# ST455: Reinforcement Learning

Lecture 9: Model-Based Reinforcement Learning

Chengchun Shi

#### **Lecture Outline**

- 1. What is Model-Based RL
- 2. How to implement Model-Based RL
- 3. Simulation-Based Search
- 4. Mastering the Game of Go

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### Recap: Planning vs Learning

Two fundamental problems in sequential decision making

#### Planning

- A model of the environment (e.g., state transition, reward function) is known
- The agent performs computations with its model, without any external interaction
- a.k.a. deliberation, reasoning, introspection, pondering, thought, search

#### Learning

- The environment is initially **unknown**
- The agent interacts with the environment
- The agent **learns** the optimal policy from experience

#### RL Algorithms We Have Covered So Far

- Dynamic Programming (Lecture 3): learn value from model (planning)
- MC, TD (Lectures 3 7): learn value from experience (learning)
- Policy Gradient (Lecture 8): learn policy from experience (learning)
- Today's lecture: Model-based RL
  - learn **model** from experience
  - use both learned model and experience to construct a value function or policy
  - combine learning with planning

#### What is a Model?

- A model  $\mathcal{M}$  is a **representation** of an MDP  $\langle \mathcal{S}, \mathcal{A}, \mathcal{P}, \mathcal{R}, \gamma \rangle$
- The state space S and action space A are usually known to us
- The discounted factor  $\gamma$  is user-specified
- ullet Only need to learn the state transition  ${\cal P}$

$$\mathcal{P}_{ss'}^{a} = \Pr(S_{t+1} = s' | S_t = s, A_t = a)$$

and reward function  $\mathcal{R}$ 

$$\mathcal{R}_{s}^{a} = \mathbb{E}(R_{t}|S_{t} = s, A_{t} = a)$$

#### Model-Free v.s. Model-Based RL

- Model-based RL
  - Learn the model (e.g., reward  $\mathcal{R}_s^a$  and transition  $\mathcal{P}_{ss'}^a$ ) from experience
  - Plan value or policy from model or integrate planning with learning
- Model-free RL
  - Learn value or policy without learning the reward and transition function
  - Rely on Bellman optimality equation
  - Examples: MC, TD, Policy gradient

# Model-Free v.s. Model-Based RL (Cont'd)

- Pros of model-based RI
- In some applications, we have a perfect model (e.g., Go, chess)
- Can handle offline data (more in the next lecture)

- Pros of model-free RL
- Dimensional reduction
- Easier to learn value than model
- # of parameters of  $Q^{\pi^{\text{opt}}}$ :  $|\mathcal{S}||\mathcal{A}|$
- # of parameters of  $\mathcal{R}_s^a$ :  $|\mathcal{S}||\mathcal{A}|$
- ullet # of parameters of  $\mathcal{P}^{a}_{ss'}$ :  $|\mathcal{S}|^{2}|\mathcal{A}|$

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#### How to Implement Model-Based RL

- First, we learn a model (reward and state transition functions) based on data
- Next, we can implement **planning** based on the learned model
- Alternatively, we can **integrate planning with learning** (Dyna)

#### How to Implement Model-Based RL

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#### **Model Learning**

- Goal: estimate  $\mathcal{R}_s^a$  and  $\mathcal{P}_{ss'}^a$  from experience  $\{S_0, A_0, R_0, \cdots, S_T\}$
- Using supervised learning

$$S_0, A_0 \rightarrow R_0, S_1$$

$$S_1, A_1 \rightarrow R_1, S_2$$

$$\vdots$$

$$S_{T-1}, A_{T-1} \rightarrow R_{T-1}, S_T$$

- Learning  $s, a \rightarrow r$  is a **regression** problem
- Learning  $s, a \rightarrow s'$  is a conditional density estimation problem
- Loss function: least square/Huber loss, KL divergence
- Compute parameter that minimizes empirical loss

# **Models for Conditional Density Estimation**

- Table lookup model
- Conditional kernel density estimation
- Gaussian process model [Williams and Rasmussen, 2006]
- Deep conditional generative learning<sup>1</sup>
  - mixture density network [Rothfuss et al., 2019]
  - normalising flows [Trippe and Turner, 2018]

<sup>&</sup>lt;sup>1</sup>https://deepgenerativemodels.github.io/notes/index.html

