

## CSCE 496/896 Lecture 7: Reinforcement Learning

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## Introduction

- Consider learning to choose actions, e.g.,
  - Robot learning to dock on battery charger
  - Learning to choose actions to optimize factory output
  - Learning to play Backgammon, chess, Go, etc.
- Note several problem characteristics:
  - Delayed reward (thus have problem of **temporal credit assignment**)
  - Opportunity for active exploration (versus exploitation of known good actions)
    - ⇒ Learner has some influence over the training data it sees
  - Possibility that state only **partially observable**

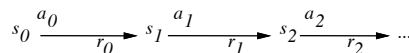
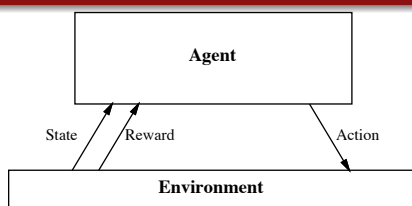
## Example: TD-Gammon (Tesauro, 1995)

- Learn to play Backgammon
- Immediate Reward:
  - +100 if win
  - 100 if lose
  - 0 for all other states
- Trained by playing 1.5 million games against itself
- Approximately equal to best human player at that time

## Outline

- Markov decision processes
- The agent's learning task
- Q learning
- Temporal difference learning
- Deep Q learning
- Example: Learning to play Atari

## Reinforcement Learning Problem



Goal: Learn to choose actions that maximize

$$r_0 + \gamma r_1 + \gamma^2 r_2 + \dots, \text{ where } 0 \leq \gamma < 1$$

## Markov Decision Processes

Assume

- Finite set of states  $S$
- Set of actions  $A$
- At each discrete time  $t$  agent observes state  $s_t \in S$  and chooses action  $a_t \in A$
- Then receives immediate reward  $r_t$ , and state changes to  $s_{t+1}$
- Markov assumption:  $s_{t+1} = \delta(s_t, a_t)$  and  $r_t = r(s_t, a_t)$ 
  - I.e.,  $r_t$  and  $s_{t+1}$  depend only on **current** state and action
  - Functions  $\delta$  and  $r$  may be nondeterministic
  - Functions  $\delta$  and  $r$  not necessarily known to agent

## Agent's Learning Task

- Execute actions in environment, observe results, and
  - Learn **action policy**  $\pi : S \rightarrow A$  that maximizes

$$E [r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \dots]$$

- from any starting state in  $S$ 
  - Here  $0 \leq \gamma < 1$  is the **discount factor** for future rewards
- Note something new:
  - Target function is  $\pi : S \rightarrow A$
  - But we have no training examples of form  $\langle s, a \rangle$
  - Training examples are of form  $\langle \langle s, a \rangle, r \rangle$
  - I.e., not told what best action is, instead told reward for executing action  $a$  in state  $s$

## Value Function

- First consider deterministic worlds
- For each possible policy  $\pi$  the agent might adopt, we can define **discounted cumulative reward** as

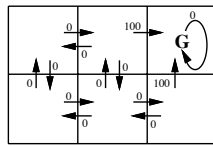
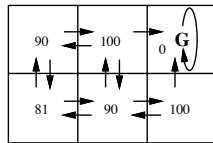
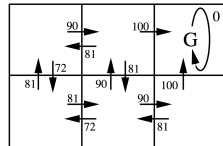
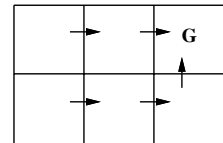
$$V^\pi(s) \equiv r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \dots = \sum_{i=0}^{\infty} \gamma^i r_{t+i},$$

where  $r_t, r_{t+1}, \dots$  are generated by following policy  $\pi$ , starting at state  $s$

- Restated, the task is to learn an **optimal policy**  $\pi^*$

$$\pi^* \equiv \operatorname{argmax}_{\pi} V^\pi(s), \quad (\forall s)$$

## Value Function


 $r(s, a)$  values

 $V^*(s)$  values

 $Q(s, a)$  values


One optimal policy

## What to Learn

- We might try to have agent learn the evaluation function  $V^{\pi^*}$  (which we write as  $V^*$ )
- It could then do a lookahead search to choose best action from any state  $s$  because

$$\pi^*(s) = \operatorname{argmax}_a [r(s, a) + \gamma V^*(\delta(s, a))],$$

i.e., choose action that maximized immediate reward + discounted reward if optimal strategy followed from then on

- E.g.,  $V^*(\text{bot. ctr.}) = 0 + \gamma 100 + \gamma^2 0 + \gamma^3 0 + \dots = 90$
- A problem:
  - This works well if agent knows  $\delta : S \times A \rightarrow S$ , and  $r : S \times A \rightarrow \mathbb{R}$
  - But when it doesn't, it can't choose actions this way

