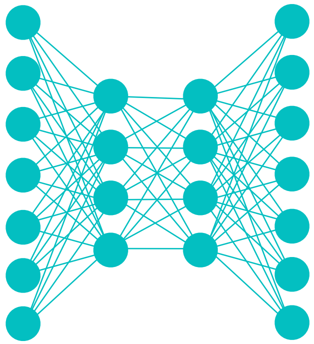
Lecture Notes for

Neural Networks and Machine Learning

Introduction to Reinforcement Learning



Logistics and Agenda

- Logistics
  - Lab Four: Cleaning up GANs
- Agenda
  - Pytorch
  - Basics of Reinforcment Learning
  - Markov Processes
  - Reinforcement Learning Categorization
  - OpenAI Gym
  - The Cross Entropy Method

Basics of Pytorch

Wait, why are we switching to Pytorch?

- Well, its good to know more than just Tensorflow
- Pytorch has some distinct advantages:
  - No need to setup a static computation graph—graph can be dynamic
    - Lazy computations happen on dynamic graph
  - Integration with numpy code on the fly is much easier and faster (compared to TF)
    - Can tradeoff computations with numpy easily, though not neccessarily optimized
- Also, all the book examples are in Pytorch… so this is nice for following along with the examples
- Keras subclassing is simlar in syntax/metaphor

Pytorch General Flow Training Flow

- Inherit from torch.nn.Module
- Define __init__ and forward
- Run epochs in a loop with explicit calls to:
  - Loss creation (for batch)
  - Backward calculation of gradient for batch
  - Step of optimizer for batch
  - Gives a great deal of flexibility to design and optimization process
- Lots of different pythonic ways to carry this out
  - Your book likes to setup steps of model through iterators (**yield** the batch, loss, etc.)

A Simple Definition (much like Keras!)

```python
import torch
import torch.nn as nn

class OurModule(nn.Module):
    def __init__(self, num_inputs, num_classes, dropout_prob=0.3):
        super(OurModule, self).__init__()
        self.pipe = nn.Sequential(
            nn.Linear(num_inputs, 5),
            nn.ReLU(),
            nn.Linear(5, 20),
            nn.ReLU(),
            nn.Linear(20, num_classes),
            nn.Dropout(p=dropout_prob),
            nn.Softmax(dim=1)
        )

    def forward(self, x):
        return self.pipe(x)

if __name__ == "__main__":
    net = OurModule(num_inputs=2, num_classes=3)
    print(net)
    v = torch.FloatTensor([[2, 3]])
    out = net(v)
    print(out)
    print("Cuda's availability is %s" % torch.cuda.is_available())
    if torch.cuda.is_available():
        print("Data from cuda: %s" % out.to('cuda'))
```

Sequential Definitions

Common Functions

The MNIST Example (not so like Keras)

Functional Definitions

```
import torch
import torch.nn as nn
import torch.nn.functional as F
import torch.optim as optim

class Net(nn.Module):
    def __init__(self):
        super(Net, self).__init__()
        self.conv1 = nn.Conv2d(1, 20, 5, 1)
        self.conv2 = nn.Conv2d(20, 50, 5, 1)
        self.fc1 = nn.Linear(4*4*50, 500)
        self.fc2 = nn.Linear(500, 10)

    def forward(self, x):
        x = F.relu(self.conv1(x))
        x = F.max_pool2d(x, 2, 2)
        x = F.relu(self.conv2(x))
        x = F.max_pool2d(x, 2, 2)
        x = x.view(-1, 4*4*50)
        x = F.relu(self.fc1(x))
        x = self.fc2(x)
        return F.log_softmax(x, dim=1)
```

Definitions

```
torch.nn.Conv2d(in_channels, out_channels, kernel_size,
stride=1, padding=0, dilation=1, groups=1, bias=True)
```

https://github.com/pytorch/examples/blob/master/mnist/main.py

Training One Epoch

```
def train(args, model, device, train_loader, optimizer, epoch):
    model.train()
    for batch_idx, (data, target) in enumerate(train_loader):
        data, target = data.to(device), target.to(device)
        optimizer.zero_grad()
        output = model(data)
        loss = F.nll_loss(output, target)
        loss.backward()
        optimizer.step()
```

Training Multiple Epochs

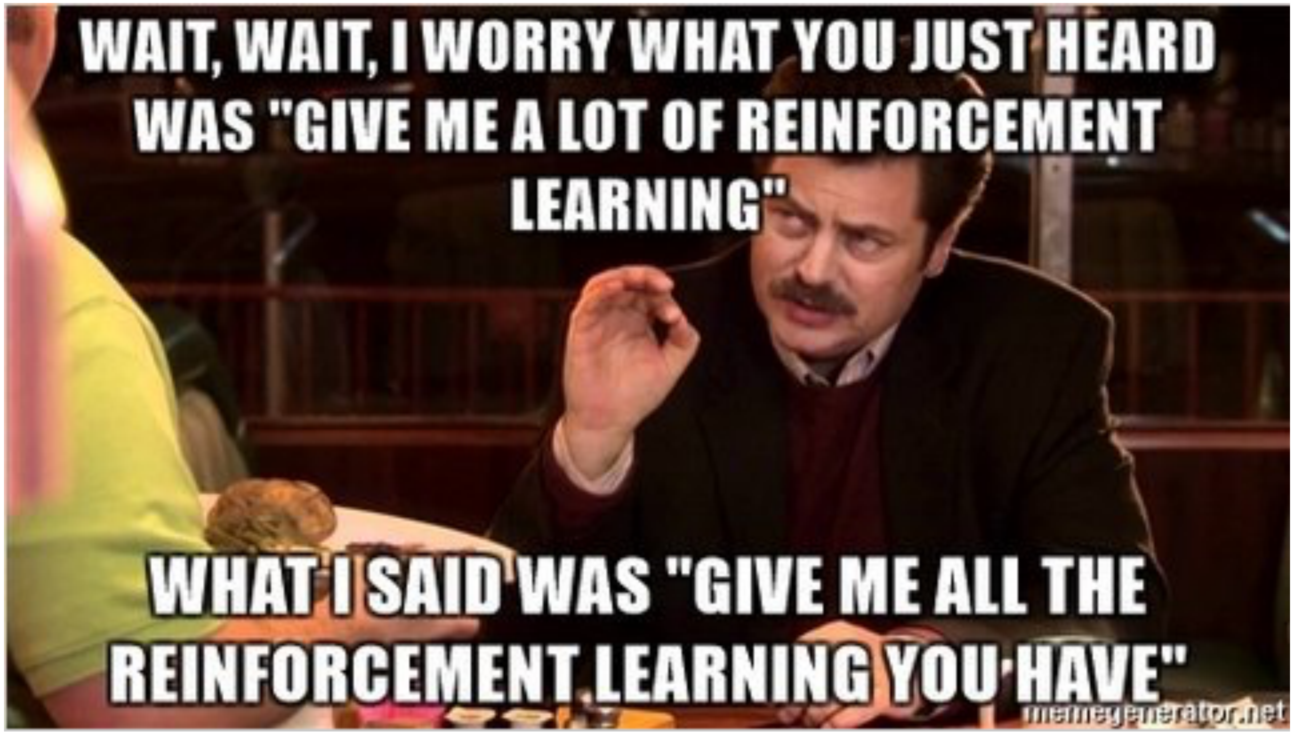
```
model = Net().to( "cpu" )
optimizer = optim.SGD(model.parameters()

for epoch in range(1, args.epochs + 1):
    train(args, model, "cpu" , train_loader, optimizer, epoch)
```

