{a_t} = \pi(s_t)$ selects an action given the current state
- The ***value function*** $Q^{\pi}(s_t, a_t)$ is the expected total reward that we will receive if we take action a_t given state s_t
- What should our goal then be?

Goal: Maximize future rewards!

- Learn the policy and value functions such that the action taken at the t-th time step a_t maximizes the expected sum of future rewards

$$Q^{\pi}(s_t, a_t) = \mathbb{E}(r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \cdots | s_t, a_t)$$

- γ is a discount factor. Why do we need it?

Goal: Maximize future rewards!

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- γ is a discount factor. Why do we need it?
  - The further into the future we look $t+1$, …, $t+\mathrm{T}$, the less certain we can be about our expected rewards r_{t+1}, …, r_{t+T}

Bellman equation

- How can we rewrite the value function in more compact form

$$Q^{\pi}(s_t, a_t) = \mathbb{E}(r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \cdots | s_t, a_t) = ?$$

Bellman equation

- How can we rewrite the value function in more compact form

$$Q^{\pi}(s_t, a_t) = \mathbb{E}(r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \cdots | s_t, a_t)$$
$$= \mathbb{E}_{s',a'}(r + \gamma Q^{\pi}(s', a') | s_t, a_t)$$

- This is the ***Bellman equation***

Bellman equation

- How can we rewrite the value function in more compact form

$$Q^{\pi}(s_t, a_t) = \mathbb{E}(r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \cdots | s_t, a_t)$$
$$= \mathbb{E}_{s',a'}(r + \gamma Q^{\pi}(s', a') | s_t, a_t)$$

- This is the ***Bellman equation***

- How can we rewrite the optimal value function $Q^*(s_t, a_t)$?

Optimal value function

- Optimal value function $Q^*(s,a)$ is attained with the optimal policy π^*

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

- After we have found the optimal policy π^* we do the optimal action

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

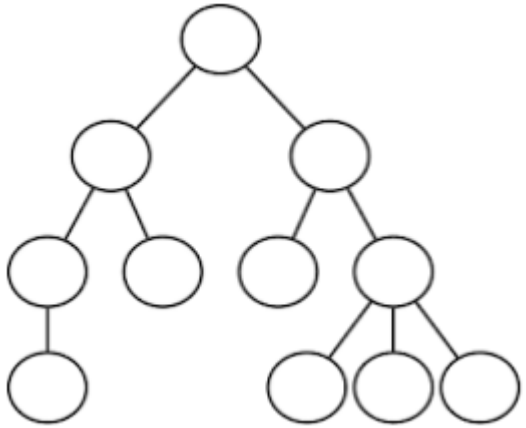
- By expanding the optimal value function

$$Q^*(s,a) = r_{t+1} + \gamma \max_{a_{t+1}} Q^*(s_{t+1}, a_{t+1})$$

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

Environment Models in RL

- The model is learnt from experience
- The model acts as a replacement for the environment
- When planning, the agent can interact with the model
- For instance look ahead search to estimate the future states given actions



Approaches to Reinforcement Learning

- Policy-based
  - Learn directly the optimal policy π^*
  - The policy π^* obtains the maximum future reward
- Value-based
  - Learn the optimal value function $Q^*(s, a)$
  - This value function applies for any policy
- Model-based
  - Build a model for the environment
  - Plan and decide using that model

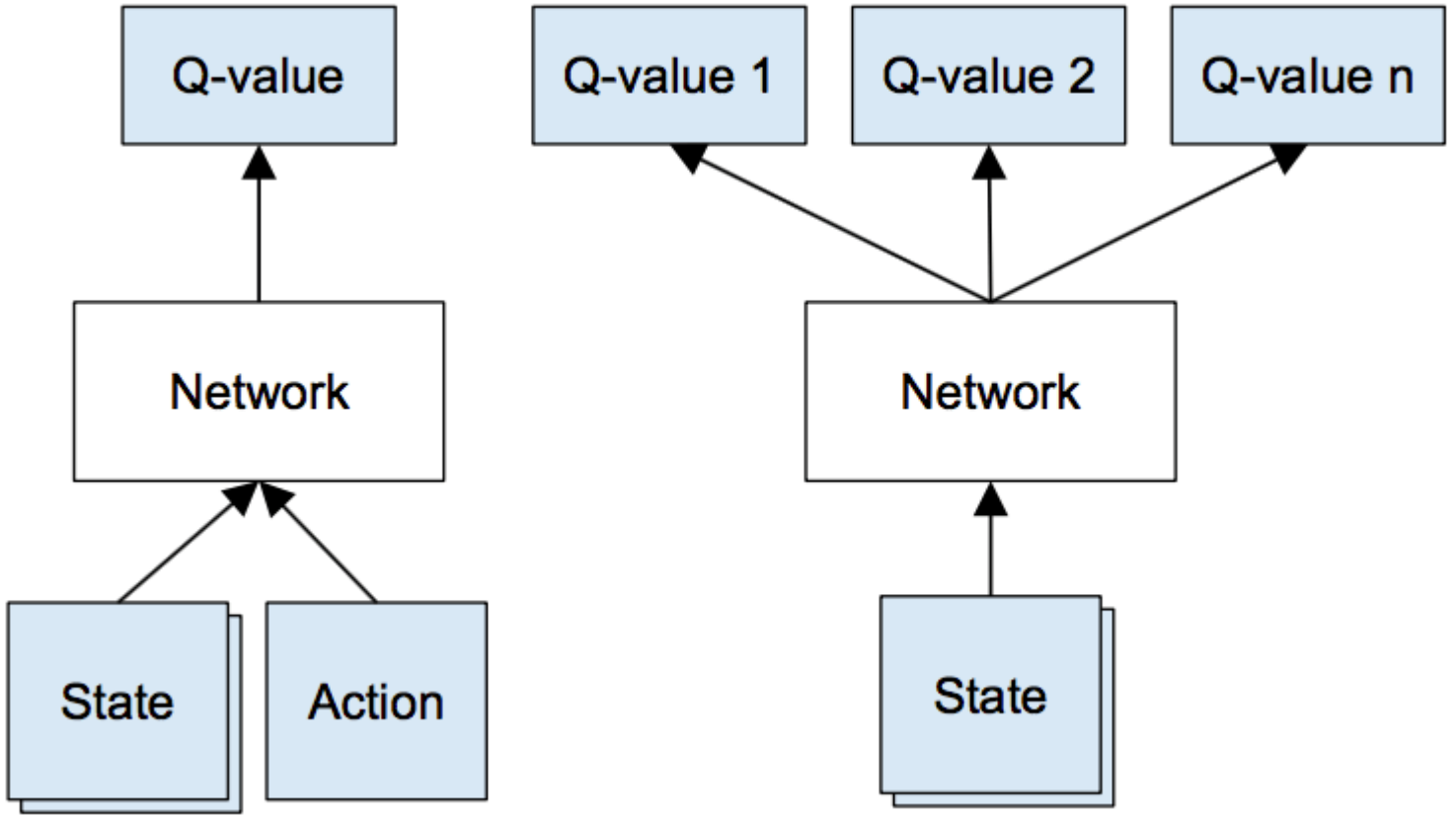
How to make RL deep?

How to make RL deep?

