

Deep Reinforcement Learning

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April 24, 2023





Outline

Sequential Decision Making

Reinforcement Learning

Markov Decision Processes Policy Iteration Other Solution Methods

Deep Reinforcement Learning

Deep Q Learning AlphaGo AlphaGo Zero



Sequential Decision Making





Sequential decision making: Multi-armed bandit problem



Action Formalize choosing a machine as **action** a at time t from a set A Reward Action a_t has a **different**¹ **unknown pdf** p(r|a) generating **reward** r_t

¹ This is not how gambling works



Sequential decision making: Multi-armed bandit problem



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Find action a producing the maximum expected reward over time t:

$$\max_{a} \mathbb{E} \left[p(r|a) \right]$$

Difference to supervised learning: No feedback on what action to choose





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- \rightarrow Estimate the joint pdf online as $\frac{1}{t} \sum_{i=1}^{t} \mathbf{r}_{i} := Q_{t}(\mathbf{a})$
- We call $Q_t(\mathbf{a})$ the action-value function, which changes with every new information



Incremental update of $Q_t(\mathbf{a})$

$$Q_{t+1}(\mathbf{a}) = \frac{1}{t} \sum_{i=1}^{t} \mathbf{r}_{i}$$

$$= \frac{1}{t} \left(\mathbf{r}_{t} + \sum_{i=1}^{t-1} \mathbf{r}_{i} \right)$$

$$= \frac{1}{t} \left(\mathbf{r}_{t} + (t-1) \frac{1}{t-1} \sum_{i=1}^{t-1} \mathbf{r}_{i} \right)$$

$$= \frac{1}{t} \left(\mathbf{r}_{t} + (t-1) Q_{t}(\mathbf{a}) \right)$$

$$= \frac{1}{t} \left(\mathbf{r}_{t} + t Q_{t}(\mathbf{a}) - Q_{t}(\mathbf{a}) \right)$$

$$= Q_{t}(\mathbf{a}) + \frac{1}{t} \left(\mathbf{r}_{t} - Q_{t}(\mathbf{a}) \right)$$





- Reward is maximized by a policy $\pi(a)$ choosing $\max_a Q_t(a)$
- We exploit a known good action
- This is a deterministic¹ policy called greedy action selection





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Exploration



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- We exploit a known good action
- This is a deterministic¹ policy called greedy action selection
- However we need to obtain samples r_a
- → This means we cannot follow the greedy action selection policy for learning
- → Sometimes explore by selecting other moves which could potentially be better

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We sample discrete actions a from $\pi(a)$, but what distributions can we use?



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 |A| is the cardinality of the set of different actions A **Epsilon Greedy**

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Softmax

$$\pi(a) = rac{\mathrm{e}^{Q_t(a)/ au_t}}{\sum_{n=1}^{|A|} \mathrm{e}^{Q_t(a_n)/ au_t}}$$

• au_t is called **temperature** and used to decrease exploration over time



So far we ...

• considered sequential decision making in a setting known as multi-armed bandits



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- found out that estimating a function Q(a) and the greedy action selection policy $\pi(a) = \max Q(a)$ maximized our reward
- learned that exploration of different actions is necessary
- assumed rewards didn't depend on a state of the world
- and our action at time t doesn't influence the rewards from a at t+1

NEXT TIME

ON DEEP LEARNING



Deep Reinforcement Learning - Part 2

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Reinforcement Learning





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- Rewards now additionally depend on the state s_t:

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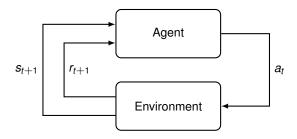
$$p(r_t|s_t,a_t)$$

- However this setting is known as contextual bandit
- In the full **reinforcement learning problem**, actions influence the state:

$$p(s_{t+1}|s_t,a_t)$$



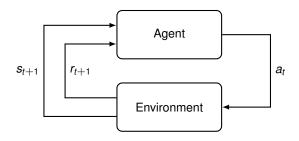




Action An action at time t from a set A

State A state s_t from a set S



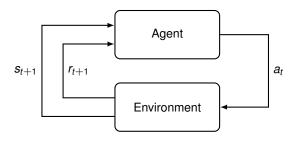


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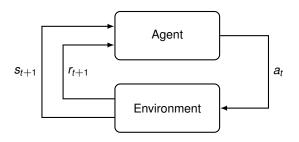
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Reward Transition produces reward $r_{t+1} \in R \subset \mathbb{R}$ according to $p(r_{t+1}|s_t, a_t)$