Utils

```
from torchvision import datasets, transforms
train_loader = torch.utils.data.DataLoader(
    datasets.MNIST('../data', train=True, download=True,
                   transform=transforms.Compose([
                       transforms.ToTensor(),        mean, std
                       transforms.Normalize((0.1307,), (0.3081,))
                   ])),
    batch_size=args.batch_size, shuffle=True, **kwargs)
```

Reinforcement Learning Basics



History of RL from Two Paths

- **Optimal Control**
  - Model processes via Markov property
  - Optimal paths through states calculated through dynamic programming
- **Animal Behavioral Learning (psychology)**
  - Animals learn by trial and error
  - Formalized by Thorndike, 1911. Strengthen through pleasure and weaken through pain
  - Motivation for many pioneering Researchers: Claude Shannon, J. Deutsch, Marvin Minsky, F. Rosenblatt, Widrow, Hoff

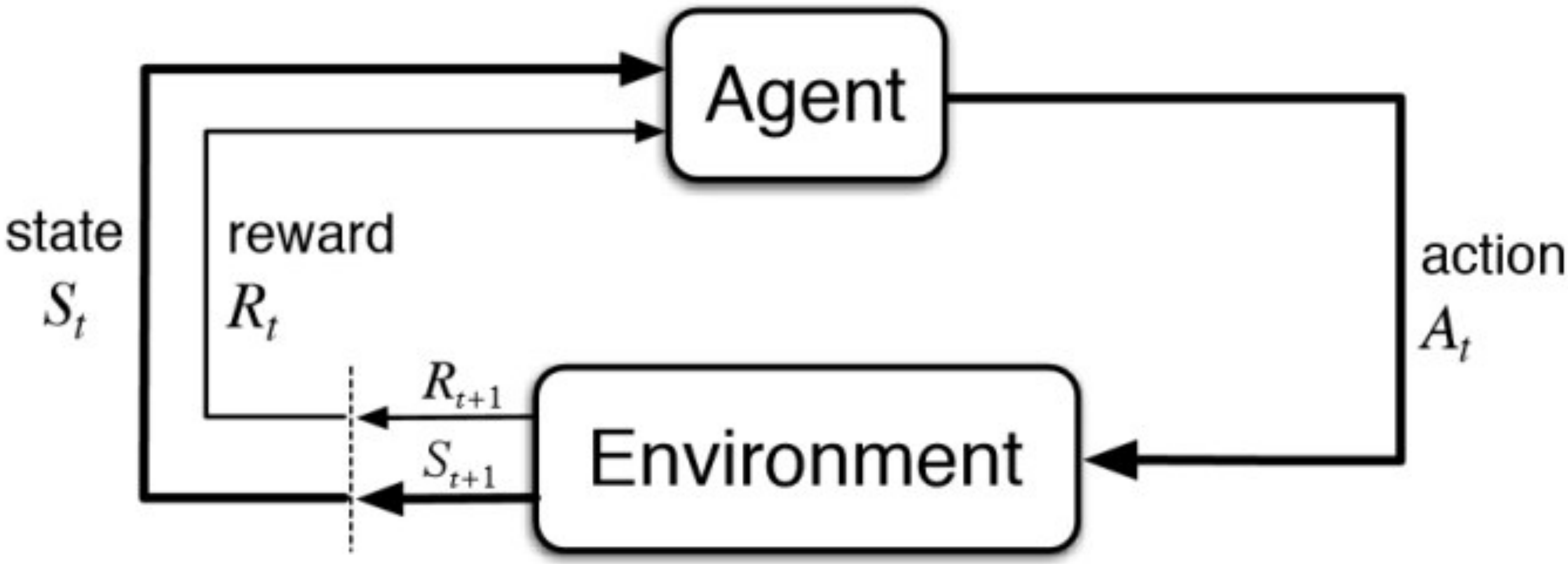
Riddles in the Dark

- Hybrid of **Supervised** and **Unsupervised** Learning
- **Reinforcement** Learning
  - Possibly specific labels given, but not without supervision
  - Uses many techniques from supervised learning, but applied towards a different objective
  - Rewards (positive and negative) are possible to assess behavior in an environment
  - Not specific to Machine Learning community

RL Landscape

- **Agent**
  - Interacts with the environment. Your model guides the Agent's decisions
- **Environment**
  - Anything that is not the agent
- **Observations**
  - What the agent knows about the environemnt
- **Actions**
  - What an agent can perform with the given environment
- **Rewards**
  - Local measure of success
  - Can compound local rewards over time

Generic Reinforcement Learning



https://www.kdnuggets.com/2018/03/5-things-reinforcement-learning.html

RL Parameters in Psychology

- One model for some human behavior, such as **learning a new topic**
- Agent: You
- Environment (be specific):
- Observations:
- Actions:
- Reward:

Conclusion: The **complexity** of the process is all entirely from the **design** and **assumptions** made in creating the **environment**, **obs**, **actions**

