Course material at:
https://github.com/lyeskhalil/mlbootcamp2022/

Advanced Topics

Friday

FASE ML Bootcamp

Based on material from various sources:
Data augmentation, Hyperparameter tuning, CNN understanding, Attention, GANs: http://cs231n.stanford.edu/schedule.html
Uncertainty in Deep Learning: https://www.gatsby.ucl.ac.uk/~balaji/balaji-uncertainty-talk-cifar-dlrl.pdf
Graph Neural Networks: http://tkipf.github.io/misc/SlidesCambridge.pdf
Reinforcement Learning: https://www.davidsilver.uk/wp-content/uploads/2020/03/deep_rl_tutorial_small_compressed.pdf

2022 Free PDF book on all of ML by Kevin Murphy (Google): https://probml.github.io/pml-book/book1.html

Tutorial: Deep Reinforcement Learning

David Silver, Google DeepMind

Reinforcement Learning in a nutshell

RL is a general-purpose framework for decision-making

- RL is for an agent with the capacity to act
- Each action influences the agent's future state
- Success is measured by a scalar reward signal
- Goal: select actions to maximise future reward

Deep Learning in a nutshell

DL is a general-purpose framework for representation learning

- Given an objective
- Learn representation that is required to achieve objective
- Directly from raw inputs
- Using minimal domain knowledge

Deep Reinforcement Learning: AI = RL + DL

We seek a single agent which can solve any human-level task

- RL defines the objective
- DL gives the mechanism
- RL + DL = general intelligence

Examples of Deep RL @DeepMind

- Play games: Atari, poker, Go, ...
- Explore worlds: 3D worlds, Labyrinth, ...
- Control physical systems: manipulate, walk, swim, ...
- Interact with users: recommend, optimise, personalise, ...

Outline

Deep Representations

- A deep representation is a composition of many functions

$$
\begin{tikzcd}
x \arrow[r] & h_1 \arrow[r] & \dots \arrow[r] & h_n \arrow[r] & y \arrow[r] & l \\
& \mathbf{w_1} \arrow[u] & \dots & \mathbf{w_n} \arrow[u] & &
\end{tikzcd}
$$

- Its gradient can be backpropagated by the chain rule

$$
\begin{tikzcd}
\frac{\partial l}{\partial x} & \frac{\partial l}{\partial h_1} \arrow[l, "\frac{\partial h_1}{\partial x}"'] \arrow[d, "\frac{\partial h_1}{\partial w_1}"'] & \dots \arrow[l, "\frac{\partial h_2}{\partial h_1}"'] & \frac{\partial l}{\partial h_n} \arrow[l, "\frac{\partial h_n}{\partial h_{n-1}}"'] \arrow[d, "\frac{\partial h_n}{\partial w_n}"'] & \frac{\partial l}{\partial y} \arrow[l, "\frac{\partial y}{\partial h_n}"'] \\
& \frac{\partial l}{\partial \mathbf{w_1}} & \dots & \frac{\partial l}{\partial \mathbf{w_n}} &
\end{tikzcd}
$$

Deep Neural Network

A deep neural network is typically composed of:

- Linear transformations

$$h_{k+1} = Wh_k$$

- Non-linear activation functions

$$h_{k+2} = f(h_{k+1})$$

- A loss function on the output, e.g.
  - Mean-squared error $l = ||y^* - y||^2$
  - Log likelihood $l = \log \mathbb{P}[y^*]$

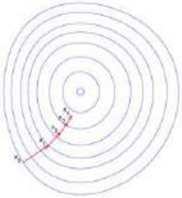
Training Neural Networks by Stochastic Gradient Descent

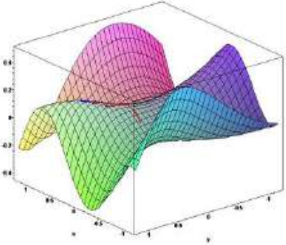
- Sample gradient of expected loss $L(\mathbf{w}) = \mathbb{E}\left[l\right]$

$$\frac{\partial l}{\partial \mathbf{w}} \sim \mathbb{E}\left[\frac{\partial l}{\partial \mathbf{w}}\right] = \frac{\partial L(\mathbf{w})}{\partial \mathbf{w}}$$