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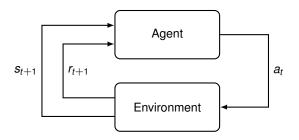
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Policy Agents choose actions a_t by a policy $\pi(a|s)$





Action An action at at time t from a set A

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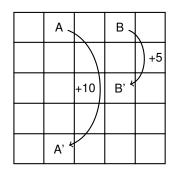
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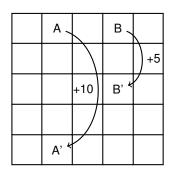
If all those sets are **finite** we call this a **finite MDP**





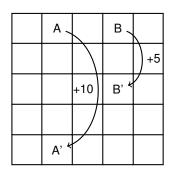
- → Here s is the field we are currently on.
- The agent can move in all four directions
- Any action which would leave the grid has $p(s_{t+1}|a_t, s_t)$ equal to a δ distribution on $s_{t+1} = s_t$ and a similarly deterministic $r_t = -1$





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- Every state we reach other than tile A' and B' deterministically causes $r_t = 0$

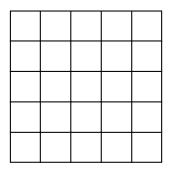




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- ullet Every state we reach other than tile A' and B' deterministically causes $r_t=0$
- On A or B any action will take us to A' or B' respectively



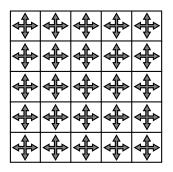
Example policy



- Policies now depend on s_t
- We can extend the **uniform random policy** to be independent from s_t



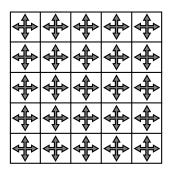
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Example policy



- Policies now depend on s_t
- We can extend the **uniform random policy** to be independent from s_t
- However there's no reason to believe that this policy is any good
- · How can we estimate good policies?



What is a good policy?

- → We have to be precise about good
- Preliminary we have to state two kinds of tasks
 - 1. Episodic tasks which have an end
 - Continuing tasks which are infinitely long
- Unify them using a terminal state in episodic tasks which only transition to themselves with deterministic $r_t = 0$
- Goal is to maximize the future return

$$\max_{\pi(s_t, a_t)} g_t = \sum_{k=t+1}^T \gamma^{k-t-1} r_k$$

- γ is a **discount** reducing influence of rewards **far** in the future
- $\gamma \in (0,1]$ meaning that $\gamma = 1$ is allowed as long as $T \neq \infty$

NEXT TIME

ON DEEP LEARNING



Deep Reinforcement Learning - Part 3

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Policy Iteration



• Before we used the action-value function Q(a)



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- Now a_t has to depend on s_t
- \rightarrow Use an oracle predicting the future reward g_t following $\pi(s_t, a_t)$ from s_t



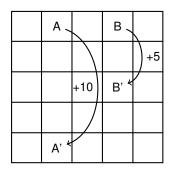


- Before we used the action-value function Q(a)
- Now a_t has to depend on s_t
- \rightarrow Use an oracle predicting the future reward g_t following $\pi(s_t, a_t)$ from s_t
- We introduce the state-value function $V_{\pi}(s)$

$$V_{\pi}(s) = \mathbb{E}_{\pi}\left[g_t|s_t
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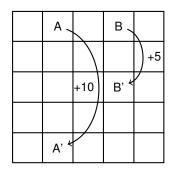




The definition of the gridworld

Recall our grid example





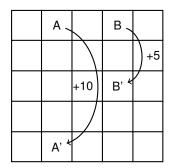
3.3	8.8	4.4	5.3	1.5
1.5	3.0	2.3	1.9	0.5
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-1.9	-1.3	-1.2	-1.4	-2.0

The definition of the gridworld

 $V_{\pi}(s)$ for the uniform random policy

- Recall our grid example
- Some edge tiles are negative since the policy can't control the move





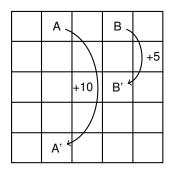
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The definition of the gridworld

 $V_{\pi}(s)$ for the uniform random policy

- Recall our grid example
- Some edge tiles are negative since the policy can't control the move
- What if we use the **greedy action selection** policy on this $V_{\pi}(s)$?
- We get a better policy!