Markov Building Blocks

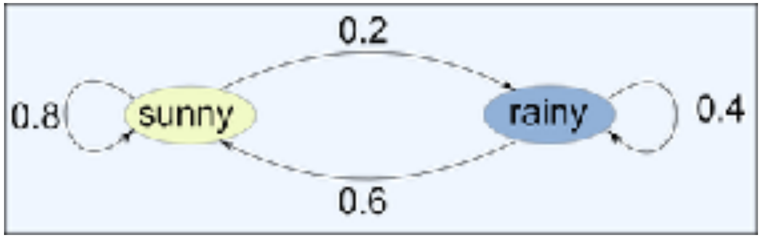
Markov Processes

- **Definition**: Any process that can be explained (or simplified) through a sequential set of states that depend only on the previous state
- **Practical Meaning**: For N states, there will be the probability of transition to any other state, encoded through an NxN transition matrix
- State sequences are not deterministic, they are sampled from the distributions
- Despite **simplicity**, they can model a number of real processes with **enough** precision

	Next State				
Previous State	0.1	0.2	0.1	0.6	0.0
	0.9	0.0	0.1	0.0	0.0
	0.0	0.4	0.0	0.4	0.2
	0.0	0.4	0.2	0.0	0.4
	0.0	0.0	0.6	0.0	0.4

MP Example from Lapan

	Sunny'	Rainy'
Sunny	0.8	0.2
Rainy	0.6	0.4

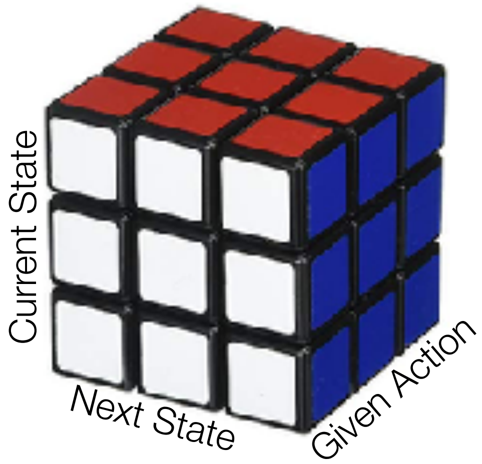


Sun+Summer	
Rainy+Summer	
Sun+Fall	
Rainy+Fall	
Sun+Else	
Rainy+Else	

Adding One Complexity Variable Can Have Large Effect on State Space

Markov Decision Processes

- **New**: Now any state to state transition can be altered by an action
- **Definition**: An MDP consists of:
  - Env. States, s_t
  - Actions for each state, $a(s_t)$
  - Reward function for each state, $r(s_t)$
  - A transition model, $P(s_{t+1}, s_t \mid a)$ a matrix of probabilities
    - Not guaranteed next state by given action



Markov Reward Process

- Total reward is given by sum of all future rewards

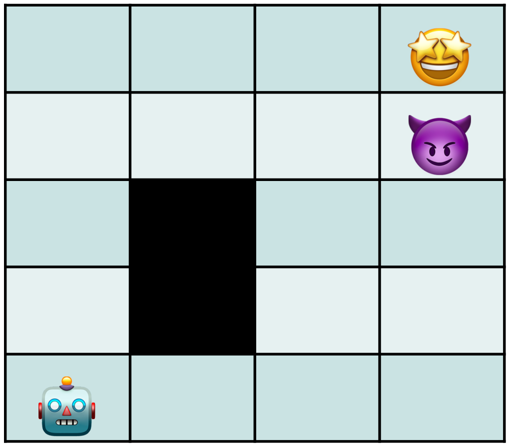
$$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} \ldots = \sum_k \gamma^k R_{t+k+1}$$

- Gamma defines far- and short-sightedness
    - Common values are **0** (short), **0.9**, **0.99**, and **1** (far)
- This reward calculation can be used to estimate the "Value" of each state based upon the average reward a state gives, $V(s) = \mathbf{E}[G \mid s_t = s]$
- Typically, this value must be estimated from the model over fixed sequences, otherwise all values can go to infinity (will return to this)

MDPs and MRPs

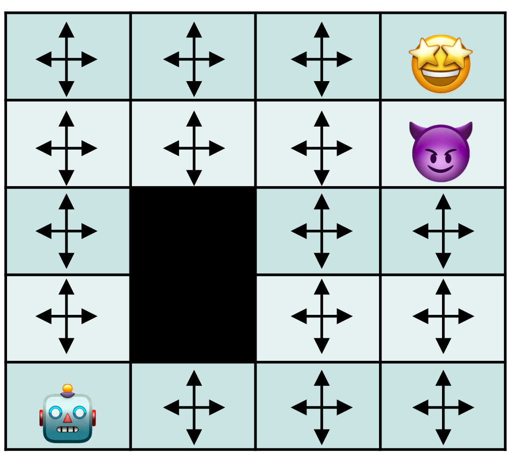
- How do we select a good action given a current state?
- If gamma is not 0, this can get really complicated as we need to look at all possible future actions
- Instead of defining what is optimal, let's instead setup a comparison of different rules (**policies**)
- A **policy** is defined as $\pi(a, s) = P(a_t = a \mid s_t = s)$
  - Given the current state, we have a certain probability of selecting each action
  - Action selection is **probabilistic**, but easy to define **deterministic** actions (*set one action to 1.0, all others to 0.0*)
- Try different policies, select one with best average reward

An Illustrative Example: Grid World

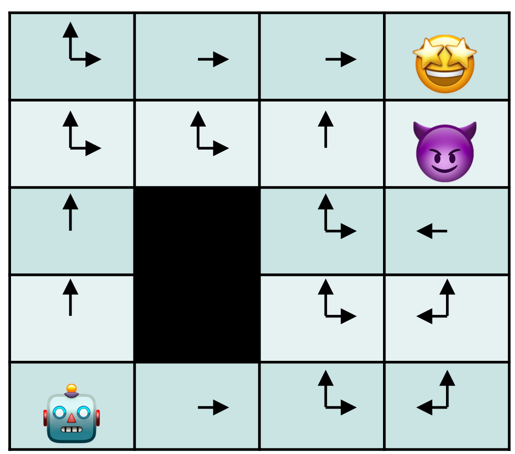


- **State**: Every square in grid
- **Action**: Move to make (l,r,u,d), with probability
- **Reward**: Goal, Death
- **Policy**: Given state, where should we move?
- **Optimal Policy**:

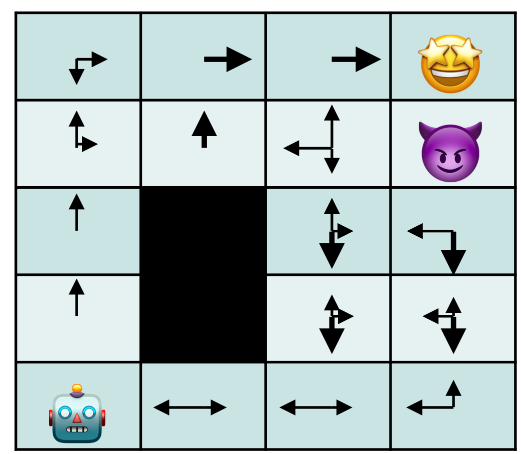
$$\pi^* = \arg\max_{\pi} \mathbf{E}\left[\sum_k \gamma^k R_{t+k+1} \mid \pi\right]$$



Random Policy

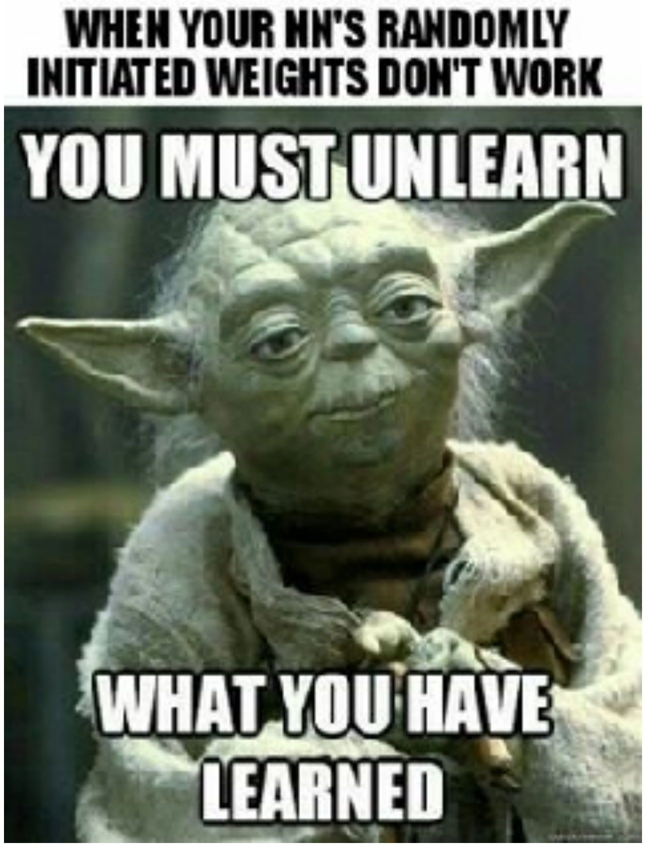


Another Policy



Another Policy

RL Categorization



Various Taxonomies

- Model-based versus Model-free
- Policy Based versus Value Based
- On-Policy, Off-Policy

- On-policy
    - We must interact with environment to learn a policy
- Off-policy
    - Can learn also from historical data or humans

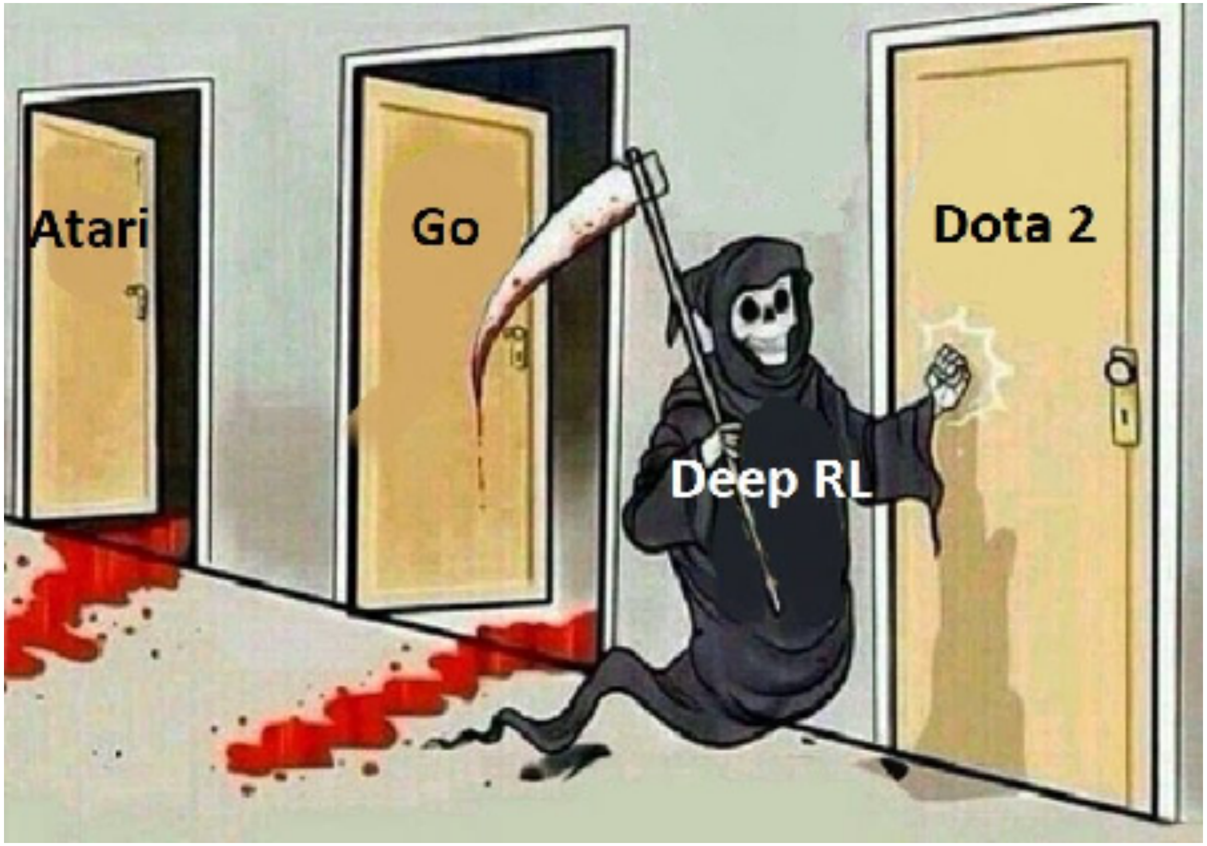
Model-based versus Model-free

- Model Based
  - Predict the next observation and reward based on an understanding of the rules in environment
  - Often look a number of moves ahead (like in chess or similar game)
  - Hard to construct in complex environemnts
- Model Free
  - Don't care what the problem is
  - Directly try to connect observations to actions (or values from which an action can be inferred)
- Mixed: Sure, like Alpha-Go