#### Table Lookup Model

- Finite MDP model
- Count visits  $N(s, a) = \sum_{t=0}^{T-1} \mathbb{I}(S_t = s, A_t = a)$  to each state-action pair

$$\widehat{\mathcal{P}}_{ss'}^{a} = \frac{1}{N(s,a)} \sum_{t=0}^{T-1} \mathbb{I}(S_t = s, A_t = a, S_{t+1} = s')$$

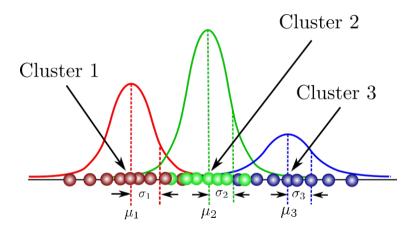
$$\widehat{\mathcal{R}}_{s}^{a} = \frac{1}{N(s,a)} \sum_{t=0}^{T-1} \mathbb{I}(S_t = s, A_t = a) R_t$$

- Alternatively
  - At each time step t, record experience tuple  $\langle S_t, A_t, R_t, S_{t+1} \rangle$
  - To sample model, based on a state-action pair (s, a), randomly pick tuple matching  $(s, a, \bullet, \bullet)$

### Mixture Density Network

- Learn a generic conditional probability mass/density function of Y given X = x, f(y|x) ( $Y = S_{t+1}$  and  $X = (S_t, A_t)$  in our RL setting)
- Combine Gaussian mixture model with deep neural networks
- Gaussian mixture model has universal approximation property to approximate any density function
- Deep neural networks have universal approximation property to approximate any mean and variance functions in Gaussian distribution

#### What is a Gaussian Mixture Model



Taken from https:

//towardsdatascience.com/gaussian-mixture-models-explained-6986aaf5a95

# Gaussian Mixture Model (Cont'd)

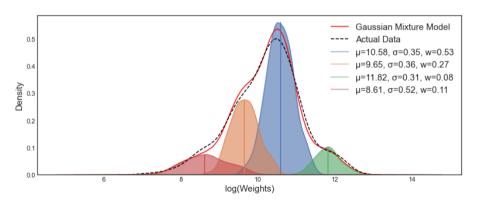
Model a probability density function f(y) by

$$f(\mathbf{y}) = \sum_{k=1}^{K} \omega_k \phi(\mathbf{y}; \mu_k, \sigma_k^2),$$

where  $\phi(\bullet; \mu, \sigma^2)$  denotes the probability density function of a Gaussian variable with mean  $\mu$  and variance  $\sigma^2$ , and  $\omega_k$  denotes the probability the variable belongs to the kth cluster

#### **Universal Approximation Property**

Gaussian mixture model approximates any probability density function as the number of clusters  $K \to \infty$ 



### Mixture Density Network

• Model a probability density function f(y) by

$$f(\mathbf{y}) = \sum_{k=1}^{K} \omega_k \phi(\mathbf{y}; \mu_k, \sigma_k^2)$$

- We want to model a **conditional** probability density function f(y|x)
- Can be modelled via a conditional Gaussian mixture model

$$f(\mathbf{y}|\mathbf{x}) = \sum_{k=1}^{K} \omega_k(\mathbf{x}) \phi(\mathbf{y}; \mu_k(\mathbf{x}), \sigma_k^2(\mathbf{x}))$$

• Use deep neural networks to parametrize  $\omega_k(\bullet)$ ,  $\mu_k(\bullet)$  and  $\sigma_k^2(\bullet)$ 

#### How to Implement Model-Based RL

- First, we learn a model (reward and state transition functions) based on data
- Next, we can implement **planning** based on the learned model
- Alternatively, we can **integrate planning with learning** (Dyna)

### Planning with Dynamic Programming

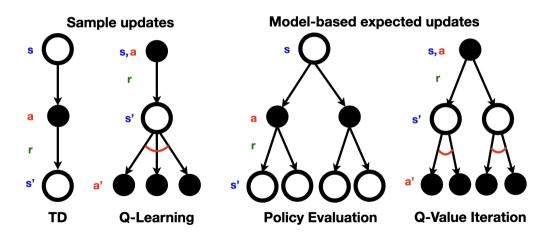
- Give a model  $\langle \widehat{\mathcal{R}}, \widehat{\mathcal{P}} \rangle$
- Use dynamic programming algorithm
  - Policy iteration

$$\pi_0 \longrightarrow V^{\pi_0} \longrightarrow \pi_1 \longrightarrow V^{\pi_1} \longrightarrow \cdots \longrightarrow \pi^{opt} \longrightarrow V^{\pi^{opt}}$$

