DSC190: Machine Learning with Few Labels

Reinforcement learning

Zhiting Hu Lecture 13, November 4, 2021



HALICIOĞLU DATA SCIENCE INSTITUTE

Recap: Knowledge driven learning

- Two general ways of integrating structured knowledge with ML:
 - Model architecture (inductive bias)
 - Integrating knowledge through learning (loss, constraints)
 - Weak supervision
 - Posterior regularization
 - Integer linear programming (ILP)

Outline

- Reinforcement Learning
- 1 Paper presentations (15 mins)
 - Kewen Zhao: Task-Agnostic Meta-Learning for Few-shot Learning

So far... Supervised Learning

Data: (x, y) x is data, y is label

Goal: Learn a *function* to map x -> y

Examples: Classification, regression, object detection, semantic segmentation, image captioning, etc.



Cat

Classification

So far... Unsupervised Learning

Data: x no labels!

Goal: Learn some underlying hidden *structure* of the data

Examples: Clustering, dimensionality reduction, feature learning, density estimation, etc.



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1-d density estimation



2-d density estimation

Today: Reinforcement Learning

Problems involving an **agent** interacting with an **environment**, which provides numeric **reward** signals

Goal: Learn how to take actions in order to maximize reward





Overview

- What is Reinforcement Learning?
- Markov Decision Processes
- Q-Learning
- Policy Gradients



Environment









Cart-Pole Problem



Objective: Balance a pole on top of a movable cart

State: angle, angular speed, position, horizontal velocityAction: horizontal force applied on the cartReward: 1 at each time step if the pole is upright



Robot Locomotion



Objective: Make the robot move forward

State: Angle and position of the joints Action: Torques applied on joints Reward: 1 at each time step upright + forward movement

Atari Games



Objective: Complete the game with the highest score

State: Raw pixel inputs of the game stateAction: Game controls e.g. Left, Right, Up, DownReward: Score increase/decrease at each time step

Go



Objective: Win the game!

State: Position of all piecesAction: Where to put the next piece downReward: 1 if win at the end of the game, 0 otherwise

How can we mathematically formalize the RL problem?



Markov Decision Process

- Mathematical formulation of the RL problem
- Markov property: Current state completely characterises the state of the world

Defined by: $(\mathcal{S}, \mathcal{A}, \mathcal{R}, \mathbb{P}, \gamma)$

- ${\cal S}$: set of possible states
- ${\boldsymbol{\mathcal{A}}}$: set of possible actions
- ${\cal R}$: distribution of reward given (state, action) pair
- ℙ : transition probability i.e. distribution over next state given (state, action) pair
- γ : discount factor

Markov Decision Process

- At time step t=0, environment samples initial state $s_0 \sim p(s_0)$
- Then, for t=0 until done:
 - Agent selects action a_t
 - Environment samples reward $r_t \sim R(. | s_t, a_t)$
 - Environment samples next state $s_{t+1} \sim P(.|s_t, a_t)$
 - Agent receives reward r_t and next state s_{t+1}

- A policy $\pi \, \textsc{is}$ a function from S to A that specifies what action to take in each state
- **Objective**: find policy π^* that maximizes cumulative discounted reward:



A simple MDP: Grid World



Set a negative "reward" for each transition (e.g. r = -1)

Objective: reach one of terminal states (greyed out) in least number of actions

A simple MDP: Grid World





Random Policy

Optimal Policy

The optimal policy π^*

We want to find optimal policy π^* that maximizes the sum of rewards.

How do we handle the randomness (initial state, transition probability...)?

The optimal policy π^*

We want to find optimal policy π^* that maximizes the sum of rewards.

How do we handle the randomness (initial state, transition probability...)? Maximize the **expected sum of rewards!**

Formally:
$$\pi^* = \arg \max_{\pi} \mathbb{E} \left[\sum_{t \ge 0} \gamma^t r_t | \pi \right]$$
 with $s_0 \sim p(s_0), a_t \sim \pi(\cdot | s_t), s_{t+1} \sim p(\cdot | s_t, a_t)$

Definitions: Value function and Q-value function

Following a policy produces sample trajectories (or paths) s_0 , a_0 , r_0 , s_1 , a_1 , r_1 , ...