- Use Deep Networks for the
  - Value function
  - Policy
  - Model

- Optimize final loss with SGD

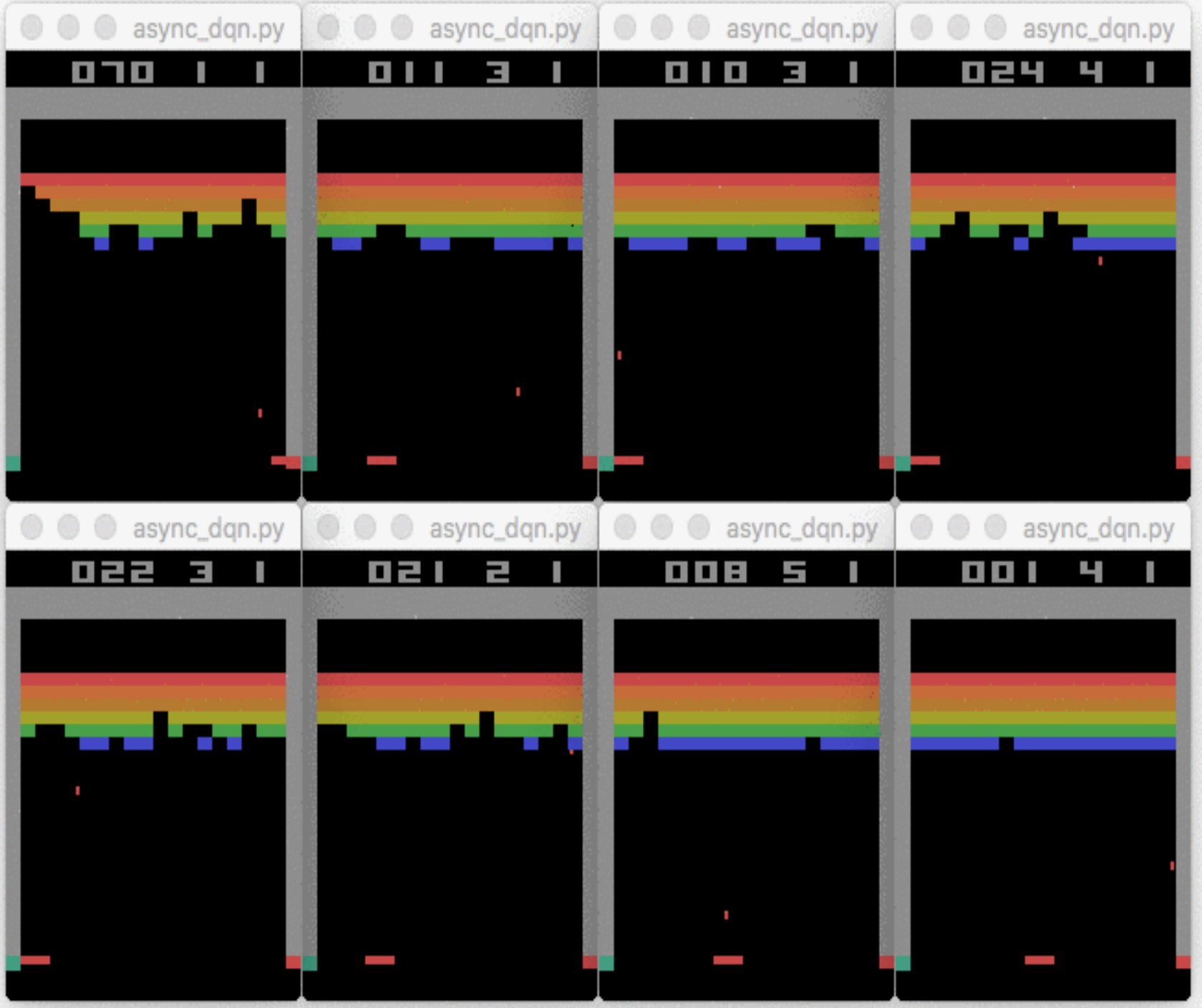
How to make RL deep?



Deep Reinforcement Learning

- Non-linear function approximator: Deep Networks
- Input is as raw as possible, e.g. image frame
  - Or perhaps several frames (When needed?)
- Output is the best possible action out of a set of actions for maximizing future reward
- **Important:** no strict need anymore to compute the actual value of the action-value function and take the maximum: $\arg\max_{\alpha} Q_{\theta}(s, a)$
- Instead, one can teach the network to return directly the optimal action

Value-based Deep RL



Q-Learning

- Optimize for Q value function

$$Q^{\pi}(s_t, a_t) = \mathbb{E}_{s'}(r + \gamma Q^{\pi}(s', a')|s_t, a_t)$$

- What does this imply in terms of learning? What do we need?

Q-Learning

- Optimize for Q value function

$$Q^{\pi}(s_t, a_t) = \mathbb{E}_{s'}(r + \gamma Q^{\pi}(s', a')|s_t, a_t)$$

- What does this imply in terms of learning? What do we need?
- Target/"Ground truth" Q values
- We set $r + \gamma \max_{a'} Q_t(s', a')$ to be the learning target
- Then we minimize the loss

$$\min \left(r + \gamma \max_{a'} Q_t(s', a') - Q_t(s, a) \right)^2$$

- In the beginning of learning the function $Q(s, a)$ is incorrect
- But the hypothesis is that as trainng progresses, so does our Q predictions

Q-Learning

- Value iteration algorithms solve the Bellman equation

$$Q_{t+1}(s,a) = \mathbb{E}_{s'}\left(r + \gamma \max_{a'} Q_t(s',a') \middle| s,a\right)$$

- In the simplest case Q_t is a table
  - To the limit iterative algorithms converge to Q^*

- However, a table representation for Q_t is not always enough. Why/when?

Q-Learning

- Value iteration algorithms solve the Bellman equation

$$Q_{t+1}(s,a) = \mathbb{E}_{s'}\left(r + \gamma \max_{a'} Q_t(s',a') \middle| s,a\right)$$

- In the simplest case Q_t is a table
  - To the limit iterative algorithms converge to Q^*

- However, a table representation for Q_t is not always enough. Why/when?
- When the state space is enormous or near infinite
  - Imagine making a table with all possible images in the rows

How to optimize?

- The objective is the mean squared-error in Q-values

$$\mathcal{L}(\theta) = \mathbb{E}[\left(\hat{Q} - Q(s, a, \theta)\right)^2]$$

where $\hat{Q} = r + \gamma \max_{a'} Q(s', a', \theta)$ is a pre-computed **scalar target value.**

- So, what does this means for the gradient? How will it look like?

How to optimize?