## Q Function

- Define new function very similar to  $V^*$ :

$$Q(s, a) \equiv r(s, a) + \gamma V^*(\delta(s, a))$$

i.e.,  $Q(s, a)$  = total discounted reward if action  $a$  taken in state  $s$  and optimal choices made from then on

- If agent learns  $Q$ , it can choose optimal action even without knowing  $\delta$

$$\begin{aligned} \pi^*(s) &= \operatorname{argmax}_a [r(s, a) + \gamma V^*(\delta(s, a))] \\ &= \operatorname{argmax}_a Q(s, a) \end{aligned}$$

- $Q$  is the evaluation function the agent will learn

Training Rule to Learn  $Q$ 

- Note  $Q$  and  $V^*$  closely related:

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

- Which allows us to write  $Q$  recursively as

$$\begin{aligned} Q(s_t, a_t) &= r(s_t, a_t) + \gamma V^*(\delta(s_t, a_t)) \\ &= r(s_t, a_t) + \gamma \max_{a'} Q(s_{t+1}, a') \end{aligned}$$

- Let  $\hat{Q}$  denote learner's current approximation to  $Q$ ; consider training rule

$$\hat{Q}(s, a) \leftarrow r + \gamma \max_{a'} \hat{Q}(s', a'),$$

where  $s'$  is the state resulting from applying action  $a$  in state  $s$

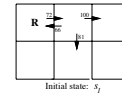
## Q Learning for Deterministic Worlds

- For each  $s, a$  initialize table entry  $\hat{Q}(s, a) \leftarrow 0$
- Observe current state  $s$
- Do forever:
  - Select an action  $a$  (greedily or probabilistically) and execute it
  - Receive immediate reward  $r$
  - Observe the new state  $s'$
  - Update the table entry for  $\hat{Q}(s, a)$  as follows:

$$\hat{Q}(s, a) \leftarrow r + \gamma \max_{a'} \hat{Q}(s', a')$$

- $s \leftarrow s'$
- Note that actions not taken and states not seen don't get explicit updates (might need to generalize)

## Updating $\hat{Q}$



$$\begin{aligned} \hat{Q}(s_1, a_{right}) &\leftarrow r + \gamma \max_{a'} \hat{Q}(s_2, a') \\ &= 0 + 0.9 \max\{66, 81, 100\} \\ &= 90 \end{aligned}$$

Can show via induction on  $n$  that if rewards non-negative and  $\hat{Q}$ s initially 0, then

$$(\forall s, a, n) \quad \hat{Q}_{n+1}(s, a) \geq \hat{Q}_n(s, a)$$

and

$$(\forall s, a, n) \quad 0 \leq \hat{Q}_n(s, a) \leq Q(s, a)$$

## Updating $\hat{Q}$ Convergence

- $\hat{Q}$  **converges to  $Q$** : Consider case of deterministic world where each  $\langle s, a \rangle$  is visited infinitely often
- Proof**: Define a **full interval** to be an interval during which each  $\langle s, a \rangle$  is visited. Will show that during each full interval the largest error in  $\hat{Q}$  table is reduced by factor of  $\gamma$
- Let  $\hat{Q}_n$  be table after  $n$  updates, and  $\Delta_n$  be the maximum error in  $\hat{Q}_n$ ; i.e.,

$$\Delta_n = \max_{s, a} |\hat{Q}_n(s, a) - Q(s, a)|$$

- Let  $s' = \delta(s, a)$

## Updating $\hat{Q}$ Convergence

- For any table entry  $\hat{Q}_n(s, a)$  updated on iteration  $n + 1$ , error in the revised estimate  $\hat{Q}_{n+1}(s, a)$  is

$$\begin{aligned} |\hat{Q}_{n+1}(s, a) - Q(s, a)| &= |(r + \gamma \max_{a'} \hat{Q}_n(s', a')) - (r + \gamma \max_{a'} Q(s', a'))| \\ &= \gamma |\max_{a'} \hat{Q}_n(s', a') - \max_{a'} Q(s', a')| \\ (*) &\leq \gamma \max_{a'} |\hat{Q}_n(s', a') - Q(s', a')| \\ (**) &\leq \gamma \max_{s', a'} |\hat{Q}_n(s', a') - Q(s', a')| \\ &= \gamma \Delta_n \end{aligned}$$

(\*) works since  $|\max_a f_1(a) - \max_a f_2(a)| \leq \max_a |f_1(a) - f_2(a)|$