Action-value function

- Before we used the action-value function Q(a)
- Now we introduced $V_{\pi}(s)$ filling a similar role



Action-value function

- Before we used the action-value function Q(a)
- Now we introduced $V_{\pi}(s)$ filling a similar role
- We can also introduce the **action-value function** $Q_{\pi}(s, a)$
- Basically this accounts for the **transition probabilities**

$$Q_{\pi}(s,a) = \mathbb{E}_{\pi}\left[g_t|s_t,a_t
ight] = \mathbb{E}_{\pi}\left[\sum_{k=t+1}^{T}\gamma^{k-t-1}r_k|s_t,a_t
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- We can state its existence without referring to a specific policy:

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• $Q^*(s, a)$ can also be defined and is related to $V^*(s_t)$ by:

$$Q^*(s,a) = \mathbb{E}[r_{t+1} + \gamma V^*(s_{t+1})]$$
 (2)



Optimal Value-function Example

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 $V_{\pi}(s)$ for the uniform random policy



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22.0	24.4	22.0	19.4	17.5
19.8	22.0	19.8	17.8	16.0
17.8	19.8	17.8	16.0	14.4
16.0	17.8	16.0	14.4	13.0
14.4	16.0	14.4	13.0	11.7

 $V_{\pi}(s)$ for the uniform random policy

• Observe that V^* is strictly positive since it's deterministic



• Policies can now be ordered: $\pi \geq \pi'$ if and only if $V_\pi(s) \geq V_{\pi'}(s), \forall s \in S$



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- Any policy π with $V_{\pi} = V^*$ is an optimal policy π^*



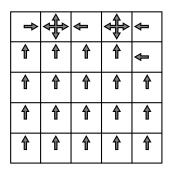
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- Given either V^* or Q^* an optimal policy is directly obtained by **greedy action** selection



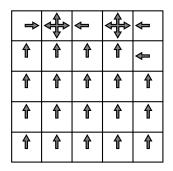
Greedy Action Selection on $V^*(s)$ or $Q^*(s, a)$



 $\pi'(s,a) =$ Greedy Action Selection on $V_{\pi}(s)$ with $\pi(s, a)$ being uniform random



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$$\pi^*(s,a) =$$
 Greedy Action Selection on $V^*(s)$



A Tool to Compute Optimal Value-functions

• We still need to compute $V^*(s)$ and $Q^*(s, a)$



A Tool to Compute Optimal Value-functions

- We still need to compute $V^*(s)$ and $Q^*(s,a)$
- For this the Bellman equations can be utilized
- They are consistency conditions for the value functions

Bellman equation for $V_{\pi}(s)$

$$V_{\pi}(s) = \sum_{a} \pi(a|s) \sum_{s_{t+1},r} p(s_{t+1},r|s,a) [r + \gamma V_{\pi}(s_{t+1})]$$



Policy Evaluation

- The Bellman equations form a system of linear equations which can be solved for small problems
- Better: **Iteratively solve**, by turning the Bellman equations into **update rules**:

$$V_{k+1}(s) = \sum_{a} \pi(a|s) \sum_{s_{l+1},r} p(s_{l+1},r|s,a) \left[r + \gamma V_k(s_{l+1}) \right]$$

For all $s \in S$



Policy Improvement

• $V_{\pi}(s)$ is used to **guide our search** for good policies



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- Another necessary step is to update the policy



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- Now iterate evaluation of the greedy policy on $V_{\pi}(s)$



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- Stop iterating if the policy stops changing
- But is this guaranteed to work?



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- In general if

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This also implies:

$$V_{\pi'}(s) \geq V_{\pi}(s)$$

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- Because we **only select greedy** we have $Q_{\pi}(s, a) > V_{\pi}(s)$ before convergence
- So iteratively updating $V_{\pi}(s)$ and using **greedy action selection** is quaranteed to work here
- We terminate if the policy no longer changes



- We consider changing a single action a_t in state s_t but following π
- In general if

$$Q_{\pi}(s,\pi'(s)) \geq V_{\pi}(s)\,, orall s \in S \implies \pi' \geq \pi$$

$$V_{\pi'}(s) \geq V_{\pi}(s)$$

- Because we **only select greedy** we have $Q_{\pi}(s, a) > V_{\pi}(s)$ before convergence
- So iteratively updating $V_{\pi}(s)$ and using **greedy action selection** is quaranteed to work here
- We terminate if the policy no longer changes
- Last remark: If we don't loop over all $s \in S$ for policy evaluation, but update the policy directly this algorithm is called **Value iteration**