Value iteration

$$V^{\pi_0} \longrightarrow V^{\pi_1} \longrightarrow V^{\pi_2} \longrightarrow \cdots \longrightarrow V^{\pi^{opt}} \longrightarrow \pi^{opt}$$

#### **Difference From Model-Free Methods**



### Planning with Model-Free RL

- A simple but powerful approach to planning
- Use the model only to generate samples
- **Sample** experience from model:

$$\mathbf{S}' \sim \widehat{\mathcal{P}}_{\mathbf{S}, \bullet}^{\mathbf{A}}$$
 and  $R = \widehat{\mathcal{R}}_{\mathbf{S}}^{\mathbf{A}}$ 

- Apply model-free RL to samples
  - MC control
  - SARSA
  - Q-learning
- This is often more efficient than dynamic programming-based method

#### Planning with an Inaccurate Model

- Model-based RL computes  $\pi^{opt}$  with respect to the model  $\langle \mathcal{S}, \mathcal{A}, \widehat{\mathcal{R}}, \widehat{\mathcal{P}}, \widehat{\gamma} \rangle$
- Quality of the estimated policy depends heavily on the accuracy of the model
- When model is inaccurate, planning yields a suboptimal policy
- Solution 1: when model is wrong, using model-free RL
- **Solution** 2: integrate planning with learning

#### How to Implement Model-Based RL

- First, we learn a model (reward and state transition functions) based on data
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### Real and Simulated Experience

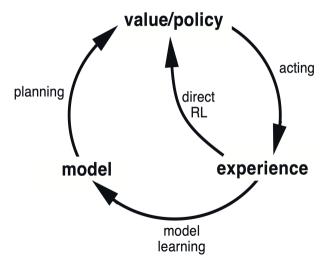
- We consider two sources of experience
- **Real experience**: Sampled from environment (true MDP)

$$\{S_0, A_0, R_0, \cdots, S_T\}$$

• **Simulated experience**: Sampled from model (estimated MDP)

$$\mathbf{S}' \sim \widehat{\mathcal{P}}_{\mathbf{S},\bullet}^{\mathbf{A}}$$
 and  $R = \widehat{\mathcal{R}}_{\mathbf{S}}^{\mathbf{A}}$ 

# Dyna



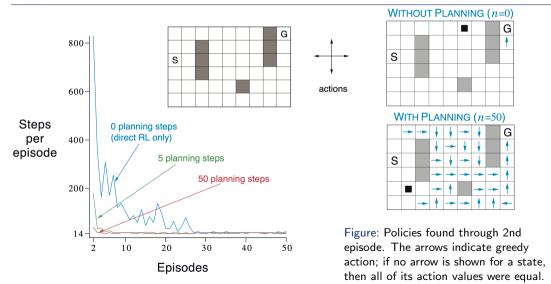
### Dyna-Q Algorithm

- Initialize Q(s, a) and model(s, a) for all s and a
- **do** forever:
  - (a)  $s \leftarrow$  current (non-terminal) state
  - (b)  $\mathbf{a} \leftarrow \varepsilon$ -greedy( $\mathbf{s}, \mathbf{Q}$ )
  - (c) Execute action a; observe reward r and next state s'
  - (d)  $Q(s, a) \leftarrow Q(s, a) + \alpha[r + \gamma \max_{a'} Q(s', a') Q(s, a)]$
  - (e)  $model(s, a) \leftarrow (r, s')$
  - (f) Repeat *n* times:
    - s ← random previously observed state
    - $a \leftarrow$  random action previously taking in s

$$(r, s') \sim \mathsf{model}(s, a)$$

$$Q(s, a) \leftarrow Q(s, a) + \alpha[r + \gamma \max_{a'} Q(s', a') - Q(s, a)]$$

### Dyna-Q on a Simple Maze



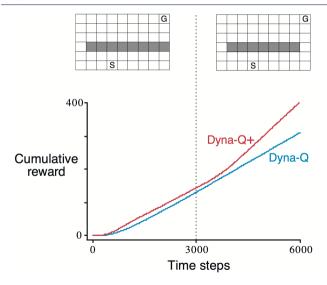
# Dyna-Q<sup>+</sup>

- Motivation: models maybe incorrect; leads to sub-optimal policies
  - Limited sample size for a given state-action pair
  - the environment changes and new behavior has not been observed
- Idea: encourage long-untried actions
  - For each state—action pair, check how many times have elapsed since it was last tried
  - Use **bonus reward** in action selection:

$$\boldsymbol{a} \leftarrow \boldsymbol{\varepsilon} - \operatorname{greedy}(\boldsymbol{s}, \boldsymbol{Q} + \kappa \sqrt{\tau}),$$