- The objective is the mean squared-error in Q-values

$$\mathcal{L}(\theta) = \mathbb{E}[\left(\hat{Q} - Q(s, a, \theta)\right)^2]$$

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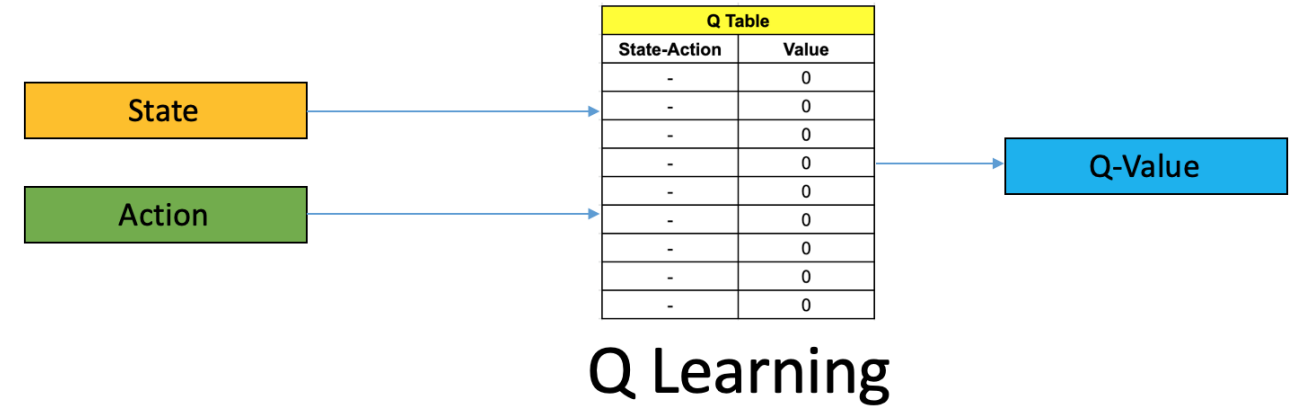
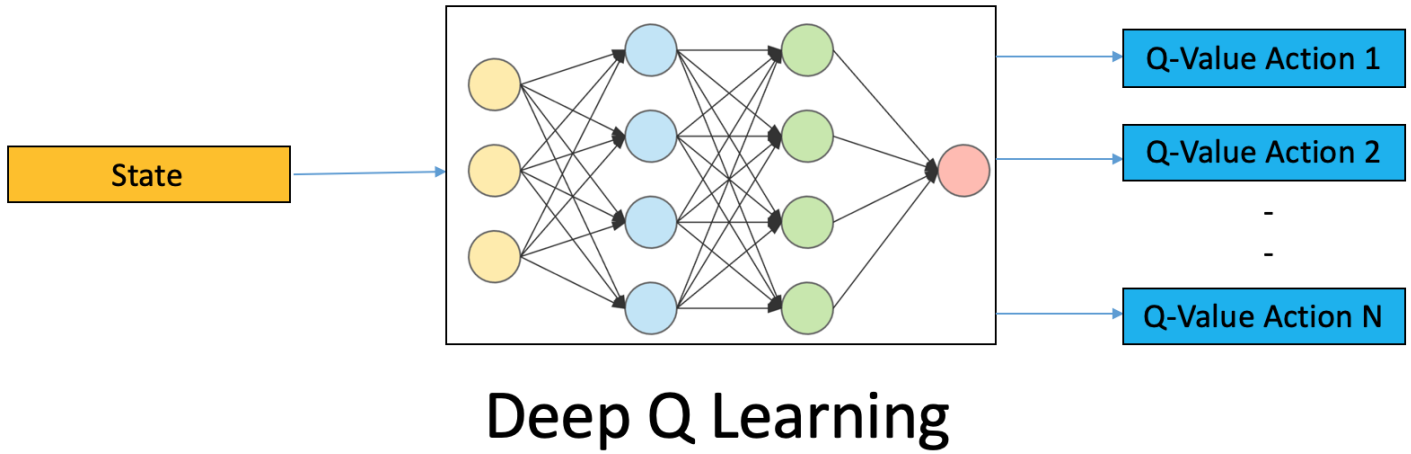
- So, what does this means for the gradient? How will it look like?
- The Q-Learning gradient then becomes

$$\frac{\partial \mathcal{L}}{\partial \theta} = \mathbb{E}[-2 \cdot \left(\hat{Q} - Q(s, a, \theta)\right) \frac{\partial Q(s, a, \theta)}{\partial \theta}]$$

- Backprop to get the gradient
- Optimize end-to-end with SGD

A system perspective





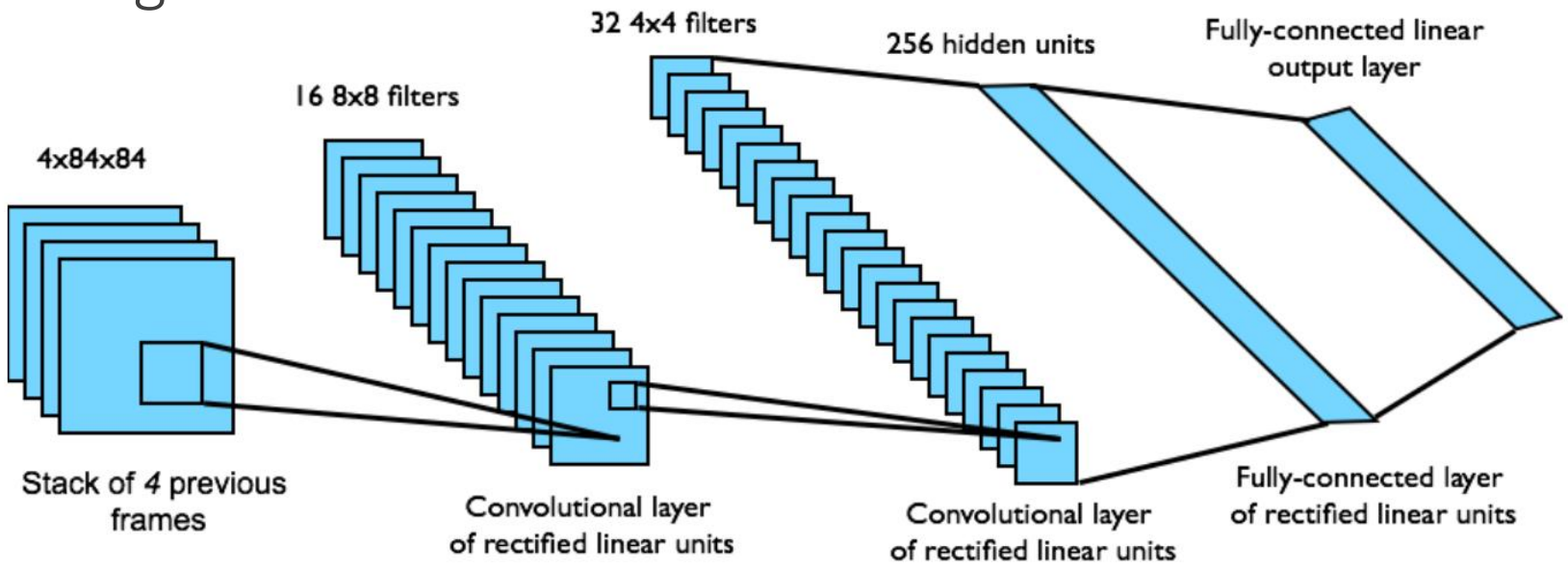
https://www.analyticsvidhya.com/blog/2019/04/introduction-deep-q-learning-python/

Algorithmically

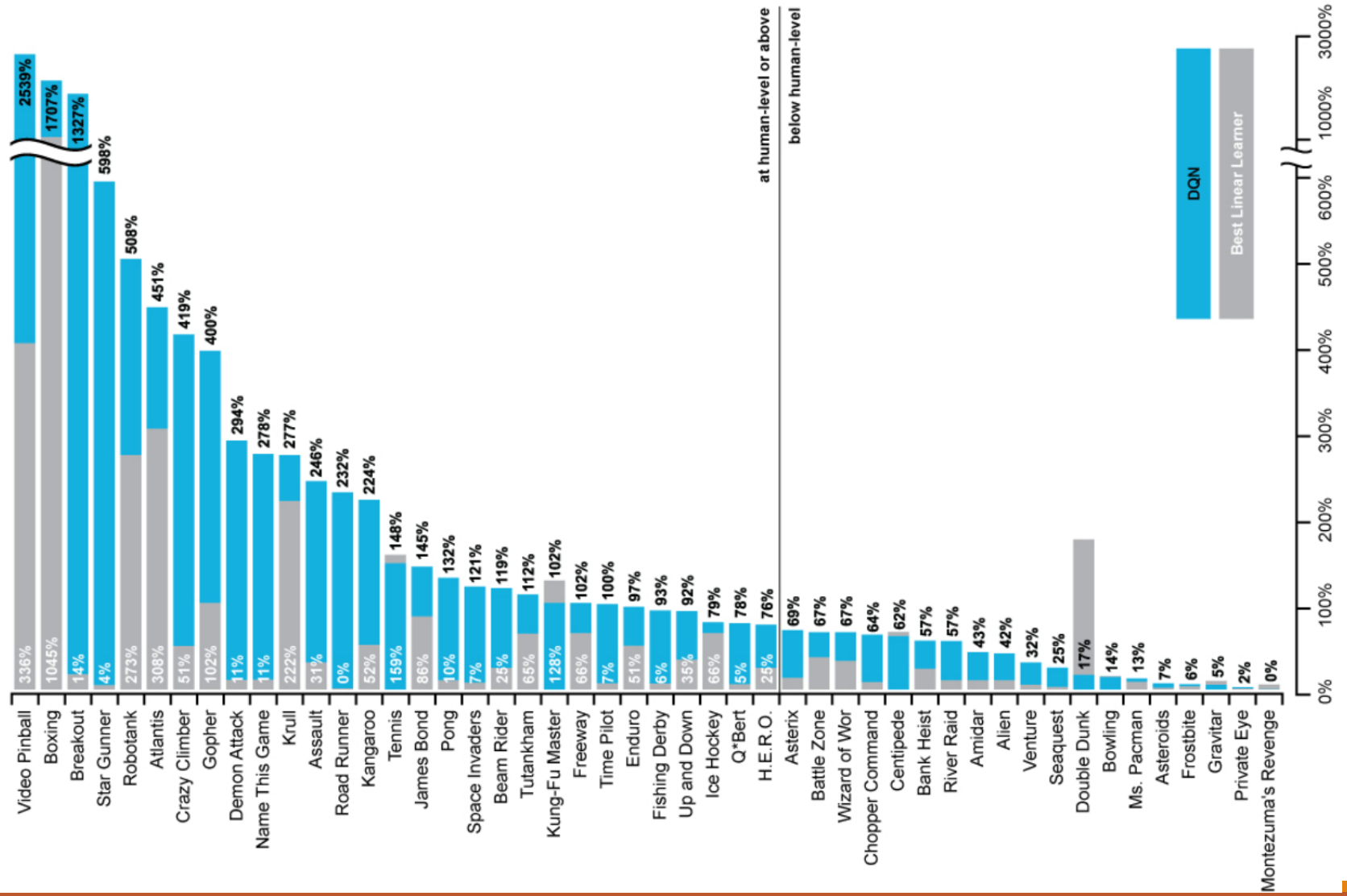
1. Do a feedforward pass for the current state s to predict Q-values for all actions
2. Select an action
   a. either by ε-greedy policy
   b. or the one with the best Q value $a = \max_{a'} Q(s', a', \theta)$
3. Perform the action, get a new state *s'* with reward *r*. Store the <*s, a, r, s'*>
4. Set Q-value target to $\mathrm{r} + \gamma \max_{a'} Q(s', a', \theta)$
   - use the max calculated in step 2
   - For all other action classes, set the Q-value target to the same as originally returned from step 1
   - Makes the error 0 for those action classe → Zero gradient
5. Update the weights using backpropagation
   (in fact, between step 3 and 4 you probably should do experience replay)