NEXT TIME

ON DEEP LEARNING



Deep Reinforcement Learning - Part 4

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April 24, 2023





Other Solution Methods



 Both policy iteration and value iteration require using the updated policies during learning to obtain better approximations to $V^*(s)$



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- Both policy iteration and value iteration require using the updated policies during learning to obtain better approximations to $V^*(s)$
- For this reason we call them on-policy algorithms
- Additionally we assumed the **state-transition** pdf and **reward** pdf are known
- Can we relax this?
- Yes. The methods differ mostly how they perform policy evaluation



Monte Carlo Techniques

Properties

- Only for episodic tasks
- Off-policy learns $V^*(s)$ by following any **arbitrary** $\pi(s,a)$
- Does not need information about dynamics of the environment



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- Does not need information about dynamics of the environment

Scheme

- Generate an episode by using some policy
- Loop backwards over the episode accumulating the expected future reward $g_t = g_{t+1} + r_{t+1}$
- If a state was **not yet** visited append g_t to a list returns(s_t)
- Update $V_{s_t} = \frac{1}{N} \sum_{n=1}^{N} returns_n(s_t)$



Temporal Difference Learning

Properties

- On-policy
- Does not need information about dynamics of the environment



Temporal Difference Learning

Properties

- On-policy
- Does not need information about dynamics of the environment

Scheme

- Loop and follow $\pi(s_t, a_t)$
- Use a from $\pi(s_t, a_t)$, observe r_t, s_{t+1}
- Update: $V_{t+1}(s) = V_t(s) + \alpha [r_t + \gamma V_t(s_{t+1}) V_t(s_t)]$

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Temporal Difference Learning

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- Update: $V_{t+1}(s) = V_t(s) + \alpha [r_t + \gamma V_t(s_{t+1}) V_t(s_t)]$
- Converges to the optimal solution
- A variant of this estimates $Q_{(s,a)}$ and is known as SARSA



Q Learning

Properties

- Off-policy
- Temporal difference type of method
- Does not need information about dynamics of the environment



Q Learning

Properties

- Off-policy
- Temporal difference type of method
- Does not need information about dynamics of the environment

Scheme

- Loop and follow $\pi(s_t, a_t)$ derived from $Q_t(s, a)$ e.g. ϵ -greedy
- Use a from $\pi(s_t, a_t)$, observe r_t, s_{t+1}
- Update: $Q_{t+1}(s, a) = Q_t(s_t, a_t) + \alpha \left[r_t + \gamma \max_{a} Q_t(s_{t+1}, a_t) Q_t(s_t, a_t) \right]$



If you have Universal Function Approximators

• What about just parametrizing $\pi(s_t, a_t, \mathbf{w})$ by weights \mathbf{w} and use some loss-function L?



If you have Universal Function Approximators

- What about just parametrizing $\pi(s_t, a_t, \mathbf{w})$ by weights \mathbf{w} and use some loss-function 1?
- → Known as policy gradient and this instance is called REINFORCE



If you have Universal Function Approximators

- What about just parametrizing $\pi(s_t, a_t, \mathbf{w})$ by weights \mathbf{w} and use some loss-function 1?
- → Known as policy gradient and this instance is called REINFORCE
- Generate an episode using $\pi(s_t, a_t, \mathbf{w})$
- Go forwards in the episode: t = 0, ..., T 1
- $\mathbf{w} = \mathbf{w} + \eta \gamma^t g_t \nabla_{\mathbf{w}} \ln \left(\pi(\mathbf{a}_t | \mathbf{s}_t, \mathbf{w}) \right)$

NEXT TIME

ON DEEP LEARNING



Deep Reinforcement Learning - Part 5

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Deep Reinforcement Learning





Deep Q Learning



Atari Games: Human-level control through deep reinforcement learning [4]

- Volodymyr Mnih et al. (Google DeepMind) 2013/2015
- Idea: Let a neural network play Atari games!
- Input: Current and three subsequent video frames from game
- Processed by network trained with reinforcement learning
- Goal: learn best controller movements



Atari Pac-Man



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- Goal: learn best controller movements
- Convolutional layers for frame processing, fully-connected for final decision making

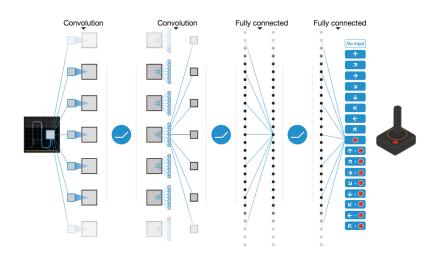


Atari Pac-Man

Source: Human-level control through deep reinforcement learning [4]