(\*\*) works since max will not decrease

## Updating $\hat{Q}$ Convergence

- Also,  $\hat{Q}_0(s, a)$  and  $Q(s, a)$  are both bounded  $\forall s, a$   
 $\Rightarrow \Delta_0$  bounded
- Thus after  $k$  full intervals, error  $\leq \gamma^k \Delta_0$
- Finally, each  $\langle s, a \rangle$  visited infinitely often  $\Rightarrow$  number of intervals infinite, so  $\Delta_n \rightarrow 0$  as  $n \rightarrow \infty$

## Nondeterministic Case

- What if reward and next state are non-deterministic?
- We redefine  $V, Q$  by taking expected values:

$$\begin{aligned} V^\pi(s) &\equiv \mathbb{E}[r_t + \gamma r_{t+1} + \gamma^2 r_{t+2} + \dots] \\ &= \mathbb{E}\left[\sum_{i=0}^{\infty} \gamma^i r_{t+i}\right] \end{aligned}$$

$$\begin{aligned} Q(s, a) &\equiv \mathbb{E}[r(s, a) + \gamma V^*(\delta(s, a))] \\ &= \mathbb{E}[r(s, a)] + \gamma \mathbb{E}[V^*(\delta(s, a))] \\ &= \mathbb{E}[r(s, a)] + \gamma \sum_{s'} P(s' | s, a) V^*(s') \\ &= \mathbb{E}[r(s, a)] + \gamma \sum_{s'} P(s' | s, a) \max_{a'} Q(s', a') \end{aligned}$$

## Nondeterministic Case

- $Q$  learning generalizes to nondeterministic worlds
- Alter training rule to

$$\hat{Q}_n(s, a) \leftarrow (1 - \alpha_n) \hat{Q}_{n-1}(s, a) + \alpha_n [r + \gamma \max_{a'} \hat{Q}_{n-1}(s', a')]$$

where

$$\alpha_n = \frac{1}{1 + \text{visits}_n(s, a)}$$

- Can still prove convergence of  $\hat{Q}$  to  $Q$ , with this and other forms of  $\alpha_n$  (Watkins and Dayan, 1992)

## Temporal Difference Learning

- $Q$  learning: reduce error between successive  $Q$  estimates
- $Q$  estimate using one-step time difference:

$$Q^{(1)}(s_t, a_t) \equiv r_t + \gamma \max_a \hat{Q}(s_{t+1}, a)$$

- Why not two steps?

$$Q^{(2)}(s_t, a_t) \equiv r_t + \gamma r_{t+1} + \gamma^2 \max_a \hat{Q}(s_{t+2}, a)$$

- Or  $n$ ?

$$Q^{(n)}(s_t, a_t) \equiv r_t + \gamma r_{t+1} + \dots + \gamma^{(n-1)} r_{t+n-1} + \gamma^n \max_a \hat{Q}(s_{t+n}, a)$$

## Temporal Difference Learning

- Blend all of these ( $0 \leq \lambda \leq 1$ ):

$$\begin{aligned} Q^\lambda(s_t, a_t) &\equiv (1 - \lambda) [Q^{(1)}(s_t, a_t) + \lambda Q^{(2)}(s_t, a_t) + \lambda^2 Q^{(3)}(s_t, a_t) + \dots] \\ &= r_t + \gamma [(1 - \lambda) \max_a \hat{Q}(s_{t+1}, a) + \lambda Q^\lambda(s_{t+1}, a_{t+1})] \end{aligned}$$

- TD( $\lambda$ ) algorithm uses above training rule
  - Sometimes converges faster than  $Q$  learning
  - Converges for learning  $V^*$  for any  $0 \leq \lambda \leq 1$  (Dayan, 1992)
  - Tesauro's TD-Gammon uses this algorithm

## Representing $\hat{Q}$

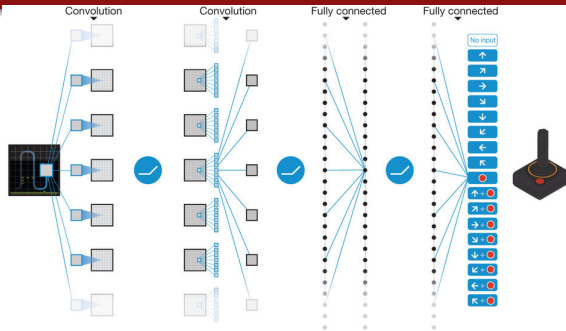
- Convergence proofs assume that  $\hat{Q}(s, a)$  represented **exactly**
  - E.g., as an array
- How well does this scale to real problems?
- What can we do about it?