Deep Q Networks on Atari

- End-to-end learning from raw pixels
- Input: last 4 frames
- Output: 18 joystick positions
- Reward: change of score



Deep Q Networks on Atari



Stability in Deep Reinforcement Learning

Stability problems

- Naively, Q-Learning oscillates or diverges with neural networks
- Why?

Stability problems

- Naively, Q-Learning oscillates or diverges with neural networks
- Why?
- Sequential data breaks IID assumption
  - Highly correlated samples break SGD
- However, this is not specific to RL, as we have seen earlier

Stability problems

- Naively, Q-Learning oscillates or diverges with neural networks
- Why?

Stability problems

- The learning objective is

$$\mathcal{L}(\theta) = \mathbb{E}[(r + \gamma \max_{a'} Q(s', a', \theta) - Q(s, a, \theta))^2]$$

- The target depends on the Q function also. This means that if we update the current Q function with backprop, the target will also change
- Non-stationarity (BIG problem)
- Plus, we know neural networks are highly non-convex
- Policy changes will change fast even with slight changes in the Q function
  - Policy might oscillate
  - Distribution of data might move from one extreme to another

Stability problems

- Naively, Q-Learning oscillates or diverges with neural networks
- Why?

Stability problems

- Not easy to control the scale of the Q values→ gradients are unstable Q
- Remember, the Q function is the output of a neural network
- There is no guarantee that the outputs will lie in a certain range
  - Unless care is taken
- Naïve Q gradients can be too large, or too small → generally unstable and unreliable
- Where else did we observe a similar behavior?

Improving stability: Experience replay

- Replay memory/Experience replay
- Store memories $< s, a, r, s' >$
- Train using random stored memories instead of the latest memory transition
- Breaks the temporal dependencies – SGD works well if samples are roughly independent
- Learn from all past policies

Experience replay

- Take action a_t according to ε-greedy policy
- Store transition $(s_t, a_t, r_{t+1}, s_{t+1})$ in replay memory D
- Sample random mini-batch of transitions (s, a, r, s') from D
- Optimize mean squared error using the mini-batch

$$\mathcal{L}(\theta) = \mathbb{E}_{(s,a,r,s')\sim D}\left[\left(r + \gamma \max_{a'} Q(s', a', \theta) - Q(s, a, \theta)\right)^2\right]$$

- Effectively, update your network using random past inputs (experience), not the ones the agent currently sees

Improving stability: Freeze target Q network

- Instead of having "moving" targets, have two networks
  - One Q-Learning and one Q-Target networks
- Copy the Q network parameters to the target network every K iterations
  - Otherwise, keep the old parameters between iterations
  - The targets come from another (Q-Target) network with slightly older parameters
- Optimize the mean squared error as before, only now the targets are defined by the "older" Q function

$$\mathcal{L}(\theta) = \mathbb{E}[\left(r + \gamma \max_{a'} Q(s', a', \theta_{old}) - Q(s, a, \theta)\right)^2]$$

- Avoids oscillations

Improving stability: Take care of rewards

- Clip rewards to be in the range $[-1, +1]$
- Or normalize them to lie in a certain, stable range
- Can’t tell the difference between large and small rewards