- Adjust $\mathbf{w}$ down the sampled gradient

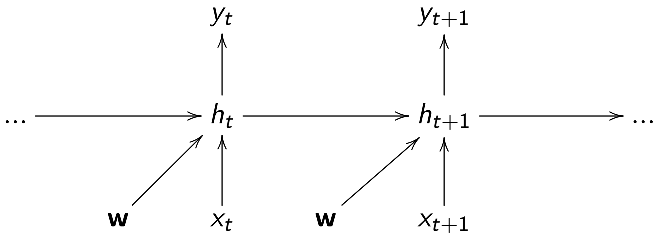
$$\Delta w \propto \frac{\partial l}{\partial \mathbf{w}}$$



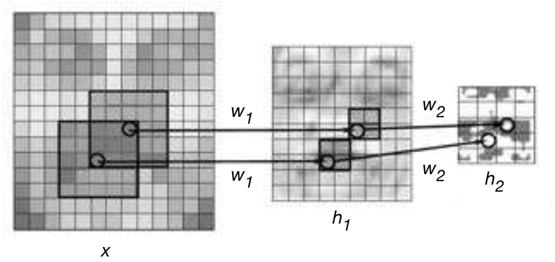


Weight Sharing

Recurrent neural network shares weights between time-steps

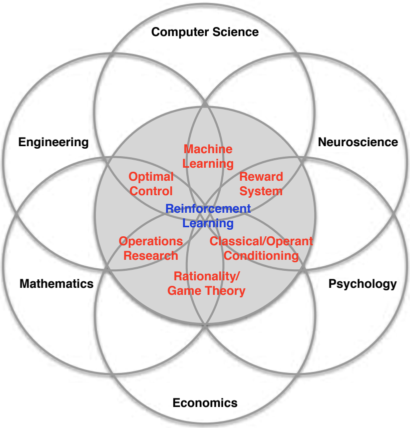


Convolutional neural network shares weights between local regions

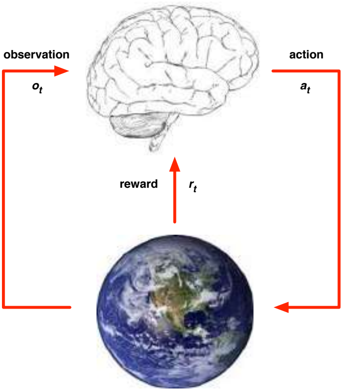


Outline

Many Faces of Reinforcement Learning



Agent and Environment



- At each step t the agent:
  - Executes action a_t
  - Receives observation o_t
  - Receives scalar reward r_t
- The environment:
  - Receives action a_t
  - Emits observation o_{t+1}
  - Emits scalar reward r_{t+1}

State

- Experience is a sequence of observations, actions, rewards

$$o_1, r_1, a_1, ..., a_{t-1}, o_t, r_t$$

- The state is a summary of experience

$$s_t = f(o_1, r_1, a_1, ..., a_{t-1}, o_t, r_t)$$

- In a fully observed environment

$$s_t = f(o_t)$$

Major Components of an RL Agent

- An RL agent may include one or more of these components:
  - Policy: agent's behaviour function
  - Value function: how good is each state and/or action
  - Model: agent's representation of the environment

Policy

- A policy is the agent's behaviour
- It is a map from state to action:
  - Deterministic policy: $a = \pi(s)$
  - Stochastic policy: $\pi(a|s) = \mathbb{P}[a|s]$

Value Function

- A value function is a prediction of future reward
  - "How much reward will I get from action a in state s?"
- Q-value function gives expected total reward
  - from state s and action a
  - under policy π
  - with discount factor γ

$$Q^{\pi}(s, a) = \mathbb{E}\left[r_{t+1} + \gamma r_{t+2} + \gamma^2 r_{t+3} + \ldots \mid s, a\right]$$

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- Value functions decompose into a Bellman equation

$$Q^{\pi}(s, a) = \mathbb{E}_{s', a'}\left[r + \gamma Q^{\pi}(s', a') \mid s, a\right]$$