Policy Based versus Value Based

- Policy Based
  - Directly approximate the policy of the agent
  - Policy is typically a probability distribution of actions that we sample from for next action
- Value Based
  - Calculate an intermediate value function for all possible actions
  - Choose the best action based on value function

OpenAI Gym



Object Oriented RL

- Basics:
    - Define object instance for Agent() and the Env()
    - Define what observations will return
    - Run env.step(action)
    - Get new observations and reward from env
- `action_space` and `observation_space`
    - Possible actions to execute, Observations to get
    - Discrete or continuous?
    - Can actions be given simultaneously?

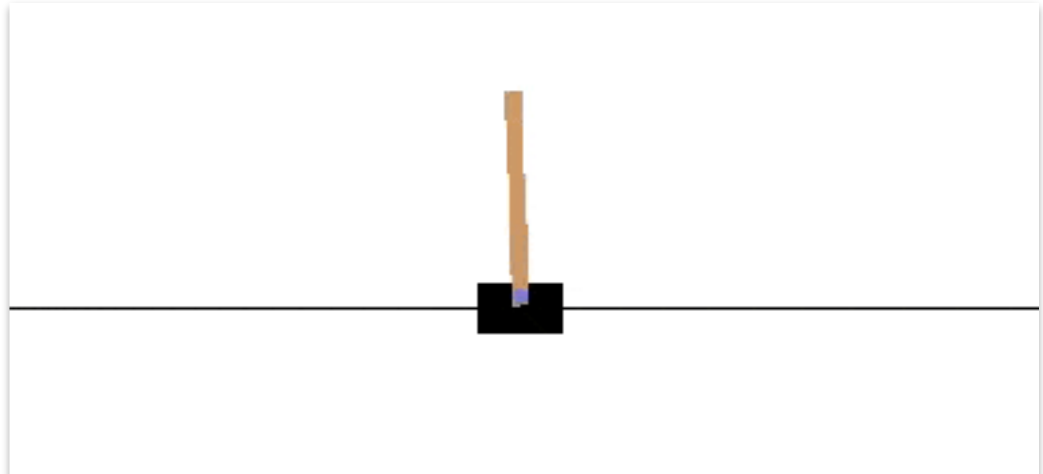
Basics of Cartpole

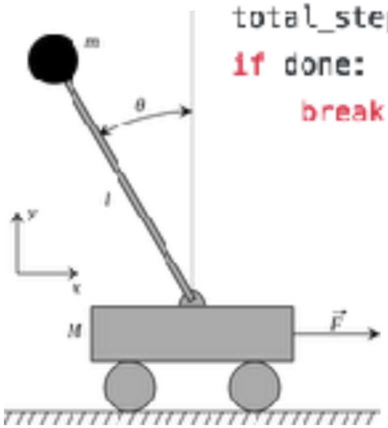
```
import gym


if __name__ == "__main__":
    env = gym.make("CartPole-v0")

    total_reward = 0.0
    total_steps = 0
    obs = env.reset()

    while True:
        action = env.action_space.sample()
        obs, reward, done, _ = env.step(action)
        total_reward += reward
        total_steps += 1
        if done:
            break
```





Action Space: One input, [0, 1] pull left or pull right

Obs Space: Dynamic state variables (continuous and four dimensional)

End: When more than 15 degrees off or too far from center

Reward: +1 for each time step

Wrapping the Environment

- When you want some extra action, observation, reward processing
- Expose function with `ActionWrapper`, `RewardWrapper`, `ObservationWrapper`

```
class RandomActionWrapper(gym.ActionWrapper):
    def __init__(self, env, epsilon=0.1):
        super(RandomActionWrapper, self).__init__(env)
        self.epsilon = epsilon

    def action(self, action):
        if random.random() < self.epsilon:
            print("Random!")
            return self.env.action_space.sample()
        return action
```

```
if __name__ == "__main__":
    env = RandomActionWrapper(gym.make("CartPole-v0"))

    obs = env.reset()
    total_reward = 0.0

    while True:
        obs, reward, done, _ = env.step(0)
        total_reward += reward
        if done:
            break
```

Might return different action than user supplied with small probability

Lecture Notes for

Neural Networks and Machine Learning

Intro to Reinforcement Learning

Next Time:
CrossEntropy and Q-Learning

Reading: Lamar CH4-CH6

Lecture Notes for

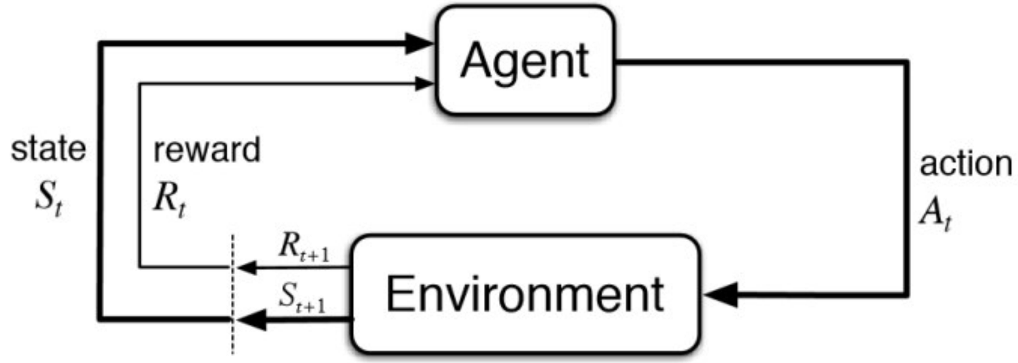
Neural Networks and Machine Learning

Cross Entropy and Value Iteration

Logistics and Agenda

- Logistics
  - Paper for Class
- Agenda
  - The Cross Entropy Method
  - Value Iteration
  - Q-Learning