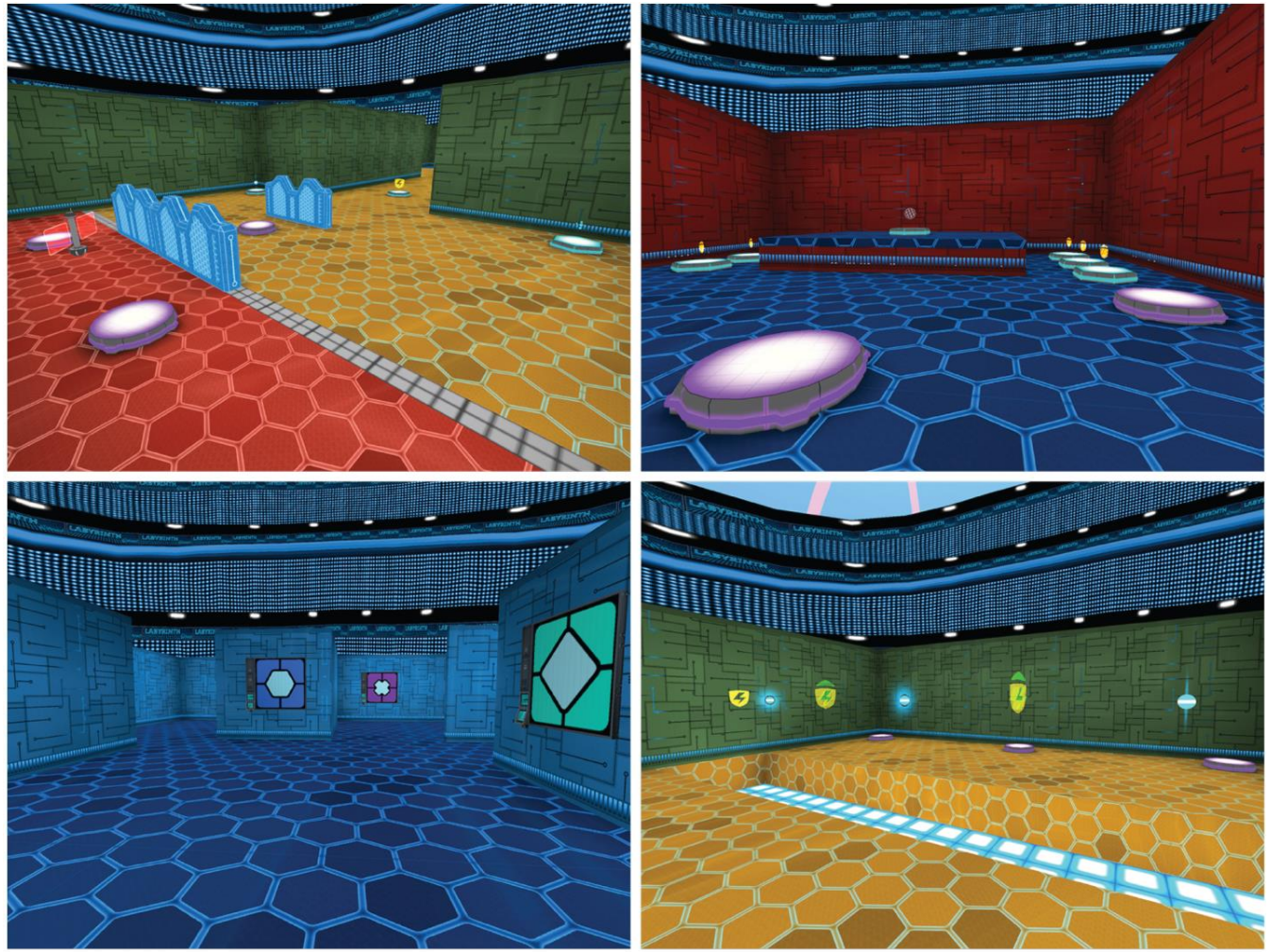
Results

	Q-learning	Q-learning + Target Q	Q-learning + Replay	Q-learning + Replay + Target Q
Breakout	3	10	241	**317**
Enduro	29	142	831	**1006**
River Raid	1453	2868	4103	**7447**
Seaquest	276	1003	823	**2894**
Space Invaders	302	373	826	**1089**

Some extra tricks

- Skipping frames
  - Saves time and computation
  - Anyways, from one frame to the other there is often very little difference
- ε-greedy behavioral policy with annealed temperature during training
  - Select random action (instead of optimal) with probability ε
  - In the beginning of training our model is bad, no reason to trust the “optimal” action
- Alternatively: Exploration vs exploitation
  - early stages → strong exploration
  - late stages → strong exploitation

Policy-based Deep RL

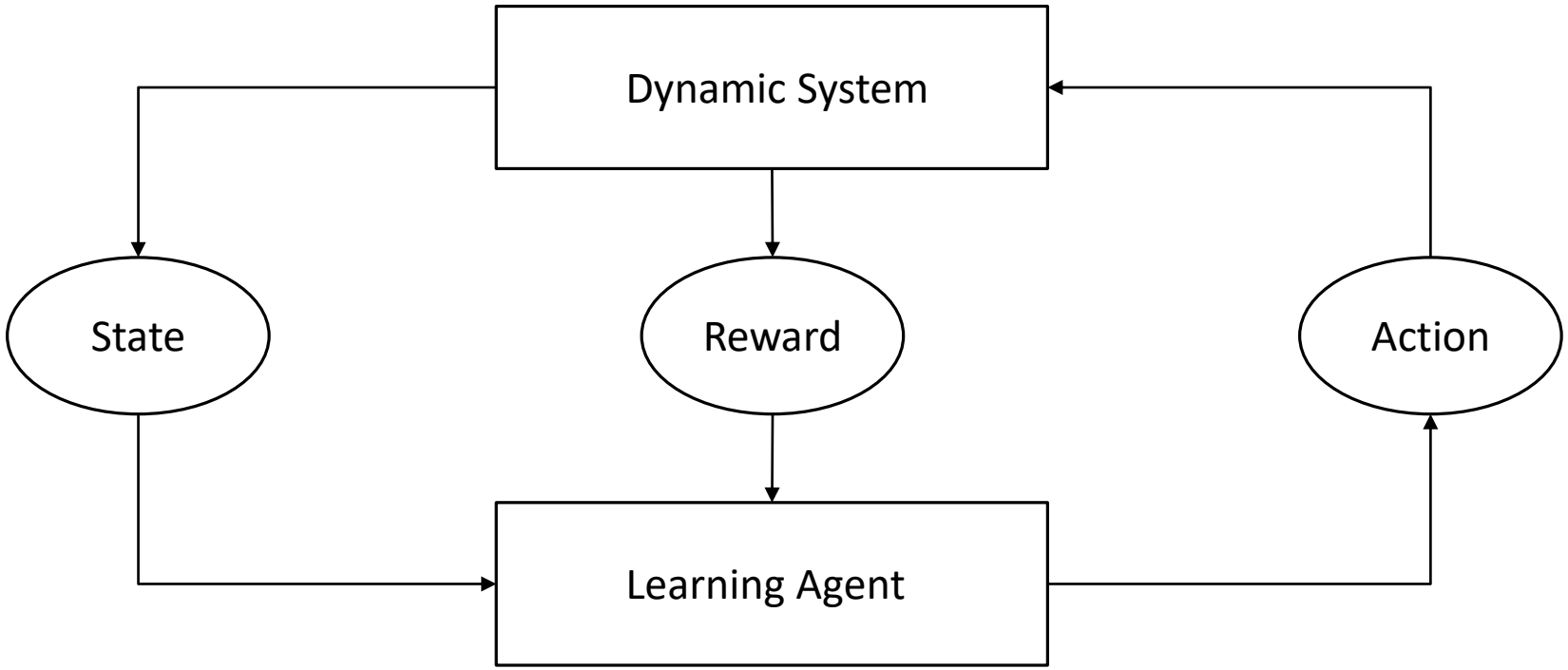


Policy Optimization

- Problems with modelling the Q-value function
  - Often too expensive → must take into account all possible states, actions →Imagine when having continuous or high-dimensional action spaces
  - Not always good convergence ← Oscillations
- Often learning directly a policy $\pi_\theta(a|s)$ that gives the best action without knowing what its expected future reward is easier
- Also, allows for stochastic policies ← no exploration/exploitation dilemma
- Model optimal *action value* with a non-linear function approximator

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

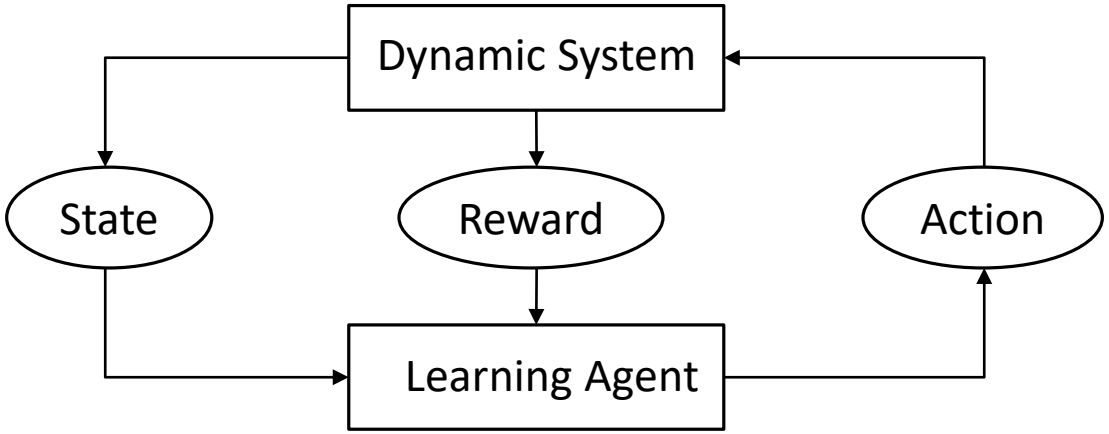
Policy Optimization

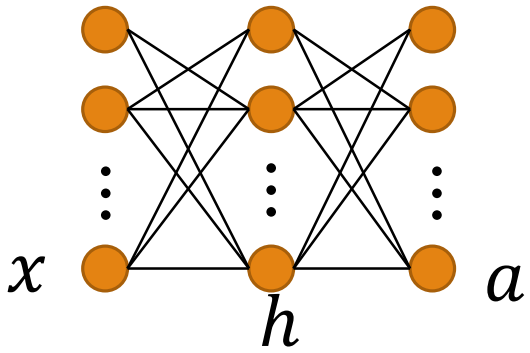


$\pi_\theta(a|s)$

Slide inspired by P. Abbeel

Policy Optimization





$\pi_w(a|s)$

- Train learning agent for the optimal policy $\pi_w(a|s)$ given states s and possible actions a
- The policy class can be either deterministic or stochastic