Learning Atari Games



Source: Human-level control through deep reinforcement learning [4]



Learning Atari Games

- Deep Q-network: Deep network that applies Q-learning
- State s_t of the game: current + 3 previous frames (image stack)
- 18 outputs associated with an action
- → Each output estimates optimal action value for "its" action given the input
- Instead of label & cost function, update to maximize reward
- Reward: +1/-1 when game score increased/decreased, 0 otherwise
- ϵ -greedy policy with ϵ decreasing to a low value during training
- Semi-gradient form of Q-learning to update network weights w
- Uses mini-batches to accumulate weight updates



Target Network

Weight update:

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \alpha \left[r_{t+1} + \gamma \max_{a} \hat{q}(s_{t+1}, a, \mathbf{w}_t) - \hat{q}(s_t, a_t, \mathbf{w}_t) \right] \cdot \nabla \mathbf{w}_t \hat{q}(s_t, a_t, \mathbf{w}_t)$$

- Problem: The target $\gamma \max_{a} \hat{q}(s_{t+1}, a, \mathbf{w}_{t})$ is a function of \mathbf{w}_{t} .
- → Target changes simultaneously with the weights we want to learn!
- → Training can oscillate or diverge

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Target Network

Weight update:

$$\mathbf{w}_{t+1} = \mathbf{w}_t + \alpha \left[r_{t+1} + \gamma \max_{a} \hat{q}(s_{t+1}, a, \mathbf{w}_t) - \hat{q}(s_t, a_t, \mathbf{w}_t) \right] \cdot \nabla \mathbf{w}_t \hat{q}(s_t, a_t, \mathbf{w}_t)$$

- Problem: The target $\gamma \max_{a} \hat{q}(s_{t+1}, a, \mathbf{w}_{t})$ is a function of \mathbf{w}_{t} .
- → Target changes simultaneously with the weights we want to learn!
- → Training can oscillate or diverge
- Idea: Use a second target network:
- After each C steps, copy weights of action-value network to a duplicate network and keep them fixed
- Use output \bar{q} of "target network" as a target to stabilize:

$$\gamma \max_{a} \bar{q}(s_{t+1}, a, \mathbf{w}_t)$$



Experience Replay

Goal: Reduce correlation between updates

- After performing action a_t for image stack s_t (state) and receiving reward r_t, add (s_t, a_t, r_t, s_{t+1}) to replay memory
- → Memory accumulates experiences
- To update the network, draw random samples from memory, instead of taking the most recent ones
- → Removes dependence on current weights
- → Increases stability



Atari Breakout Example



Video on learning Atari Breakout. Click here



AlphaGo



Mastering the game of Go with deep neural networks and tree search [1]

- Go is an ancient Chinese boardgame: Black plays against white for control over the board
- Simple rules but extremely high number of possible moves and situations
- Performance on par with professional human players thought years away



Traditional Go board



Challenges in Go

- Go is a "perfect information" game: No hidden information and no chance
- Theoretically, we can construct a full game tree and traverse it with Minimax to find the best moves



Challenges in Go

- Go is a "perfect information" game: No hidden information and no chance
- Theoretically, we can construct a full game tree and traverse it with Minimax to find the best moves
- Problem: High number of legal moves (≈ 250 chess ≈ 35)
- Games involve many moves (\approx 150)
- → Exhaustive search is infeasible!



Challenges in Go (cont.)

- Search tree can be pruned if we have an accurate evaluation function
- For chess (DeepBlue) already extremely complex and based on massive human input
- For Go: "No simple yet reasonable evaluation function will ever be found for Go." (Müller 2002) [5]



Challenges in Go (cont.)

- Search tree can be pruned if we have an accurate evaluation function
- For chess (DeepBlue) already extremely complex and based on massive human input
- For Go: "No simple yet reasonable evaluation function will ever be found for Go." (Müller 2002) [5]
- Still: AlphaGo beat Lee Sedol and Ke Jie, two of the world's strongest players in 2016 and 2017!