## Deep $Q$ Learning

- We already have machinery to approximate functions based on labeled samples
- Search for a **deep  $Q$  network** (DQN) to implement function  $Q_\theta$  approximating  $Q$
- Each training instance is  $\langle s, a \rangle$  with label  $y(s, a) = r + \gamma \max_{a'} Q_\theta(s', a')$ 
  - I.e., take action  $a$  in state  $s$ , get reward  $r$  and observe new state  $s'$
  - Then use  $Q_\theta$  to compute label  $y(s, a)$  and update as usual
- Convergence proofs break, but get scalability to large state space

## DQN Example: Playing Atari (Mnih et al., 2015)

- Applied same architecture and hyperparameters to 49 Atari 2600 games
  - System learned effective policy for each, very different, game
  - No game-specific modifications
- State description consists of raw input from emulator
- Frames rescaled to  $84 \times 84$ , single channel
- Each state is sequence of four most recent frames
- Rather than take  $s$  and  $a$  as inputs, network takes  $s$  and gives prediction of  $Q(s, a)$  for all  $a$  as outputs
- Clipped positive rewards to  $+1$  and negative to  $-1$
- Evaluated each policy's performance against professional human tester

DQN Example: Playing Atari (Mnih et al., 2015)  
Architecture

- Input:  $84 \times 84 \times 4$ , 3 convolutional layers, two dense
- Conv:  $32 \ 20 \times 20$ ,  $64 \ 9 \times 9$ ,  $64 \ 7 \times 7$
- 512 units in dense layers
- 18 outputs: Output  $i$  is estimate of  $Q(s_i, a_i)$

DQN Example: Playing Atari (Mnih et al., 2015)  
Training

- Reward signal at time  $t$ :  $+1$  if score increased,  $-1$  if decreased,  $0$  otherwise
- Action in game selected via  $\epsilon$ -greedy policy: With probability  $\epsilon$  choose action u.a.r., with probability  $(1 - \epsilon)$  choose  $\arg\max_a Q_\theta(s, a)$
- Chosen action  $a_t$  run in emulator, which returns reward  $r_t$  and next frame for state  $s_{t+1}$
- Update:

$$\theta_{t+1} = \theta_t + \alpha \left[ r_t + \gamma \max_{a'} Q_{\theta_t}(s_{t+1}, a') - Q_{\theta_t}(s_t, a_t) \right] \nabla Q_{\theta_t}(s_t, a_t)$$

- Trained with RMSProp, mini-batch size of 32

DQN Example: Playing Atari (Mnih et al., 2015)  
Modifications

Deep RL systems can be unstable or divergent, so Mnih:

1. Used **experience replay**: Rather than train on consecutive tuples, tuple  $(s_t, a_t, r_t, s_{t+1})$  from game play added to **replay memory**
  - Replay memory sampled u.a.r. for training mini-batches
  - Independent instances in mini-batches reduces correlations in training data
  - Trained **off-policy** (policy trained is not the one choosing actions in game)
2. Used separate **target network**  $\tilde{\theta}$  to generate labels:

$$\theta_{t+1} = \theta_t + \alpha \left[ r_t + \gamma \max_{a'} Q_{\tilde{\theta}}(s_{t+1}, a') - Q_{\theta_t}(s_t, a_t) \right] \nabla Q_{\theta_t}(s_t, a_t)$$

Copied  $\theta$  into  $\tilde{\theta}$  every  $C$  updates

3. **Clipped** error term  $[r_t + \dots - Q_{\theta_t}(s_t, a_t)]$  to  $[-1, 1]$

DQN Example: Playing Atari (Mnih et al., 2015)  
Pseudocode

**Algorithm 1: deep Q-learning with experience replay.**

Initialize replay memory  $D$  to capacity  $N$

Initialize action-value function  $Q$  with random weights  $\theta$

Initialize target action-value function  $\tilde{Q}$  with weights  $\theta^- = \theta$

**For** episode  $= 1, M$  **do**

Initialize sequence  $s_1 = \{x_1\}$  and preprocessed sequence  $\phi_1 = \phi(s_1)$

**For**  $t = 1, T$  **do**

With probability  $\epsilon$  select a random action  $a_t$

otherwise select  $a_t = \arg\max_a Q(\phi(s_t), a; \theta)$

Execute action  $a_t$  in emulator and observe reward  $r_t$  and image  $x_{t+1}$

Set  $s_{t+1} = s_t, a_t, x_{t+1}$  and preprocess  $\phi_{t+1} = \phi(s_{t+1})$

Store transition  $(\phi_t, a_t, r_t, \phi_{t+1})$  in  $D$

Sample random minibatch of transitions  $(\phi_j, a_j, r_j, \phi_{j+1})$  from  $D$

Set  $y_j = \begin{cases} r_j + \gamma \max_{a'} \tilde{Q}(\phi_{j+1}, a'; \theta^-) & \text{if episode terminates at step } j+1 \\ r_j + \gamma \max_{a'} Q(\phi_{j+1}, a'; \theta^-) & \text{otherwise} \end{cases}$