Slides inspired by P. Abbeel

Policy Optimization

- Use a deep networks as non-linear approximator that finds optimal policy by maximizing $Q(s, a; \theta)$

$$\mathcal{L}(w) = Q(s, a; w)$$
$$= \mathbb{E}[r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \cdots | \pi_w(s_t, a_t)]$$

- If policy is deterministic

$$\frac{\partial \mathcal{L}}{\partial w} = \mathbb{E}\left[\frac{\partial \log \pi(a|s, w)}{\partial w} Q^{\pi}(s, a)\right]$$

- If policy is stochastic $a = \pi(s)$

$$\frac{\partial \mathcal{L}}{\partial w} = \mathbb{E}\left[\frac{\partial Q^{\pi}(s, a)}{\partial a} \frac{\partial a}{\partial w}\right]$$

- To compute gradients use the log-derivative trick (REINFORCE algorithm (Williams, 1992))

$$\nabla_\theta \log p(x; \theta) = \frac{\nabla_\theta p(x; \theta)}{p(x; \theta)}$$

Policy Optimization

- Use a deep networks as non-linear approximator that finds optimal policy by maximizing $Q(s, a; \theta)$

$$\mathcal{L}(w) = Q(s, a; w)$$
$$= \mathbb{E}[r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \cdots | \pi_w(s_t, a_t)]$$

- We can rewrite the score function as $\mathcal{L}(w) = \mathbb{E}_{\pi_w}[R(\tau)]$

Expected future reward given a policy

- Note: $\mathcal{L}(w)$ is the score, not loss → we want to maximize it

$$\frac{\partial \mathcal{L}}{\partial w} = \nabla_w \mathbb{E}_{\pi_w}[R(\tau)] = \sum_t \nabla_w \pi_w(t) R(t)$$

- We use the log-derivative trick

$$\nabla_\theta \log p(x; \theta) = \frac{\nabla_\theta p(x; \theta)}{p(x; \theta)}$$

Policy gradients

- Given stochastic policy $\pi(a|s,w)$

$$\frac{\partial \mathcal{L}(w)}{\partial w} = \mathbb{E}\left[\frac{\partial \log \pi(a|s,w)}{\partial w} Q^{\pi}(s,a)\right]$$

  - Since we have a stochastic/random quantity/variable, i.e., the policy ($\pi(a|s,w)$), this means that to compute our loss we must take expectations w.r.t. that RV

- Given deterministic policy $a = \pi(s)$

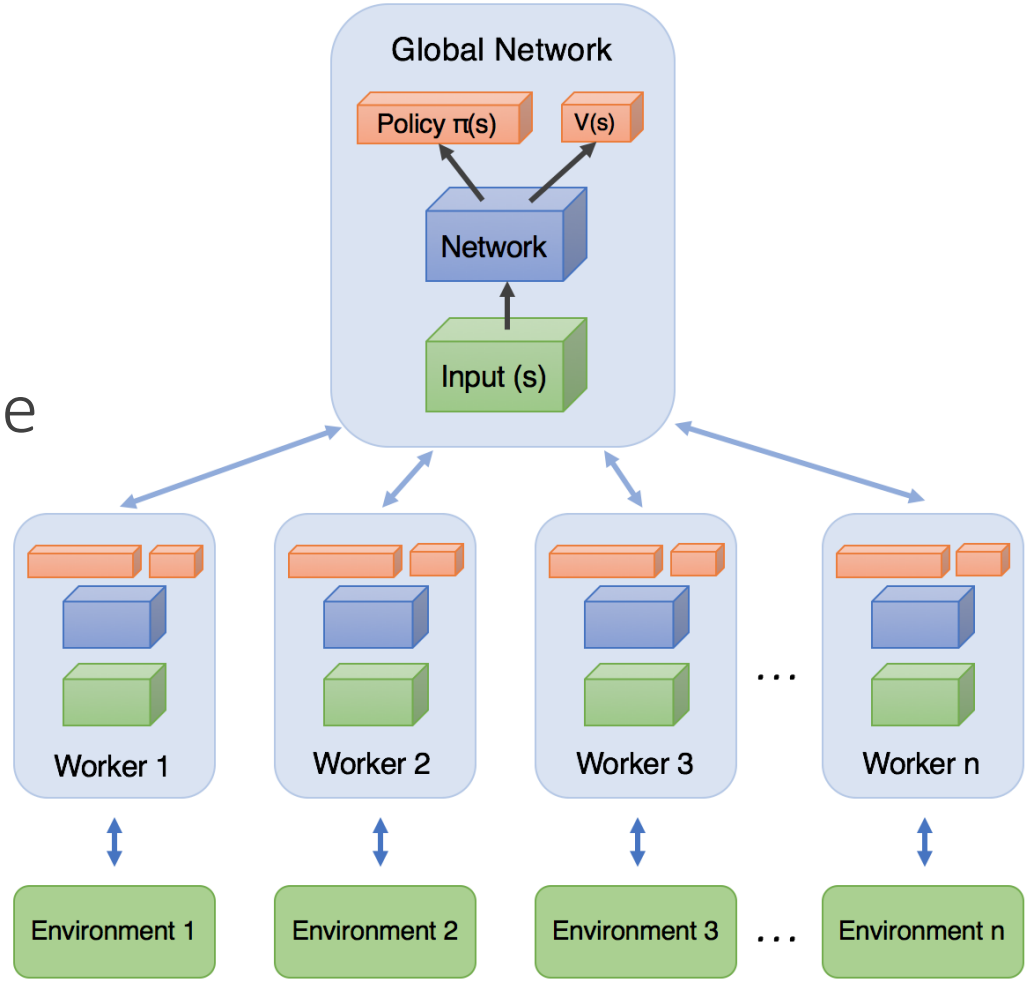
$$\frac{\partial \mathcal{L}(w)}{\partial w} = \mathbb{E}\left[\frac{\partial Q^{\pi}(s,a)}{\partial a}\frac{\partial a}{\partial w}\right]$$