Optimal Value Functions

- An optimal value function is the maximum achievable value

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

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- Optimal value maximises over all decisions. Informally:

$$\begin{aligned} Q^*(s, a) &= r_{t+1} + \gamma \max_{a_{t+1}} r_{t+2} + \gamma^2 \max_{a_{t+2}} r_{t+3} + \ldots \\ &= r_{t+1} + \gamma \max_{a_{t+1}} Q^*(s_{t+1}, a_{t+1}) \end{aligned}$$

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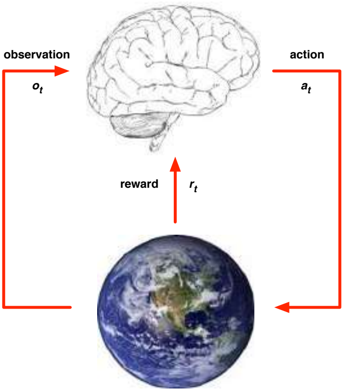
- Formally, optimal values decompose into a Bellman equation

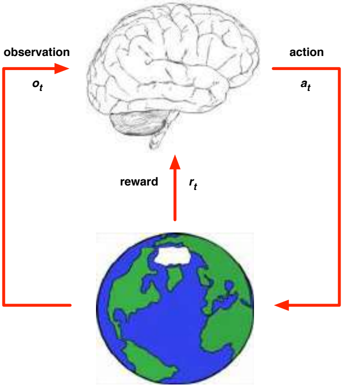
$$Q^*(s,a) = \mathbb{E}_{s'}\left[r + \gamma \max_{a'} Q^*(s',a') \mid s, a \right]$$

Value Function Demo

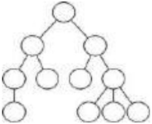
Model



Model



- Model is learnt from experience
- Acts as proxy for environment
- Planner interacts with model
- e.g. using lookahead search



Approaches To Reinforcement Learning

Value-based RL

- Estimate the optimal value function $Q^*(s, a)$
- This is the maximum value achievable under any policy

Policy-based RL

- Search directly for the optimal policy π^*
- This is the policy achieving maximum future reward

Model-based RL

- Build a model of the environment
- Plan (e.g. by lookahead) using model

Deep Reinforcement Learning

- Use deep neural networks to represent
  - Value function
  - Policy
  - Model
- Optimise loss function by stochastic gradient descent

Outline

Introduction to Deep Learning

Introduction to Reinforcement Learning

Value-Based Deep RL

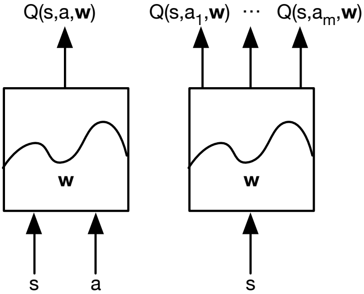
Policy-Based Deep RL

Model-Based Deep RL

Q-Networks

Represent value function by Q-network with weights **w**

$$Q(s, a, \mathbf{w}) \approx Q^*(s, a)$$



Q-Learning

- Optimal Q-values should obey Bellman equation

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

- Treat right-hand side $r + \gamma \max_{a'} Q(s',a',\mathbf{w})$ as a target
- Minimise MSE loss by stochastic gradient descent

$$l = \left(r + \gamma \max_{a'} Q(s',a',\mathbf{w}) - Q(s,a,\mathbf{w})\right)^2$$

Q-Learning

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- Converges to Q^* using table lookup representation