Perform a gradient descent step on  $(y_j - Q(\phi_j, a_j; \theta))^2$  with respect to the network parameters  $\theta$

Every  $C$  steps reset  $\tilde{Q} = Q$

**End For**

**End For**

## DQN Example: Playing Atari (Mnih et al., 2015)

## During Training

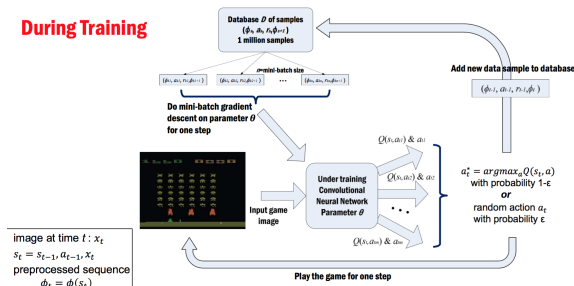
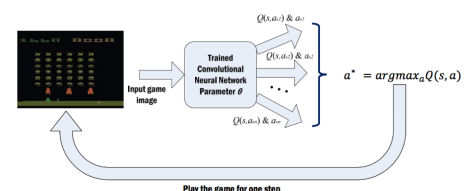


image at time  $t$ :  $x_t$   
 $s_t = x_{t-1}, a_{t-1}, x_t$   
 preprocessed sequence  
 $\phi_t = \phi(s_t)$

## DQN Example: Playing Atari (Mnih et al., 2015)

## After Training



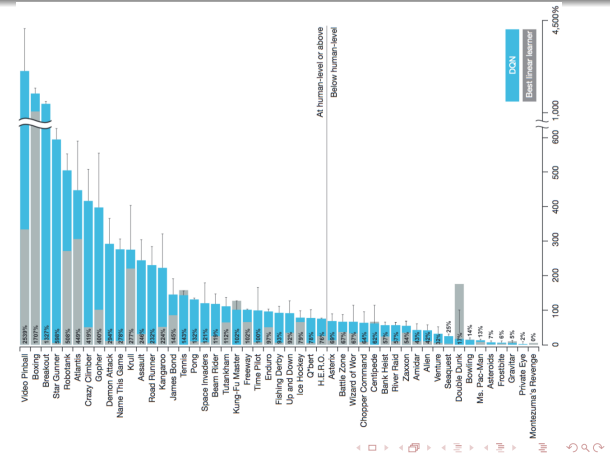
## DQN Example: Playing Atari (Mnih et al., 2015)

### Results

- Trained on each game for 50 million frames, no transfer learning
- Testing: Averaged final score over 30 sessions/game
- Measured performance of DQN RL and linear learner RL (with custom features) vs. human player:  $100(\text{RL} - \text{random}) / (\text{human} - \text{random})$ 
  - i.e., human=100%, random=0%
- DQN outperformed linear learner on all but 6 games, outperformed human on 22, and comparable to human on 7
- Shortcoming: Performance poor (near random) when long-term planning required, e.g., Montezuma's revenge

## DQN Example: Playing Atari (Mnih et al., 2015)

### Results



## Go Example

- One of the most complex board games humans have
- Checkers has about  $10^{18}$  distinct states, Backgammon:  $10^{20}$ , Chess:  $10^{47}$ , Go:  $10^{170}$ 
  - Number of atoms in the universe around  $10^{81}$
  - Another issue: Difficult to quantify goodness of a board configuration
- AlphaGo:** Used RL and human knowledge to defeat professional player
- AlphaGo Zero:** Improved on AlphaGo without human knowledge
- AlphaZero:** Generalized to chess and shogi with general RL

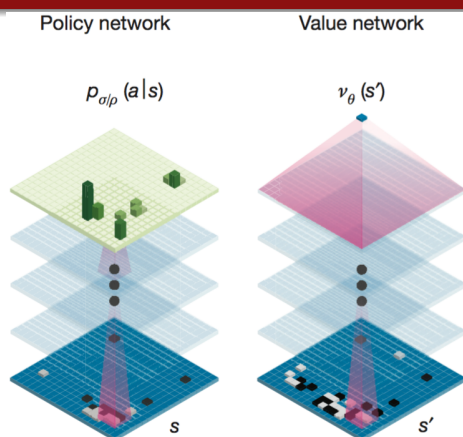
## AlphaGo (Silver et al., 2016)

### Overview

- Input:  $19 \times 19 \times 48$  image stack representing player's and opponent's board positions, number of opponent's stones that could be captured there, etc.
- Training
  - Supervised learning** (classification) of policy networks  $p_\pi$  and  $p_\sigma$  based on expert moves for states
  - Transfer learning** from  $p_\sigma$  to policy network  $p_p$
  - Reinforcement learning** to refine  $p_p$  via **policy gradient** and **self-play**
  - Regression** to learn value network  $v_\theta$
- Live play
  - Uses these networks in **Monte Carlo tree search** to choose actions during games
- 99.8% winning rate vs other Go programs and defeated human Go champion 5-0