for continuous a and differentiable Q

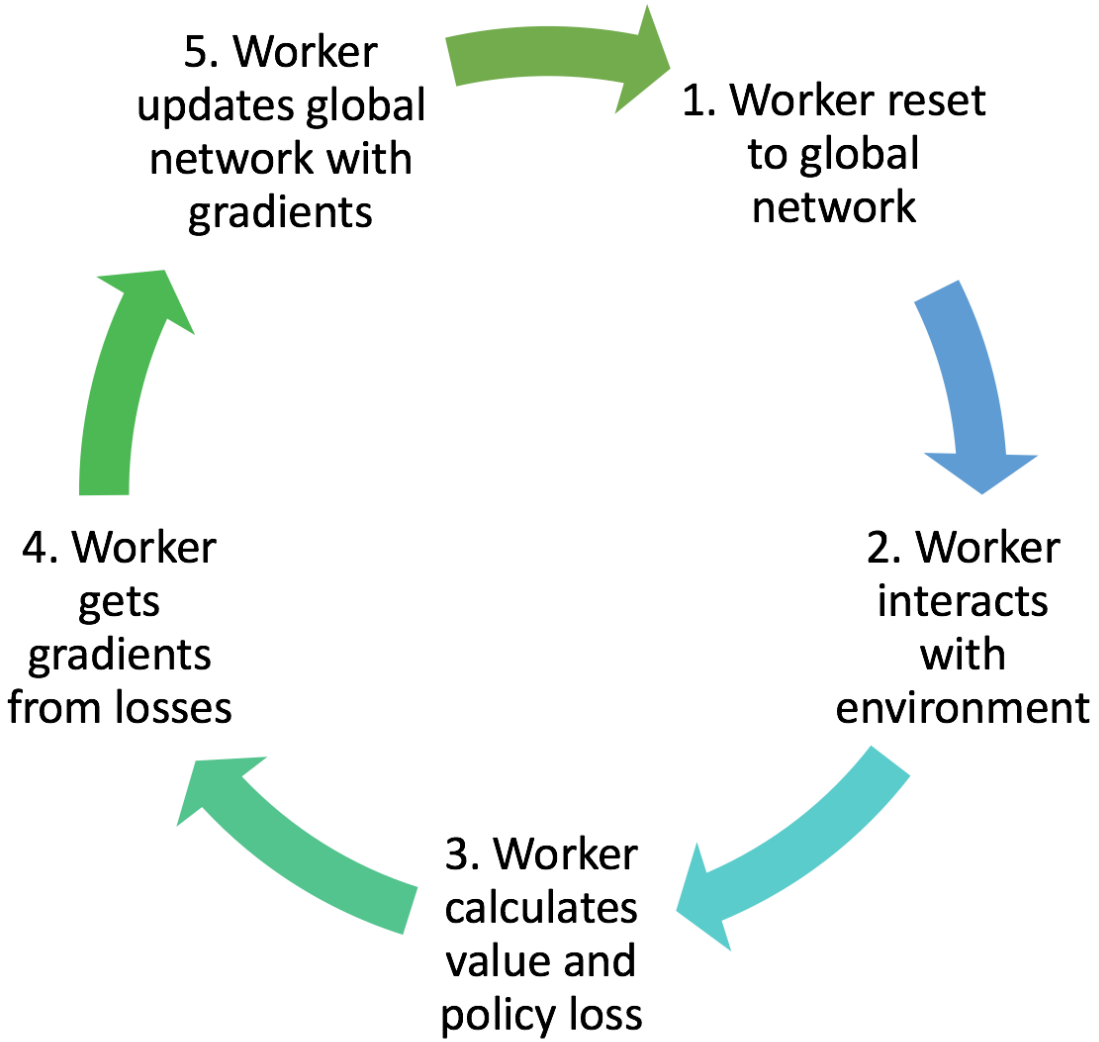
  - Since the policy is deterministic, we simply need to take gradients of the final objective (Q^{π}) w.r.t. the optimized variables (w), taking into account all computational paths (via $a = \pi(s)$)

Asynchronous Advantage Actor-Critic (A3C)

- Learn both
  - Policy function and
  - Value function
- Multiple agents trained at the same time
- Global Network consists of
  - ConvNet to model spatial correlations
  - LSTM to model temporal correlations



A3C Training



A3C Training

- Estimate Value function

$$V(s, v) = \mathbb{E}[r_{t+1} + \gamma r_{t+2} + \cdots | s]$$

- Estimate the Q value after n steps

$$q_t = r_{t+1} + \gamma r_{t+2} + \cdots + \gamma^{n-1} r_{t+n} + \gamma^n V(s_{t+n}, v)$$

- Update actor by

$$\frac{\partial \mathcal{L}_{actor}}{\partial w} = \frac{\partial \log \pi(a_t | s_t, w)}{\partial w} (q_t - V(s_t, v))$$

Advantage Estimates

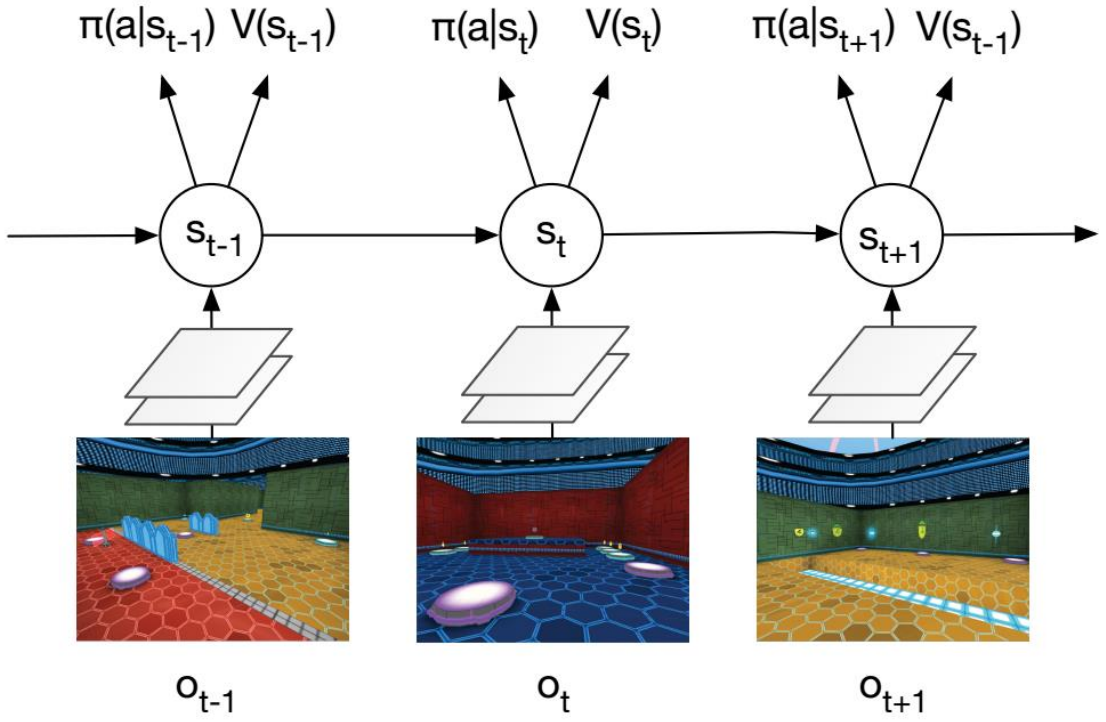
- Discounted future rewards $R = \gamma(r)$
  - The model must learn how good the actions taken are

- With Advantage Estimates $A = R - V(s)$
  - Now just how good the actions taken are
  - Also, how much better the actions where than expected

- Model will focus on the areas of the parameter space that it was lacking

A3C in labyrinth

- End-to-end learning of softmax policy from pixels
- Observations are the raw pixels
- The state is implemented as an LSTM
- Outputs value $V(s)$ and softmax over actions $\pi(a|s)$
- Task
  - Collect apples (+1)
  - escape (+10)
- Demo