Last Time



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$$\pi^* = \arg\max_{\pi} \mathbb{E}\left[\sum_k \gamma^k R_{t+k+1} \mid \pi\right]$$

Random Policy

Another Policy

Another Policy

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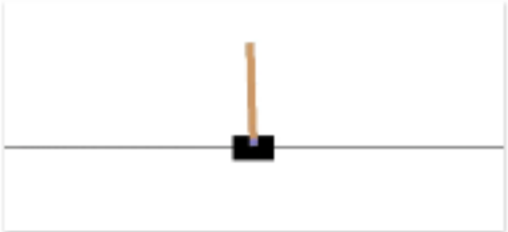

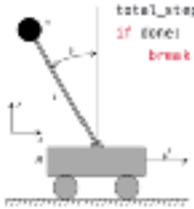

Action Space: One input, [0, 1] pull left or pull right

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Reward: +1 for each time step

Cross Entropy Method

Optimize Best Random Models

- Create a random neural network
- Let it interact with the environment (randomly)
  - For some set of episodes (e.g., 20)
  - Use network output to sample from possible actions
  - Run episode to completion
- Calculate reward for each episode
- Keep best episodes (some percentile, e.g., best five)
- For the given best episodes, develop loss function incentivizing the actions taken based upon the input observations

Cross Entropy Method

- Model based or Model Free?
  - Model Free (no assumptions of problem)
- Value or Policy Based?
  - Policy Based (randomly sample actions based on policy)
- On-policy or Off-Policy?
  - On-Policy (need to interact with environment to get better)
- Has some similarity to **Simulated Annealing** Optimization

How to Make this more Mathy?

- If we have all possible policies p(x) and a reward function H(x), then maximize

$$\mathbf{E}_{x \leftarrow p(x)}[H(x)] = \mathbf{E}_{x \leftarrow q(x)}[\frac{p(x)}{q(x)} H(x)]$$

- We can approximate the distribution by: $\frac{1}{N} \sum_i \frac{p(x_i)}{q(x_i)} H(x_i)$
- Proven that this is optimized when $\mathbf{KL}(q(x) \,||\, p(x)H(x))$ is minimized. But its intractable, so we drop terms … and end up just optimizing (neg) cross entropy of samples

$$\pi_{k+1} = \arg\max_{\pi_k} \mathbf{E}_{z \leftarrow \pi_k}[\underbrace{\mathbf{1}_{R(z) > \psi}}_{\text{Performance Measure}} \log \pi_k]$$

Review: Basics of Cartpole

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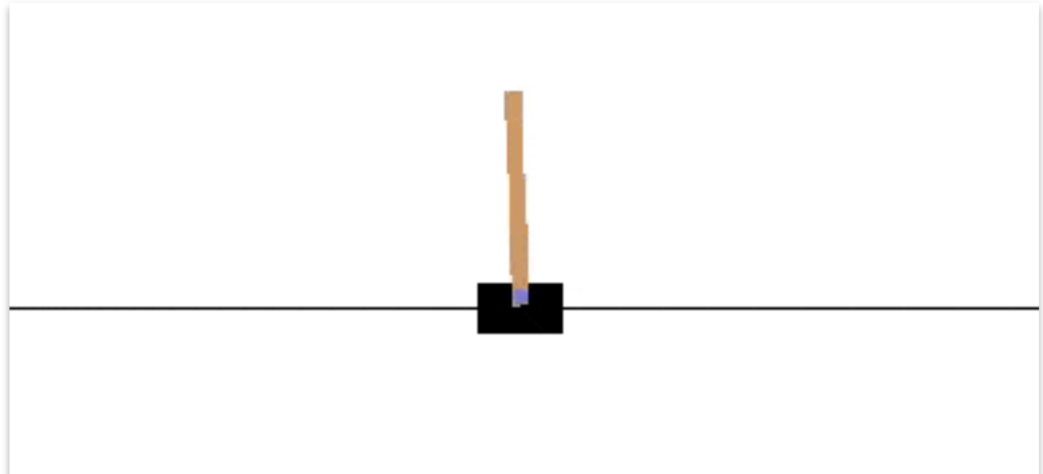

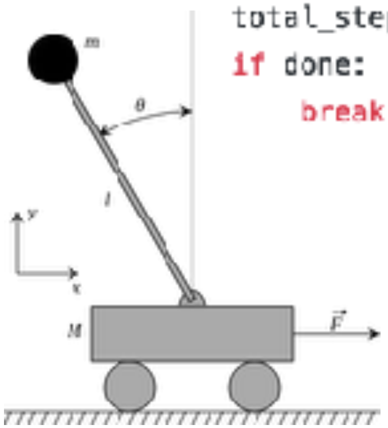

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Cross Entropy Reinforcement Learning

M. Lapan Implementation for CartPole and Frozen Lake

```
Follow Along:
08a_Basics_Of_Reinforcement_Learning.ipynb
```

Value Iteration

State Value Review

- Given: $$G_t = R_{t+1} + \gamma R_{t+2} + \gamma^2 R_{t+3} \ldots = \sum_k \gamma^k R_{t+k+1}$$
- $V(s) = \mathbf{E}[G \mid s_t = s]$, expected Value of a given state over all future iterations
- **Important**: we can only calculate this exactly if we know:
    - all the rewards for all the states
    - the probabilities of transitioning to a given state from selecting an action
    - likelihood of successful action
    - Most of the time **we know none of this** when we approach the problem, because it assumes a model of the system

The Bellman Equation

- For the case when each action is successful and state is discrete:

$$V_0 = \max_{a \in 1 \ldots N} (r_a + \gamma V_a)$$

current value is immediate reward plus value of next state with highest value

- Which feels like cheating because we assume we know V_a … just go with it for now
- General extension for when actions are probabilistic:

$$V_0 = \max_{a \in A} \mathbf{E}[r_{s,a} + \gamma V_s] = \max_{a \in A} \sum_{s \in S} p_{a,0 \to s} \cdot (r_{s,a} + \gamma V_s)$$