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How good is a state?

The value function at state s, is the expected cumulative reward from following the policy from state s: $V^{\pi}(s) = \mathbb{E}\left[\sum \gamma^{t} r_{t} | s_{0} = s, \pi\right]$

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How good is a state-action pair?

The **Q-value function** at state s and action a, is the expected cumulative reward from taking action a in state s and then following the policy:

$$Q^{\pi}(s,a) = \mathbb{E}\left[\sum_{t\geq 0} \gamma^t r_t | s_0 = s, a_0 = a, \pi
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Bellman equation

The optimal Q-value function Q* is the maximum expected cumulative reward achievable from a given (state, action) pair:

$$Q^*(s,a) = \max_{\pi} \mathbb{E}\left[\sum_{t \geq 0} \gamma^t r_t | s_0 = s, a_0 = a, \pi
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$$Q^*(s,a) = \max_{\pi} \mathbb{E}\left[\sum_{t \ge 0} \gamma^t r_t | s_0 = s, a_0 = a, \pi\right]$$

Q* satisfies the following **Bellman equation**:

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

Intuition: if the optimal state-action values for the next time-step Q*(s',a') are known, then the optimal strategy is to take the action that maximizes the expected value of $r + \gamma Q^*(s',a')$

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The optimal policy π^* corresponds to taking the best action in any state as specified by Q^{*}

Value iteration algorithm: Use Bellman equation as an iterative update

$$Q_{i+1}(s,a) = \mathbb{E}\left[r + \gamma \max_{a'} Q_i(s',a')|s,a\right]$$

 Q_i will converge to Q^* as i -> infinity

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Not scalable. Must compute Q(s,a) for every state-action pair. If state is e.g. current game state pixels, computationally infeasible to compute for entire state space!

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Solution: use a function approximator to estimate Q(s,a). E.g. a neural network!

Solving for the optimal policy: Q-learning

Q-learning: Use a function approximator to estimate the action-value function

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

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If the function approximator is a deep neural network => deep q-learning!

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Q-learning: Use a function approximator to estimate the action-value function

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

function parameters (weights)

If the function approximator is a deep neural network => deep q-learning!
Remember: want to find a Q-function that satisfies the Bellman Equation:

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

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Forward Pass

Loss function:
$$L_i(\theta_i) = \mathbb{E}_{s,a \sim \rho(\cdot)} \left[(y_i - Q(s,a;\theta_i))^2 \right]$$

where $y_i = \mathbb{E}_{s' \sim \mathcal{E}} \left[r + \gamma \max_{a'} Q(s',a';\theta_{i-1}) | s, a \right]$

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Backward Pass

Gradient update (with respect to Q-function parameters θ):

$$\nabla_{\theta_i} L_i(\theta_i) = \mathbb{E}_{s,a \sim \rho(\cdot); s' \sim \mathcal{E}} \left[r + \gamma \max_{a'} Q(s',a';\theta_{i-1}) - Q(s,a;\theta_i)) \nabla_{\theta_i} Q(s,a;\theta_i) \right]$$

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close to the target value (y) it

should have, if Q-function

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(and optimal policy π^*)

Case Study: Playing Atari Games



Objective: Complete the game with the highest score

State: Raw pixel inputs of the game stateAction: Game controls e.g. Left, Right, Up, DownReward: Score increase/decrease at each time step

Q(s,a; heta) : neural network with weights heta



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Q(s,a; heta) : neural network with weights heta



Q(s,a; heta): neural network with weights heta

A single feedforward pass to compute Q-values for all actions from the current state => efficient!