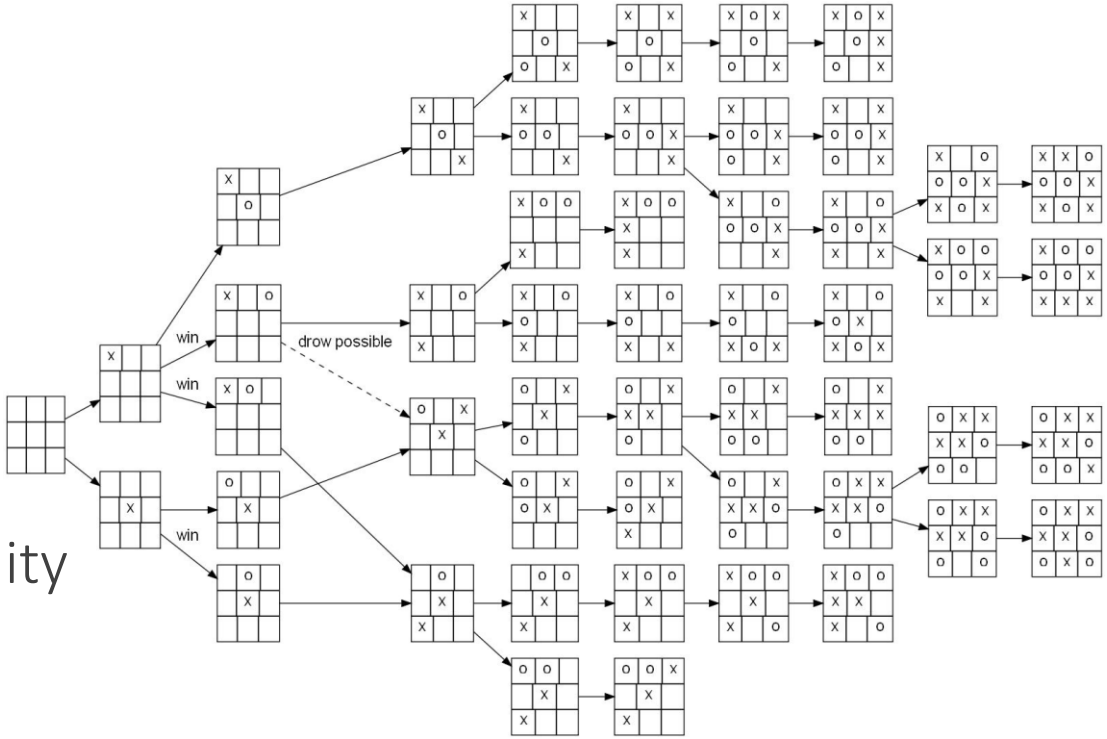
Model-based Deep RL

Learning models of the environment

- Often quite challenging because of cumulative errors
- Errors in transition models accumulate over trajectories
- Planning trajectories are different from executed trajectories
- At the end of a long trajectory final rewards are wrong
- Can be better if we know the rules

AlphaGo

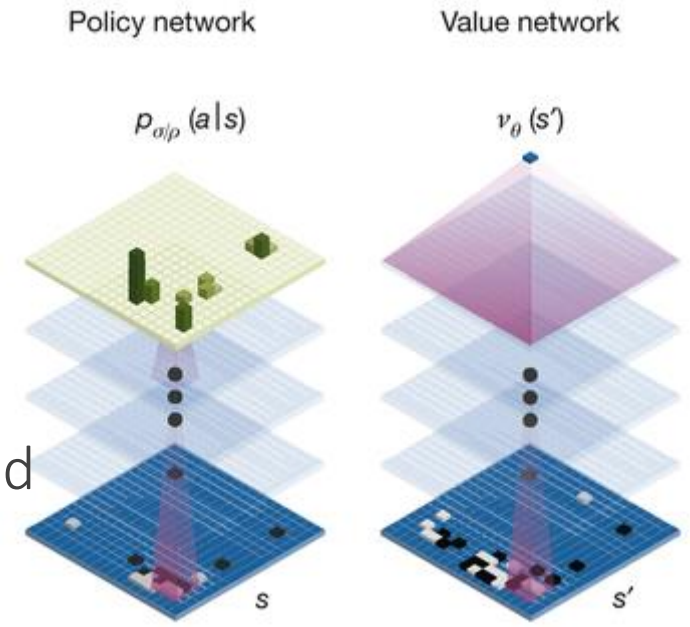
- At least $10^{10^{48}}$ possible game states
  - Chess has 10^{120}
- Monte Carlo Tree Search used mostly
  - Start with random moves and evaluate how often they lead to victory
  - Learn the value function to predict the quality of a move
  - Exploration-exploitation trade-off



Tic-Tac-Toe possible game states

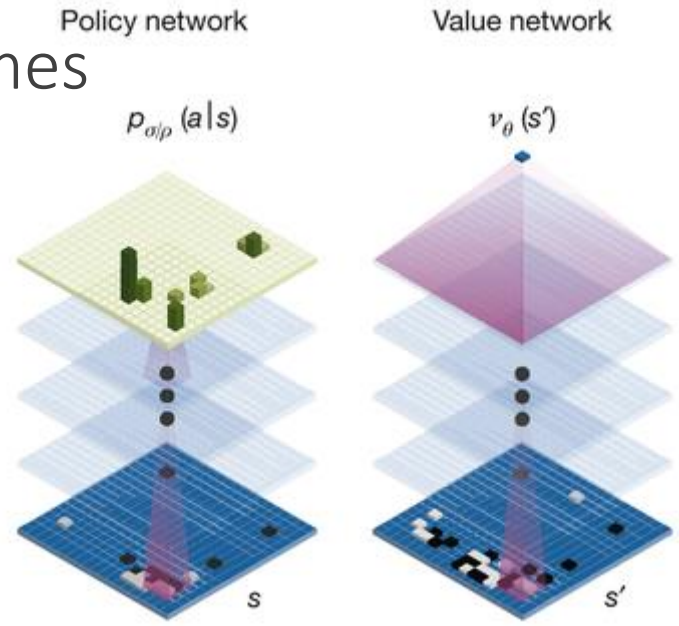
AlphaGo

- AlphaGo relies on a tree procedure for search
- AlphaGo relies on ConvNets to guide the tree search
- A ConvNet trained to predict human moves achieved 57% accuracy
  - Humans make intuitive moves instead of thinking too far ahead
- For Deep RL we don't want to predict human moves
  - Instead, we want the agent to learn the optimal moves
- Two policy networks (one per side) + One value network
- Value network trained on 30 million positions while policy networks play



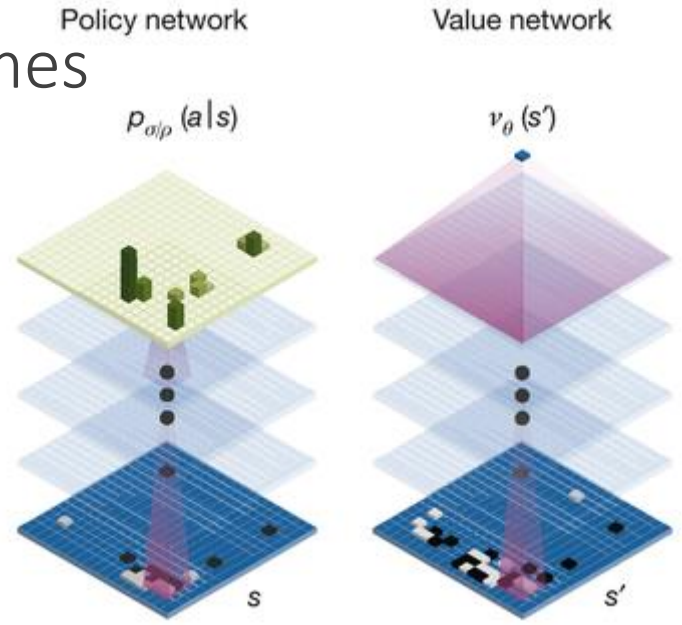
AlphaGo

- Both humans and Deep RL agents play better end games
  - Maybe a fundamental cause?
- In the end the value of a state is computed equally from Monte Carlo simulation and the value network output
  - Combining intuitive play and thinking ahead
- Where is the catch?



AlphaGo

- Both humans and Deep RL agents play better end games
  - Maybe a fundamental cause?
- In the end the value of a state is computed equally from Monte Carlo simulation and the value network output
  - Combining intuitive play and thinking ahead
- Where is the catch?
- State is not the pixels but positions
- Also, the game states and actions are highly discrete



Exam and theses

- What is allowed
  - 1 A4 page with whatever you want on it (handwritten or printed)
- What is not allowed
  - Everything else (internet, phones, messaging, etc)
- And if you are interested in the coming months in research in any of the topics discussed in the course
  - especially in temporal sequences, deep dynamics, video, causality, generative models and/or oncology (together with the Netherlands Cancer Insitute)

  Drop me a line (egavves@uva.nl)

Summary

- Reinforcement Learning
- Q-Learning
- Deep Q-Learning
- Policy-based Deep RL
- Model-based Deep RL
- Making Deep RL stable