-probabilities of getting to next state x (current value is immediate reward plus value of next state)
-$p_{a,0 \to s}$ probability of getting to state s from state 0, given that you perform action a

- To select action with best value we need reward matrix, $r_{s,a}$ and action transition matrix $p_{a,0 \to s}$

Defining the Q-Function

$$V_0 = \max_{a \in A} \mathbf{E}[r_{s,a} + \gamma V_s] = \max_{a \in A} \sum_{s \in S} p_{a,0 \rightarrow s} \cdot (r_{s,a} + \gamma V_s)$$

- Define intermediate function Q

$$Q(s,a) = \sum_{s' \in S} p_{a,s \rightarrow s'} \cdot (r_{s,a} + \gamma V_{s'})$$

- With some nice properties/relations:

$$V_s = \max_{a \in A} Q(s,a)$$

$$Q(s,a) = r_{s,a} + \gamma \max_{a' \in A} Q(s', a')$$

Value Iteration (Value Based)

- **Direct**:
  - Initialize V(s) to all zeros
  - Take a series of random steps
  - Perform for each state: $V(s) \leftarrow \max_{a \in A} \sum_{s' \in S} p_{a,s \to s'} \cdot (r_{s,a} + \gamma V(s'))$
  - Repeat until V(s) stops changing
- **Q-Function Variant**:
  - Initialize Q(s,a) to all zeros
  - Take a series of random steps
  - For each state and action: $Q(s,a) \leftarrow \sum_{s' \in S} p_{a,s \to s'} \cdot (r_{s,a} + \gamma \max_{a'} Q(s', a'))$
  - Repeat until Q is not changing

Need to estimate $p_{a,s \to s'}$
Via observed **Transitions**

This Update Will **Converge to Optimal Policy**

Value Iteration Reinforcement Learning

M. Lapan Implementation for
and Frozen Lake

```
Follow Along:
08a_Basics_Of_Reinforcement_Learning.ipynb
```

Some Limitations

- Q function can get really big for large states and action spaces
- Infinite when the spaces are continuous
  - We will solve this by using a neural network to approximate the Q function
- Transition matrix, similarly, can get gigantic for large state and action spaces
  - We will solve this by dropping the transition probabilities in Q function update
- This Variant is known as Q-Learning

Lecture Notes for

Neural Networks and Machine Learning

CE and Value Iteration

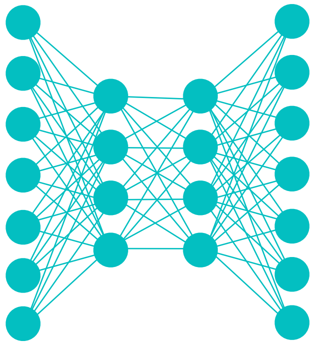
Next Time:
Deep Q-Learning

Reading: Lapan CH6, CH7

Lecture Notes for

Neural Networks and Machine Learning

Deep Q-Learning



Last Time

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- Proven that this is optimized when $\mathbf{KL}(q(x) \parallel p(x)H(x))$ is minimized. But its intractable, so we drop terms … and end up just optimizing (neg) cross entropy of samples

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Performance Measure

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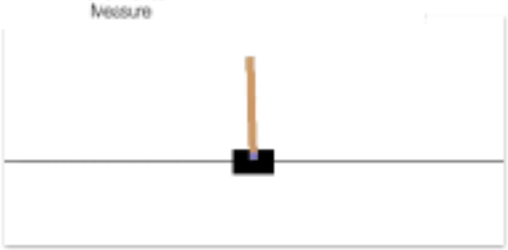
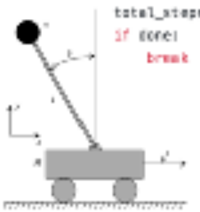
    obs = env.reset()