## AlphaGo (Silver et al., 2016)

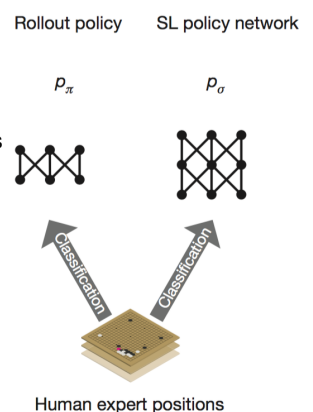
### Overview



## AlphaGo (Silver et al., 2016)

### Supervised Learning

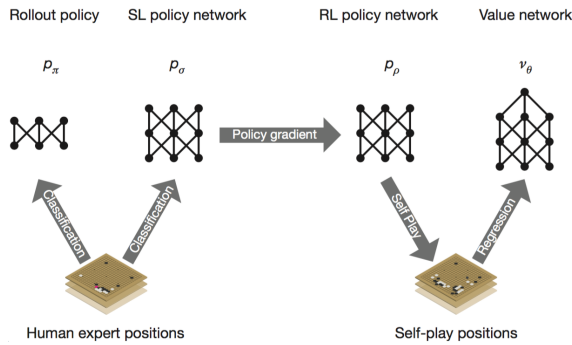
- Supervised learning** of policies  $p_\pi$  and  $p_\sigma$
- Board positions from **KGS Go Server**, labels are experts' moves
- Supervised learning of policies  $p_\pi$  and  $p_\sigma$
- $p_\sigma$  is full network (accuracy 57%, 3ms/move),  $p_\pi$  is simpler (accuracy 24% 2μs/move)



## AlphaGo (Silver et al., 2016)

### Transfer Learning

Transfer learning of  $p_\sigma$  to  $p_\rho$  (same arch., copy parameters)



## AlphaGo (Silver et al., 2016)

### Reinforcement Learning

- Trained  $p_\rho$  via play against  $p_{\bar{\rho}}$  (randomly selected earlier version of  $p_\rho$ )
- For state  $s_t$ , **terminal reward**  $z_t = +1$  if game ultimately won from  $s_t$  and  $-1$  otherwise
- Note  $p_\rho$  does not compute value of actions like Q-learning does
  - It **directly** implements a policy that outputs  $a_t$  given  $s_t$
  - Use **policy gradient** method to train:
    - If agent chooses action  $a_t$  in state  $s_t$  and ultimately wins 90% of the time, what should happen to  $p_\rho(a_t | s_t)$ ?
    - How can we make that happen?

## AlphaGo (Silver et al., 2016)

### Policy Gradient

- **REINFORCE: REward Increment = Nonnegative Factor times Offset Reinforcement times Characteristic Eligibility**
- Perform **gradient ascent** to increase probability of actions that on average lead to greater rewards:

$$\Delta \rho_j = \alpha (r - b_s) \frac{\partial \log p_\rho(a | s)}{\partial \rho_j},$$

$\alpha$  is learning rate,  $r$  is reward,  $a$  is action taken in state  $s$ , and  $b_s$  is **reinforcement baseline** (independent of  $a$ )

- $b$  keeps expected update same but reduces variance
- E.g., if all actions from  $s$  good,  $b_s$  helps differentiate
- Common choice:  $b_s = \hat{v}(s)$  = estimated value of  $s$

## AlphaGo (Silver et al., 2016)

### Policy Gradient

- AlphaGo uses REINFORCE with baseline  $b_s = v_\theta(s)$ ,  $r = z_t$ , and sums over all game steps  $t = 1, \dots, T$
- Average updates over games  $i = 1, \dots, n$

$$\Delta \rho = \frac{\alpha}{n} \sum_{i=1}^n \sum_{t=1}^T (z_t^i - v_\theta(s_t^i)) \nabla_\rho \log p_\rho(a_t^i | s_t^i)$$

## AlphaGo (Silver et al., 2016)

### Value Learning

- $v_\theta(s)$  approximates  $v^{p_\rho}(s)$  = value of  $s$  under policy  $p_\rho$
- Regression problem on state-outcome pairs  $(s, z)$
- Train with MSE
- Analogous to experience replay, mitigated overfitting by drawing each instance from a unique self-play game:
  - 1 Choose time step  $U$  uniformly from  $\{1, \dots, 450\}$
  - 2 Play moves  $t = 1, \dots, U$  from  $p_\sigma$
  - 3 Choose move  $a_U$  uniformly
  - 4 Play moves  $t = U + 1, \dots, T$  from  $p_\rho$
  - 5 Instance  $(s_{U+1}, z_{U+1})$  added to train set