Last FC layer has 4-d output (if 4 actions), corresponding to $Q(s_t, a_1)$, $Q(s_t, a_2)$, $Q(s_t, a_3)$, $Q(s_t, a_4)$

Number of actions between 4-18 depending on Atari game

Remember: want to find a Q-function that satisfies the Bellman Equation:

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

Forward Pass

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close to the target value (y) it should have, if Q-function corresponds to optimal Q* (and optimal policy π^*)

Backward Pass

Gradient update (with respect to Q-function parameters θ):

$$\nabla_{\theta_i} L_i(\theta_i) = \mathbb{E}_{s,a \sim \rho(\cdot); s' \sim \mathcal{E}} \left[r + \gamma \max_{a'} Q(s',a';\theta_{i-1}) - Q(s,a;\theta_i)) \nabla_{\theta_i} Q(s,a;\theta_i) \right]$$

Training the Q-network: Experience Replay

Learning from batches of consecutive samples is problematic:

- Samples are correlated => inefficient learning
- Current Q-network parameters determines next training samples (e.g. if maximizing action is to move left, training samples will be dominated by samples from left-hand size) => can lead to bad feedback loops

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Address these problems using **experience replay**

- Continually update a replay memory table of transitions (s_t, a_t, r_t, s_{t+1}) as game (experience) episodes are played
- Train Q-network on random minibatches of transitions from the replay memory, instead of consecutive samples

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Each transition can also contribute to multiple weight updates => greater data efficiency

Algorithm 1 Deep Q-learning with Experience Replay

Initialize replay memory \mathcal{D} to capacity N Initialize action-value function Q with random weights for episode = 1, M do Initialise sequence $s_1 = \{x_1\}$ and preprocessed sequenced $\phi_1 = \phi(s_1)$ for t = 1, T do With probability ϵ select a random action a_t otherwise select $a_t = \max_a Q^*(\phi(s_t), a; \theta)$ 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 \mathcal{D} Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from \mathcal{D} Set $y_j = \begin{cases} r_j & \text{for terminal } \phi_{j+1} \\ r_j + \gamma \max_{a'} Q(\phi_{j+1}, a'; \theta) & \text{for non-terminal } \phi_{j+1} \end{cases}$ Perform a gradient descent step on $(y_j - Q(\phi_j, a_j; \theta))^2$ according to equation 3 end for end for

Algorithm 1 Deep Q-learning with Experience Replay Initialize replay memory \mathcal{D} to capacity N Initialize replay memory, Q-network Initialize action-value function Q with random weights for episode = 1, M do Initialise sequence $s_1 = \{x_1\}$ and preprocessed sequenced $\phi_1 = \phi(s_1)$ for t = 1, T do With probability ϵ select a random action a_t otherwise select $a_t = \max_a Q^*(\phi(s_t), a; \theta)$ 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 \mathcal{D} Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from \mathcal{D} Set $y_j = \begin{cases} r_j & \text{for terminal } \phi_{j+1} \\ r_j + \gamma \max_{a'} Q(\phi_{j+1}, a'; \theta) & \text{for non-terminal } \phi_{j+1} \end{cases}$ Perform a gradient descent step on $(y_j - Q(\phi_j, a_j; \theta))^2$ according to equation 3 end for end for

Algorithm 1 Deep Q-learning with Experience Replay Initialize replay memory \mathcal{D} to capacity N Initialize action-value function Q with random weights ——— Play M episodes (full games) for episode = 1, M do Initialise sequence $s_1 = \{x_1\}$ and preprocessed sequenced $\phi_1 = \phi(s_1)$ for t = 1, T do With probability ϵ select a random action a_t otherwise select $a_t = \max_a Q^*(\phi(s_t), a; \theta)$ 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 \mathcal{D} Sample random minibatch of transitions $(\phi_j, a_j, r_j, \phi_{j+1})$ from \mathcal{D} Set $y_j = \begin{cases} r_j & \text{for terminal } \phi_{j+1} \\ r_j + \gamma \max_{a'} Q(\phi_{j+1}, a'; \theta) & \text{for non-terminal } \phi_{j+1} \end{cases}$ Perform a gradient descent step on $(y_j - Q(\phi_j, a_j; \theta))^2$ according to equation 3 end for end for

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What is a problem with Q-learning? The Q-function can be very complicated!

Example: a robot grasping an object has a very high-dimensional state => hard to learn exact value of every (state, action) pair

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Example: a robot grasping an object has a very high-dimensional state => hard to learn exact value of every (state, action) pair

But the policy can be much simpler: just close your hand Can we learn a policy directly, e.g. finding the best policy from a collection of policies?