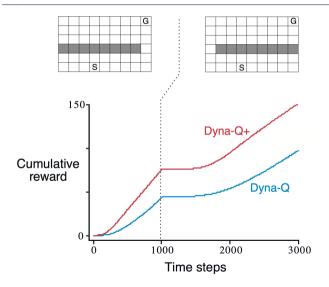
for some small  $\kappa > 0$ .  $\tau(s, a)$  denotes the times have elapsed since (s, a) was last tried

#### Dyna-Q with an Inaccurate Model



- The changed environment is easier
- The left environment was used for the first 3000 steps
- The right environment was used for the rest

### Dyna-Q with an Inaccurate Model (Cont'd)



- The changed environment is harder
- The left environment was used for the first 1000 steps
- The right environment was used for the rest

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### Two Ways of Planning

#### Background planning

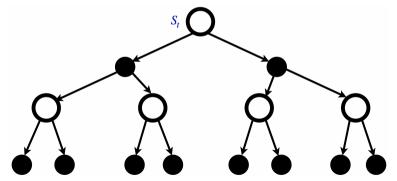
- Planning is used well before an action is selected
- Need to select actions fo each state, not current state
- Examples: policy iteration and value iteration in Lecture 3

#### Decision-time planning

- Planning is started and completed after encountering each new state S<sub>t</sub>
- As a computation to determine A<sub>t</sub>
- On the next step planning begins anew with  $S_{t+1}$  to produce  $A_{t+1}$ , and so no

#### **Simulation-Based Search**

- Decision-time planning to select the **best** action
- Build a **search tree** with the current state  $S_t$  at the root
- Simulate episodes of experience from now with the model
- Apply model-free RL to simulate trajectories



### Simple Monte-Carlo Search

- ullet Given a model  ${\mathcal M}$  and a **simulation policy**  $\pi$
- For each action  $a \in A$ 
  - 1. Simulate K episodes from current state  $S_t$

$$\left\{\boldsymbol{S_{t}, a, R_{t}^{k}, S_{t+1}^{k}, A_{t+1}^{k}, R_{t+1}^{k}, \cdots, S_{T}^{k}}\right\}_{k=1}^{K} \sim \mathcal{M}, \pi$$

2. Evaluate actions by mean return (Monte-Carlo Evaluation)

$$Q(oldsymbol{S_t}, oldsymbol{a}) = rac{1}{K} \sum_{k=1}^K G_t 
ightarrow Q^\pi(oldsymbol{S_t}, oldsymbol{a})$$

Select action with maximum value

$$A_t = \arg\max_{a \in \mathcal{A}} Q(S_t, a)$$

## Monte-Carlo Tree Search (Evaluation)

- Given a model M
- Simulate K episodes from current states  $S_t$  using current policy  $\pi$

$$\left\{\boldsymbol{S}_{t}, \boldsymbol{A}_{t}^{k}, \boldsymbol{R}_{t}^{k}, \boldsymbol{S}_{t+1}^{k}, \boldsymbol{A}_{t+1}^{k}, \boldsymbol{R}_{t+1}^{k}, \cdots, \boldsymbol{S}_{T}^{k}\right\}_{k=1}^{K} \sim \mathcal{M}, \boldsymbol{\pi}$$

- Build a search tree containing visited states and actions
- Evaluate states Q(s, a) by mean return of episodes from s, a

$$Q(s, a) = \frac{1}{N(s, a)} \sum_{k=1}^{K} \sum_{u=t}^{T} \mathbb{I}(S_u = s, A_u = a) G_u \rightarrow Q^{\pi}(s, a)$$

After search is finished, select current action with maximum value in search tree

$$A_t = \arg\max_{a \in A} Q(S_t, a)$$

### Monte-Carlo Tree Search (Simulation)

- In MCTS, the simulation policy (rollout policy)  $\pi$  that simulates data **improves**
- Repeat (each simulation)
  - **Evaluate** states Q(s, a) by Monte-Carlo evaluation
  - Improve simulation policy, e.g., by  $\varepsilon$ -greedy(Q)
  - Monte-Carlo control applied to simulated experience
- Converges to the optimal search tree,  $Q(s, a) o Q^{\pi^{\mathrm{opt}}}(s, a)$