## AlphaGo (Silver et al., 2016)

### Live Play

- Now, we're ready for live play
- Rather than exclusively using  $p_\rho$  or  $v_\theta$  to determine actions, will instead base action choice on a **rollout algorithm**
- Use the functions learned to simulate game play from state  $s$  forward in time ("rolling it out") and computing statistics about the outcome
- Repeat as much as time limit allows, then choose most favorable action
  - ⇒ **Monte Carlo Tree Search (MCTS)**



## AlphaGo (Silver et al., 2016)

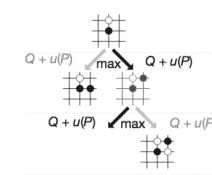
### Monte Carlo Tree Search

- Given current state  $s$ , MCTS runs four operations:
  - Selection:** Given a tree rooted at  $s$ , follow **tree policy** to traverse and select a leaf node
  - Expansion:** Expand selected leaf by adding children
  - Evaluation (simulation):** Perform rollout to end of game
    - Use  $p_\pi$  to speed up this part
  - Backup:** Use rollout results to update action values of tree
- Each tree edge  $((s, a)$  pair) has statistics:
  - Prior probability**  $P(s, a)$
  - Action values**  $W_v(s, a)$  and  $W_r(s, a)$
  - Value counts**  $N_v(s, a)$  and  $N_r(s, a)$
  - Mean action value**  $Q(s, a)$
- After many parallel simulations, choose action maximizing  $N_v(s, a)$

## AlphaGo (Silver et al., 2016)

### Monte Carlo Tree Search: Selection

#### a Selection



- Before reaching leaf state, choose action

$$a_t = \operatorname{argmax}_a (Q(s_t, a) + u(s_t, a))$$

where

$$u(s, a) = cP(s, a) \frac{\sqrt{\sum_b N_r(s, b)}}{1 + N_r(s, a)}$$

- I.e., if  $(s_t, a_t)$  has been evaluated a lot relative to other actions from  $s_t$ ,  $N_r(s_t, a_t)$  is large and  $a_t$  is evaluated mainly by  $Q$
- Otherwise, exploration is encouraged
- To avoid all searches choosing same actions: When  $(s_t, a_t)$  chosen, update stats as if  $n_{vl}$  games lost

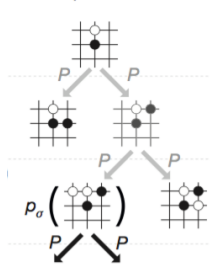
$$N_r(s_t, a_t) = N_r(s_t, a_t) + n_{vl}$$

$$W_r(s_t, a_t) = W_r(s_t, a_t) - n_{vl}$$

## AlphaGo (Silver et al., 2016)

### Monte Carlo Tree Search: Expansion

#### b Expansion



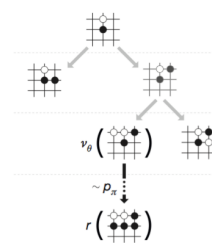
- If  $N_r(s, a) > n_{thr}$ , expand next state  $s'$  in tree

$$[N_v(s', a) = N_r(s', a) = 0, W_v(s', a) = W_r(s', a) = 0, P(s', a) = p_\sigma(a | s')]$$

## AlphaGo (Silver et al., 2016)

### Monte Carlo Tree Search: Evaluation

#### c Evaluation

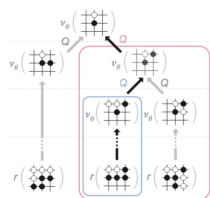


- Expand from leaf  $s_L$  until game ends
- At each time  $t \geq L$ , **each player** chooses  $a_t \sim p_\pi$
- At game's end, compute  $z_t = \pm 1$  for all  $t$

## AlphaGo (Silver et al., 2016)

### Monte Carlo Tree Search: Backup

#### d Backup



At end of simulated game, update statistics for all steps  $t \leq L$

- Undo virtual loss and update  $z$ :

$$N_r(s_t, a_t) = N_r(s_t, a_t) - n_{vl} + 1$$

$$W_r(s_t, a_t) = W_r(s_t, a_t) + n_{vl} + z_t$$

- After leaf evaluation done:

$$N_v(s_t, a_t) = N_v(s_t, a_t) + 1$$

$$W_v(s_t, a_t) = W_v(s_t, a_t) + v_\theta(s_L)$$

- Take weighted average for final action value:

$$Q(s, a) = (1 - \lambda) \left( \frac{W_v(s, a)}{N_v(s, a)} \right) + \lambda \left( \frac{W_r(s, a)}{N_r(s, a)} \right)$$