Formally, let's define a class of parametrized policies: $\Pi = \{\pi_{\theta}, \theta \in \mathbb{R}^m\}$

For each policy, define its value:

$$J(\theta) = \mathbb{E}\left[\sum_{t \ge 0} \gamma^t r_t | \pi_{\theta}\right]$$

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How can we do this?

Gradient ascent on policy parameters!

Mathematically, we can write:

$$J(\theta) = \mathbb{E}_{\tau \sim p(\tau;\theta)} [r(\tau)]$$
$$= \int_{\tau} r(\tau) p(\tau;\theta) d\tau$$

Where r(r) is the reward of a trajectory $au = (s_0, a_0, r_0, s_1, \ldots)$

Expected reward:

$$J(\theta) = \mathbb{E}_{\tau \sim p(\tau;\theta)} [r(\tau)]$$
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$$= \int_{\tau} r(\tau) p(\tau; \theta) d\tau$$
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Now let's differentiate this: ∇_{θ}

$$\partial J(\theta) = \int_{\tau} r(\tau) \nabla_{\theta} p(\tau; \theta) \mathrm{d}\tau$$

Expected reward: $J(\theta) = \mathbb{E}_{\theta}$

$$) = \mathbb{E}_{\tau \sim p(\tau;\theta)} [r(\tau)]$$
$$= \int_{\tau} r(\tau) p(\tau;\theta) d\tau$$

Now let's differentiate this: $\nabla_{\theta} J(\theta) = \int_{\tau} r(\tau) \nabla_{\theta} p(\tau; \theta) d\tau$

Intractable! Gradient of an expectation is problematic when p depends on
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However, we can use a nice trick:
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Now let's differentiate this: $\nabla_{\theta} J(\theta) = \int r(\tau) \nabla_{\theta} p(\tau; \theta) d\tau$

Intractable! Gradient of an expectation is problematic when p depends on θ

However, we can use a nice trick: $\nabla_{\theta} p(\tau; \theta) = p(\tau; \theta) \frac{\nabla_{\theta} p(\tau; \theta)}{p(\tau; \theta)} = p(\tau; \theta) \nabla_{\theta} \log p(\tau; \theta)$ If we inject this back:

$$\begin{aligned} \nabla_{\theta} J(\theta) &= \int_{\tau} \left(r(\tau) \nabla_{\theta} \log p(\tau; \theta) \right) p(\tau; \theta) \mathrm{d}\tau \\ &= \mathbb{E}_{\tau \sim p(\tau; \theta)} \left[r(\tau) \nabla_{\theta} \log p(\tau; \theta) \right] \end{aligned} \begin{array}{c} \text{Can estimate with} \\ \text{Monte Carlo sampling} \end{aligned}$$

Can we compute those quantities without knowing the transition probabilities?

We have: $p(\tau; \theta) = \prod_{t \ge 0} p(s_{t+1}|s_t, a_t) \pi_{\theta}(a_t|s_t)$
REINFORCE algorithm

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Thus:

$$\log p(\tau;\theta) = \sum_{t \ge 0} \log p(s_{t+1}|s_t, a_t) + \log \pi_{\theta}(a_t|s_t)$$

REINFORCE algorithm

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REINFORCE algorithm

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And when differentiating: $\nabla_{\theta} \log p(\tau; \theta) = \sum_{t \ge 0} \nabla_{\theta} \log \pi_{\theta}(a_t|s_t)$ Doesn't depend on transition probabilities!

Therefore when sampling a trajectory r, we can estimate J(8) with

$$\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} r(\tau) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$

Intuition

Gradient estimator:

$$\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} r(\tau) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$

Interpretation:

- If r(r) is high, push up the probabilities of the actions seen
- If r(r) is low, push down the probabilities of the actions seen

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However, this also suffers from high variance because credit assignment is really hard. Can we help the estimator?