    while True:
        action = env.action_space.sample()
        obs, reward, done, _ = env.step(action)
        total_reward += reward
        total_steps += 1
        if done:
            break
```





Action Space: One input, [0, 1] pull left or pull right

Obs Space: Dynamic state variables (continuous and four dimensional)

End: When more than 15 degrees off or too far from center

Reward: +1 for each time step

Value Iteration (Value Based)

- **Direct**:
  - Initialize V(s) to all zeros
  - Take a series of random steps
  - Perform for each state: $V(s) \leftarrow \max_{a \in A} \sum_{s' \in S} p_{a,s \to s'} \cdot (r_{s,a} + \gamma V(s'))$
  - Repeat until V(s) stops changing
- **Q-Function Variant**:
  - Initialize Q(s,a) to all zeros
  - Take a series of random steps
  - For each state and action: $Q(s,a) \leftarrow \sum_{s' \in S} p_{a,s \to s'} \cdot (r_{s,a} + \gamma \max_{a'} Q(s',a'))$
  - Repeat until Q is not changing

Need to estimate $p_{a,s \to s'}$
Via observed **Transitions**

This Update Will **Converge to Optimal Policy**

Defining the Q-Function

$$V_0 = \max_{a \in A} \mathbf{E}[r_{s,a} + \gamma V_s] = \max_{a \in A} \sum_{s \in S} p_{a,0 \to s} \cdot (r_{s,a} + \gamma V_s)$$

- Define intermediate function Q

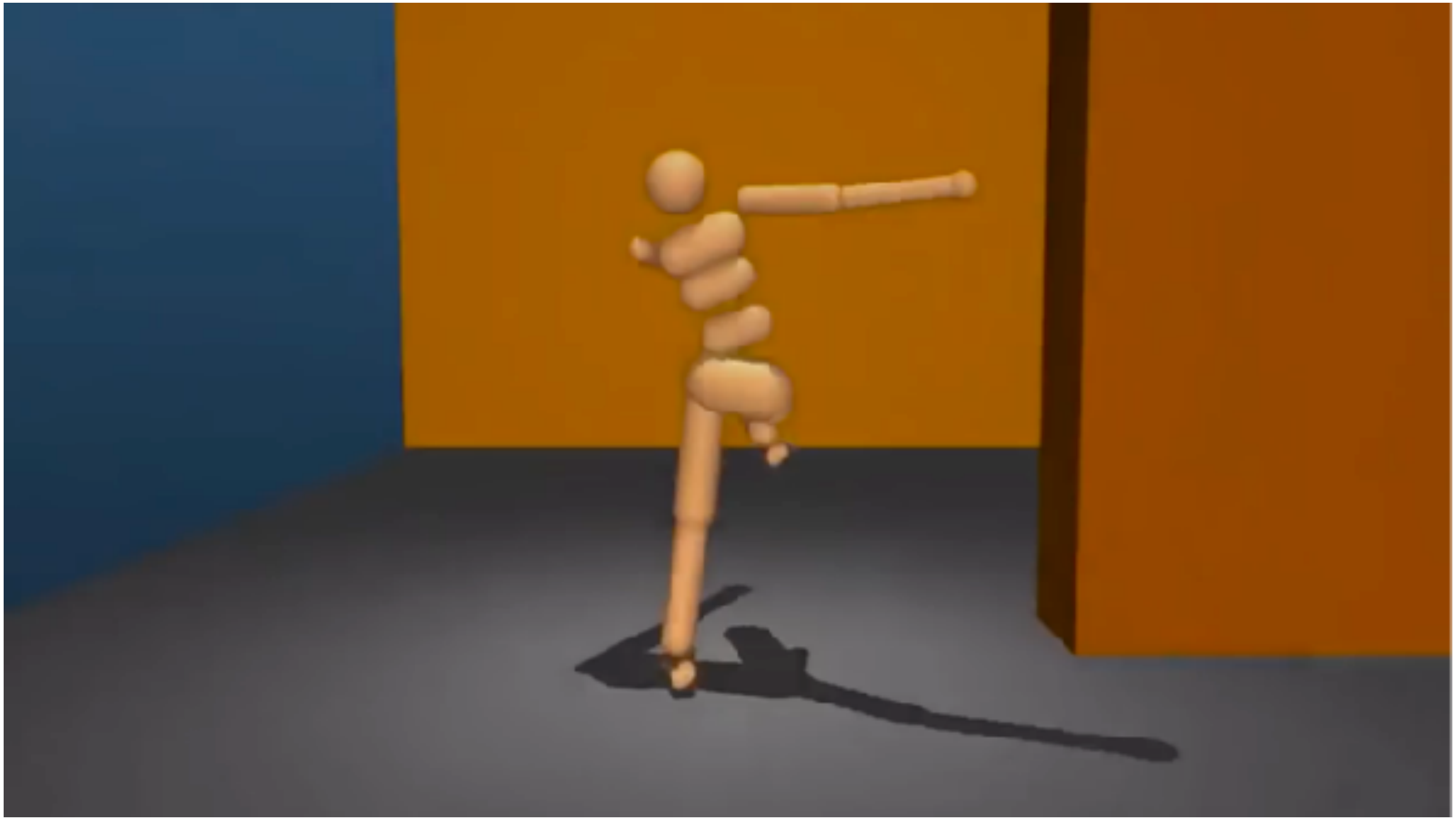
$$Q(s,a) = \sum_{s' \in S} p_{a,s \to s'} \cdot (r_{s,a} + \gamma V_{s'})$$

- With some nice properties/relations:

$$V_s = \max_{a \in A} Q(s,a)$$

$$Q(s,a) = r_{s,a} + \gamma \max_{a' \in A} Q(s',a')$$

Q-Learning



Tabular Q-Learning Algorithm

- In update, ignore the transition probability, making use of the iterative nature of Q:

$$Q(s,a) = r_{s,a} + \gamma \max_{a' \in A} Q(s',a')$$

- Add momentum to the update equation

$$Q(s,a) \leftarrow (1-\alpha)\cdot Q(s,a) + \alpha \cdot [r_{s,a} + \gamma \max_{a' \in A} Q(s',a')]$$

- Algorithm:
  - Sample (with rand) from environment, (s, a, r, s’)
  - Make **Bellman Update** with Momentum
  - Repeat until convergence

Tabular Q-Learning Reinforcement Learning

M. Lapan Implementation for and Frozen Lake

Follow Along:
`08a_Basics_Of_Reinforcement_Learning.ipynb`

Q-Learning with a Neural Network

- Want to approximate Q(s,a) when the state is potentially large. Given s_t, we want the network to give us a row of actions that we can choose from:
  $[\ Q(s_t,a_1),\ Q(s_t,a_2),\ Q(s_t,a_3),\ \ldots\ Q(s_t,a_A)\ ]$
- This allows us to make a loss function which incentives the actual Q-function behavior we desire from a sampled tuple (s, a, r, s')

$$\mathscr{L} = \left[\underbrace{Q(s,a)}_{\text{from current network params}} - [r_{s,a} + \gamma \underbrace{\max_{a' \in A} Q^*(s',a')}_{\text{from older network params (better stability)}}] \right]^2$$

Periodically Update
Params of Q^* from Q

$$\mathscr{L} = \left[Q(s,a) - [r_{s,a}] \right]^2$$

if no next state (env is done)

But we need more power!

- We need to do some **random actions** before following the policy or else we won’t learn
- Also, we need to follow the policy more and more to get to better places in the environment
- **Epsilon-Greedy** Approach:
    - Start randomly doing actions with prob epsilon
    - Slowly make epsilon smaller as training progresses
- And also we need to have larger amounts of uncorrelated training batches so we will again use **experience replay**

Deep Q-Learning
Reinforcement Learning

M. Lapan Implementation for Frozen Lake

And with Atari!

```
Follow Along:
08a_Basics_Of_Reinforcement_Learning.ipynb
```

Course Retrospective

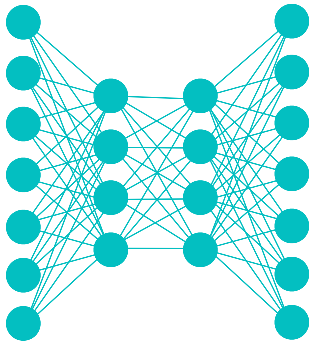
Lecture Notes for

Neural Networks and Machine Learning

Deep Q Learning

Next Time:
None!

Reading: None



Lecture Notes for

Neural Networks and Machine Learning

Deep Q-Learning

Backup slides

Title Between Topics

Example Slide

Title

Subtitle

`Follow Along: Notebook Name`