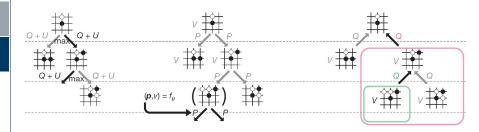


Mastering the game of Go with deep neural networks and tree search [1]

- AlphaGo was developed by Silver et al. (also Google DeepMind)
- Combination of multiple methods:
 - Deep neural networks
 - Monte Carlo tree search (MCTS)
 - Supervised learning and
 - Reinforcement learning
- First improvement compared to a full tree search: Monte Carlo Tree Search (MCTS)
- Networks to support efficient search through tree



Monte Carlo Tree Search



- Idea: Run many Monte Carlo simulations of episodes (=entire Go games) to select action (=where to place a stone)
- Starting from a root node representing the current state, MCTS iteratively extends the search tree



Monte Carlo Tree Search (cont.)

Algorithm:

- Selection: Starting at root, traverse with tree policy to a leaf node
- **Expansion**: (Optional) add one or more child nodes to the current leaf
- **Simulation**: From the current or the child node, simulate episode with actions according to rollout policy
- **Backup**: Propagate the received reward back through the tree
- Repeat for a certain amount of time, then stop
- Then, choose action from root node according to accumulated statistics
- Start again with new root node



Monte Carlo Tree Search (cont.)

- Tree policy guides in how far successful paths are frequented more often.
- Typical exploration/exploitation trade-off.
- Problem: Estimation via MCTS not accurate enough for Go.



Monte Carlo Tree Search (cont.)

- Tree policy guides in how far successful paths are frequented more often.
- Typical exploration/exploitation trade-off.
- Problem: Estimation via MCTS not accurate enough for Go.
- Ideas in AlphaGo:
 - Control tree expansion by using a neural network to find promising actions.
 - Improve value estimation by a neural network.
- More efficient extension & evaluation of search tree → better at Go!



Deep Neural Networks for Go

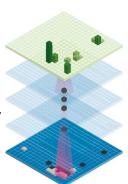
Utilization of three different networks:

- Policy network: Suggests the next move in leaf nodes for extension
- Value network: Given the current board position, get chances of winning
- Rollout policy network: Guide rollout action selection
- All networks are deep convolutional networks
- Input: Current board position and additional precomputed features



Policy Network

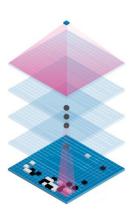
- 13 conv-layers, one output for each point on the Go board.
- Huge database of expert human moves (30 mio) available.
- Start with supervised learning: Train network to predict the next move in human expert plays
- Further train network with reinforcement learning by playing against older versions of itself. Reward when winning the game
- Older versions avoid correlation and instability
- Training time: 3 weeks on 50 GPUs + 1 day for RL





Value network

- Same architecture as policy network but just one output node
- Goal: Estimate how likely the current state leads to a win
- Training utilized self-play games of reinforcement learned policy
- → Trained using Monte-Carlo policy evaluation for 30 mio positions from these games
- Training time: 1 week on 50 GPUs





Rollout policy network

- AlphaGo could use policy network to select moves during roll-out
- Problem: Inference comparatively high: 5 ms
- Solution: Train simpler, linear network on subset of data that provides actions fast
- Speedup of ≈ 1000 compared to policy network → more simulations possible



AlphaGo Zero



AlphaGo Zero: Do we even need humans for training?

- After minor improvements, Silver et al. proposed AlphaGo Zero:
- → Solely trained with reinforcement learning & playing against itself!
- Simpler MCTS, no rollout policy
- Include MCTS in self-play games
- Multi-task training: Policy and value network share initial layers
- Further extension in Dec. '17: AlphaZero [3] able to also play chess and shoqi

NEXT TIME

ON DEEP LEARNING



Next Time

- Algorithms to learn if we don't even observe rewards
- How to benefit from adversaries
- Extensions to perform image processing tasks



Comprehensive Questions

- What is a policy?
- What are value functions?
- Explain the exploitation vs exploration dilemma.
- Describe typical solutions to the dilemma.
- What is the difference of a multi armed bandit problem to the full reinforcement learning problem?
- Describe a Markov decision process.
- Is an optimal policy necessarily unique?
- What do the Bellman equations represent?
- Describe policy iteration.
- Why does policy iteration work?
- How can you beat your friends in every Atari game?
- How can one master the game of Go?



Further Reading





Reinforcement Learning

Richard Sutton

 Link - the one real reference for Reinforcement learning in its 2018 draft, including Deep Q learning and Alpha Go details



References





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- [1] David Silver, Aja Huang, Chris J Maddison, et al. "Mastering the game of Go with deep neural networks and tree search". In: Nature 529.7587 (2016), pp. 484-489.
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