Variance reduction

Gradient estimator:

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Variance reduction Gradient estimator: $\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} r(\tau) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$

First idea: Push up probabilities of an action seen, only by the cumulative future reward from that state

$$\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} \left(\sum_{t' \ge t} r_{t'} \right) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$

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Second idea: Use discount factor γ to ignore delayed effects

$$\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} \left(\sum_{t' \ge t} \gamma^{t'-t} r_{t'} \right) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$

Variance reduction: Baseline

Problem: The raw value of a trajectory isn't necessarily meaningful. For example, if rewards are all positive, you keep pushing up probabilities of actions.

What is important then? Whether a reward is better or worse than what you expect to get

Idea: Introduce a baseline function dependent on the state. Concretely, estimator is now:

$$\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} \left(\sum_{t' \ge t} \gamma^{t'-t} r_{t'} - b(s_t) \right) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$

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A simple baseline: constant moving average of rewards experienced so far from all trajectories

How to choose the baseline? $\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} \left(\sum_{t' \ge t} \gamma^{t'-t} r_{t'} - b(s_t) \right) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$

A simple baseline: constant moving average of rewards experienced so far from all trajectories

Variance reduction techniques seen so far are typically used in "Vanilla REINFORCE"

A better baseline: Want to push up the probability of an action from a state, if this action was better than the **expected value of what we should get from that state**.

Q: What does this remind you of?

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Intuitively, we are happy with an action a_t in a state s_t if $Q^{\pi}(s_t, a_t) - V^{\pi}(s_t)$ is large. On the contrary, we are unhappy with an action if it's small.

Using this, we get the estimator:
$$\nabla_{\theta} J(\theta) \approx \sum_{t \ge 0} (Q^{\pi_{\theta}}(s_t, a_t) - V^{\pi_{\theta}}(s_t)) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$

Actor-Critic Algorithm

Problem: we don't know Q and V. Can we learn them?

Yes, using Q-learning! We can combine Policy Gradients and Q-learning by training both an **actor** (the policy) and a **critic** (the Q-function).

- The actor decides which action to take, and the critic tells the actor how good its action was and how it should adjust
- Also alleviates the task of the critic as it only has to learn the values of (state, action) pairs generated by the policy
- Can also incorporate Q-learning tricks e.g. experience replay
- **Remark:** we can define by the **advantage function** how much an action was better than expected $4\pi(a, a) = O^{\pi}(a)$

$$A^{\pi}(s,a) = Q^{\pi}(s,a) - V^{\pi}(s)$$

Actor-Critic Algorithm

Initialize policy parameters 8, critic parameters ø For iteration=1, 2 ... do Sample m trajectories under the current policy $\Delta\theta \leftarrow 0$ **For** i=1, ..., m **do For** t=1, ..., T **do** $A_t = \sum_{t' \ge t} \gamma^{t'-t} r_t^i - V_\phi(s_t^i)$ $\Delta \theta \leftarrow \Delta \theta + A_t \nabla_\theta \log(a_t^i | s_t^i)$ $\begin{aligned} \Delta \phi \leftarrow \sum_{i} \sum_{t} \nabla_{\phi} ||A_{t}^{i}||^{2} \\ \theta \leftarrow \alpha \Delta \theta \end{aligned}$ $\phi \leftarrow \beta \Delta \phi$

End for

More policy gradients: AlphaGo

Overview:

- Mix of supervised learning and reinforcement learning
- Mix of old methods (Monte Carlo Tree Search) and recent ones (deep RL)

How to beat the Go world champion:

- Featurize the board (stone color, move legality, bias, ...)
- Initialize policy network with supervised training from professional go games, then continue training using policy gradient (play against itself from random previous iterations, +1 / -1 reward for winning / losing)
- Also learn value network (critic)
- Finally, combine combine policy and value networks in a Monte Carlo Tree Search algorithm to select actions by lookahead search

[Silver et al., Nature 2016]



Key Takeaways

- Markov Decision Process (MDP)
- Q-learning
 - Bellman equation
 - Deep Q-learning, experience replay
- Policy gradients
- Guarantees:
 - Policy Gradients: Converges to a local minima of $J(\theta)$, often good enough!
 - Q-learning: Zero guarantees since you are approximating Bellman equation with a complicated function approximator

Questions?