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#### Case Study: the Game of Go



- Invented in China over 2500 years ago
- The **hardest** classic board game
- Much harder than chess:
  - Go has larger number of legal moves than chess ( $\approx$ 250 v.s.  $\approx$ 35)
  - Go involve more moves than chess ( $\approx$  150 v.s.  $\approx$  80)
  - Traditional game-tree search fails in Go

#### Rules of Go

- Two players place down white and black stones alternately
- Stones are captured according to simple rules

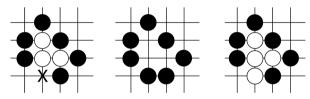


Figure: Left: the three white stones are not surrounded because point X is unoccupied. Middle: if black places a stone on X, the three white stones are captured and removed from the board. Right: if white places a stone on point X first, the capture is blocked.

- The game ends when neither player wishes to place another stone
- The player with more **territory** wins the game

#### Two-Player Zero-Sum Markov Games

- Simplest extension of MDP  $\langle S, A, B, P, R, \gamma \rangle$
- A and B are actions spaces of first and second players
- R is reward function. In Go,
  - $R_t = 0$  for all non-terminal steps
  - $R_T = 1$  if Black wins and -1 otherwise
- Let  $\pi$  and  $\nu$  be policies of the first and second players
- ullet The state-value function depends on both  $\pi$  and u

$$oldsymbol{V}^{\pi,
u}(s) = \mathbb{E}\left[\left.\sum_{t=0}^{\infty} oldsymbol{\gamma}^t R_t
ight| oldsymbol{S_0} = s, oldsymbol{A_t} \sim \pi, oldsymbol{B_t} \sim 
u
ight]$$

#### **Causal Diagram**

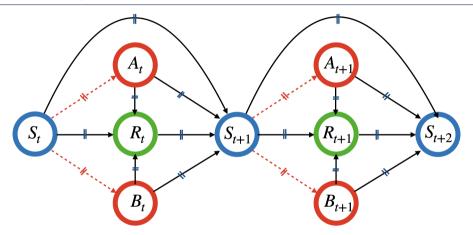


Figure: Causal diagrams for MDPs, TMDPs and POMDPs. Solid lines represent the causal relationships. Dashed lines indicate the information needed to implement the optimal policy. The parallel sign || indicates that the conditional probability function given parent nodes is equal.

#### Nash Equilibrium

• At each state s, the two players aim to solve two minimax problems

$$rg \max_{\pi} oldsymbol{V}^{\pi}(oldsymbol{s}) = rg \max_{\pi} \min_{
u} oldsymbol{V}^{\pi,
u}(oldsymbol{s})$$
  $rg \min_{
u} oldsymbol{V}^{
u}(oldsymbol{s}) = rg \min_{
u} \max_{\pi} oldsymbol{V}^{\pi,
u}(oldsymbol{s})$ 

• Under Markov and time-homogeneity assumptions, there exist stationary policies  $\pi^*$  ( $\nu^*$ ) whose values are no worse (better) than any history dependent policy

$$oldsymbol{V}^{\pi^*,
u^*}(s) = rg\max_{\pi} \min_{
u} oldsymbol{V}^{\pi,
u}(s) = rg\min_{
u} \max_{\pi} oldsymbol{V}^{\pi,
u}(s)$$

similar to the existence of the optimal stationary policy theorem in Lecture 2

• These policies reach a **Nash equilibrium** [Morgenstern and Von Neumann, 1953], i.e., no player can play better by changing his/her own policy

#### Prisoner's Dilemma

	Prisoner B stays silent (cooperates)	Prisoner B betrays (defects)
Prisoner A stays silent (cooperates)	Each serves 1 year	Prisoner A: 3 years Prisoner B: goes free
Prisoner A betrays (defects)	Prisoner A: goes free Prisoner B: 3 years	Each serves 2 years

Mutual defection is the only Nash equilibrium

### **Bellman Optimally Equation**

• Bellman optimal equation for the **state value** 

$$oldsymbol{V}^{\pi^*,
u^*}(oldsymbol{S_t}) = \max_{oldsymbol{a}} \min_{oldsymbol{b}} \mathbb{E}\left[\left.oldsymbol{R_t} + rac{\gamma}{oldsymbol{V}^{\pi^*,
u^*}}(oldsymbol{S_{t+1}})\right|oldsymbol{S_t}, oldsymbol{A_t} = oldsymbol{a}, oldsymbol{B_t} = oldsymbol{b}
ight]$$