## AlphaGo Zero (Silver et al., 2017)

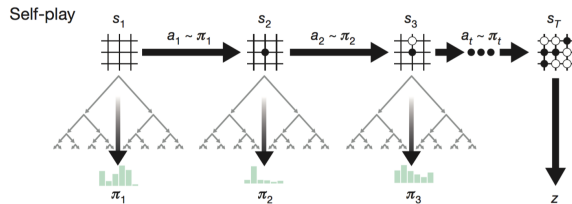
### Overview

- The "Zero" refers to zero human knowledge
- No supervised training from KGS Go data
  - Trained only via RL in self-play
  - Trained a single network  $(p, v) = f_\theta$  for both policy and value
- Integrated MCTS into training as well as live play
  - Folded lookahead search into training loop
  - Did not rollout to end of game
- Input:  $19 \times 19 \times 17$  image stack:
  - Eight of 17 binary planes indicate locations of player's stones the past 8 time steps
  - Eight of 17 binary planes indicate locations of opponent's stones the past 8 time steps
  - Final plane indicates color to play
- Discovered new Go knowledge during self-play, including previously unknown tactics



## AlphaGo Zero (Silver et al., 2017)

### Self-Play



- Play games against self, choosing actions  $a_t \sim \pi_t$  via MCTS
- Outcome of game recorded as  $z = \pm 1$

## AlphaGo Zero (Silver et al., 2017)

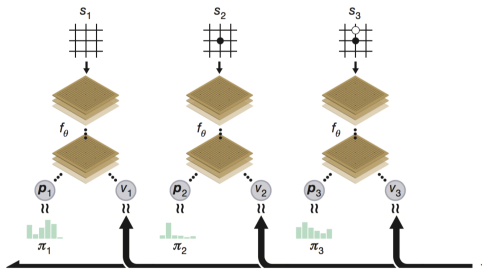
### Training

- Training is a form of **policy iteration**: Alternating between
  - **Policy evaluation**: Estimating value  $v$  of policy  $p$
  - **Policy improvement**: Improving policy wrt  $v$
- Use MCTS to map NN policy  $p$  to search policy  $\pi$
- Self-play outcomes inform updates to  $v$

## AlphaGo Zero (Silver et al., 2017)

### Training

#### Neural network training

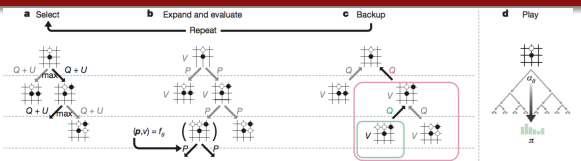


- State  $s_t$ 's targets are distribution  $\pi_t$  and reward  $z_t$
- Update network using loss function

$$\underbrace{\text{sq loss}}_{(z_t - v(s_t))^2} - \underbrace{\text{CE}}_{-\pi_t^\top \log p_t} + \underbrace{\text{regularizer}}_{+c \|\theta\|^2}$$

## AlphaGo Zero (Silver et al., 2017)

### MCTS



- MCTS similar to that of AlphaGo, but drop  $N_r$  and  $W_r$  since no rollout:  $[N(s, a), W(s, a), Q(s, a), P(s, a)]$
- (a) Select: same as before, but  $u(s, a)$  uses  $N$  instead of  $N_r$
- (b) Expand + evaluate:  $f_\theta$  compute value  $v(s)$  (modulo symmetry) for backup instead of rollout to game end
- (c) Backup: same as before, but no  $N_r$  or  $W_r$
- (d) Play policy:  $\pi(a | s_0) = N(s_0, a)^{1/\tau} / \sum_b N(s_0, b)^{1/\tau}$  ( $\tau$  controls exploration)

## AlphaZero (Silver et al., 2017b)

- AlphaGo Zero's approach applied to chess and shogi
- Same use of  $(p, v) = f_\theta(s)$  and MCTS
- Go-specific parts removed + other generalizations
- No game-specific hyperparameter tuning
  - Similar framework as Atari

Game	White	Black	Win	Draw	Loss
Chess	AlphaZero	Stockfish	25	25	0
	Stockfish	AlphaZero	3	47	0
Shogi	AlphaZero	Elmo	43	2	5
	Elmo	AlphaZero	47	0	3
Go	AlphaZero	AGO 3-day	31	—	19
	AGO 3-day	AlphaZero	29	—	21

Table 1: Tournament evaluation of AlphaZero in chess, shogi, and Go, as games won, drawn or lost from AlphaZero's perspective, in 100 game matches against Stockfish, Elmo, and the previously published AlphaGo Zero after 3 days of training. Each program was given 1 minute of thinking time per move.