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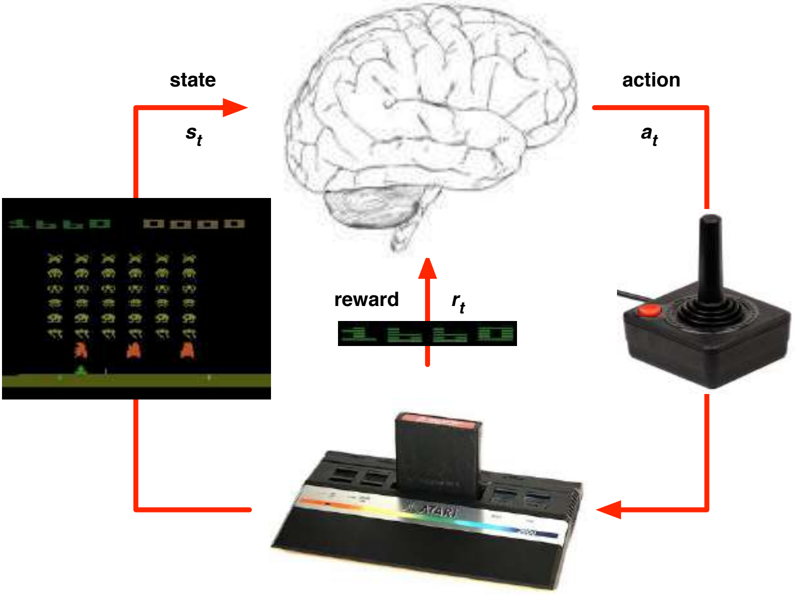
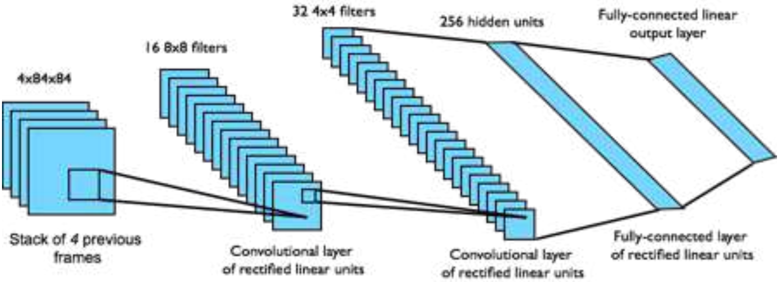
- Converges to Q^* using table lookup representation
- But diverges using neural networks due to:
  - Correlations between samples
  - Non-stationary targets

Deep Reinforcement Learning in Atari



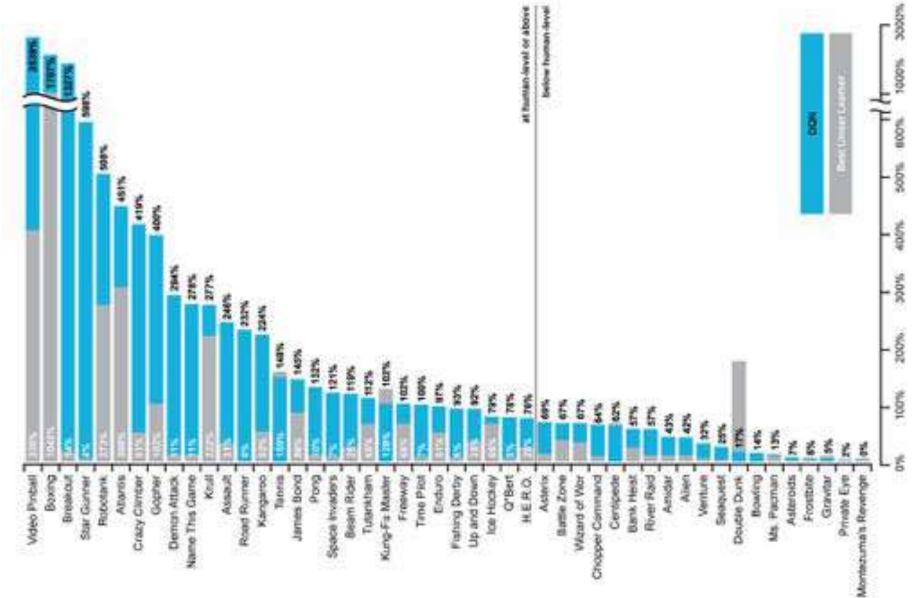
DQN in Atari

- End-to-end learning of values $Q(s, a)$ from pixels s
- Input state s is stack of raw pixels from last 4 frames
- Output is $Q(s, a)$ for 18 joystick/button positions
- Reward is change in score for that step



Network architecture and hyperparameters fixed across all games

DQN Results in Atari



DQN Atari Demo

DQN paper
www.nature.com/articles/nature14236

DQN source code:
sites.google.com/a/deepmind.com/dqn/

Conclusion

- General, stable and scalable RL is now possible
- Using deep networks to represent value, policy, model
- Successful in Atari, Labyrinth, Physics, Poker, Go
- Using a variety of deep RL paradigms