• Bellman optimal equation for the state-action value

$$Q^{\pi^*,\nu^*}(S_t, A_t, B_t) = \mathbb{E}\left[\left.R_t + \gamma \max_{\boldsymbol{a}} \min_{\boldsymbol{b}} Q^{\pi^*,\nu^*}(S_{t+1}, \boldsymbol{a}, \boldsymbol{b})\right| S_t, A_t = \boldsymbol{a}, B_t = \boldsymbol{b}\right]$$

ullet The values can be learned similarly to standard TD/Q learning algorithms for MDP [see e.g., Fan et al., 2020]

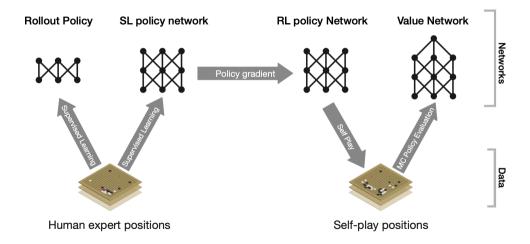
#### **AlphaGo**



#### AlphaGo Pipeline

- Based on a novel version of Monte-Carlo tree search (MCTS)
- Combined with a policy and a value function learned by RL with function approximation provided by deep CNN
- Simulate trajectories and generate the search tree using the rollout policy
- Expand search tree by selecting unexplored actions according to a policy network
- Policy network trained previously via supervised learning to predict moves contained in a database of nearly 30 million human expert moves
- Evaluate state-action value based on simulated returns (MC) and a value network
- Value network trained previously via RL

### AlphaGo Pipeline (Cont'd)



### **Input of Neural Networks**

#### Extended Data Table 2 | Input features for neural networks

Feature	# of planes	Description
Stone colour	3	Player stone / opponent stone / empty
Ones	1	A constant plane filled with 1
Turns since	8	How many turns since a move was played
Liberties	8	Number of liberties (empty adjacent points)
Capture size	8	How many opponent stones would be captured
Self-atari size	8	How many of own stones would be captured
Liberties after move	8	Number of liberties after this move is played
Ladder capture	1	Whether a move at this point is a successful ladder capture
Ladder escape	1	Whether a move at this point is a successful ladder escape
Sensibleness	1	Whether a move is legal and does not fill its own eyes
Zeros	1	A constant plane filled with 0
Player color	1	Whether current player is black

### **Policy Network**

- Training the SL policy network took approximately 3 weeks using distributed implementation of SGD on 50 processors
- The SL policy network achieved 57% accuracy; best accuracy achieved by other methods 44%
- The RL policy network is trained on a million games in a single day
- The final RL policy won more than 80% of games played against the SL policy
- It won 85% of games played against a Go program using MCTS that simulated 100,000 games per move

#### Value Network

- The value network used Monte Carlo policy evaluation based on data obtained from a large number of self-play games played using the RL policy
- To avoid overfitting and instability, and to reduce the strong correlations between
  positions encountered in self-play, the dataset consists of 30 million positions, each
  chosen randomly from a unique self-play game
- Training was done using 50 million mini-batches each of 32 positions drawn from this data set
- Training took one week on **50** GPUs

### **Rollout Policy**

- The **rollout policy** was learned prior to play by a simple linear network trained by supervised learning from a corpus of **8** million human moves
- In principle, the SL or RL policy networks could have been used in the rollouts, but the forward propagation through these deep networks took too much time for either of them to be used in rollout simulations
- The rollout policy network allowed approximately 1,000 complete game simulations per second to be run on each of the processing threads

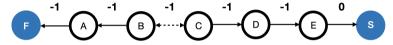
### Summary

- Model-based/Model free learning
- Integrating planning and learning
- Dyna-Q/Dyna-Q<sup>+</sup>
- Simulation-based search
- Background/Decision-time planning

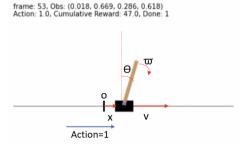
- Monte Carlo Tree Search
- Two-player zero-sum Markov games
- Nash equilibrium
- AlphaGo

#### **Seminar Exercise**

• Solution to HW8 (Deadline: Wed 12:00 pm)



Advantage Actor-Critic (with deep neural networks) to CartPole



• Implementation of Dyna-Q algorithm

#### References I

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# Questions