7.강 Deep Q-learning

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- Pytorch
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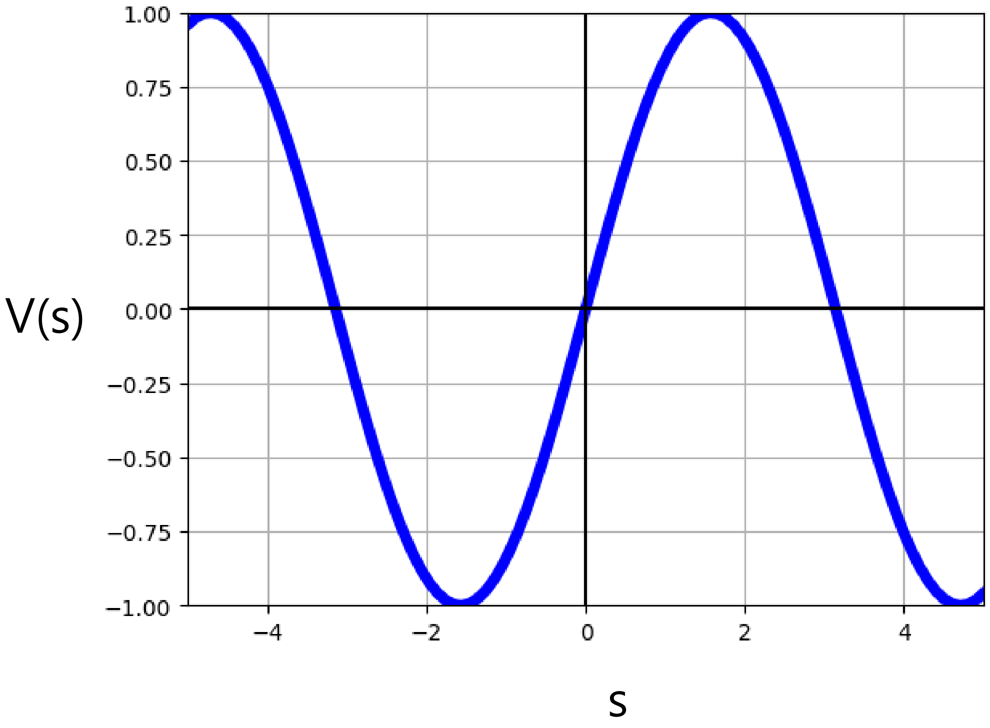
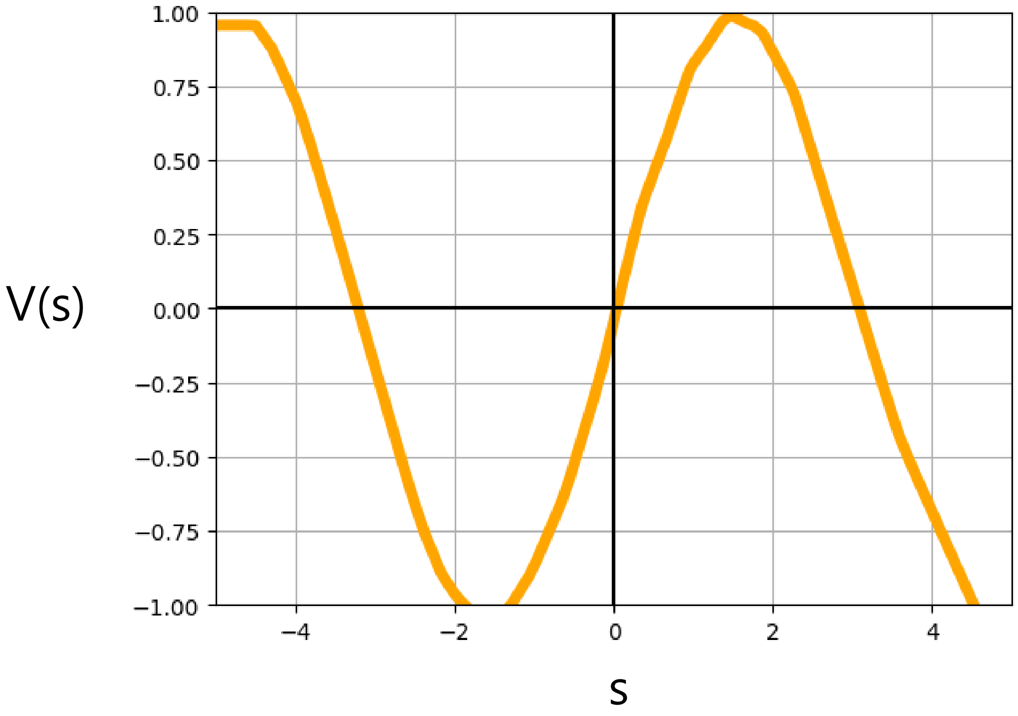
Neural Network

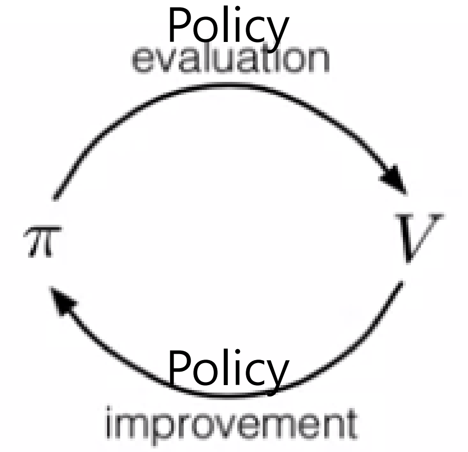
Function approximators

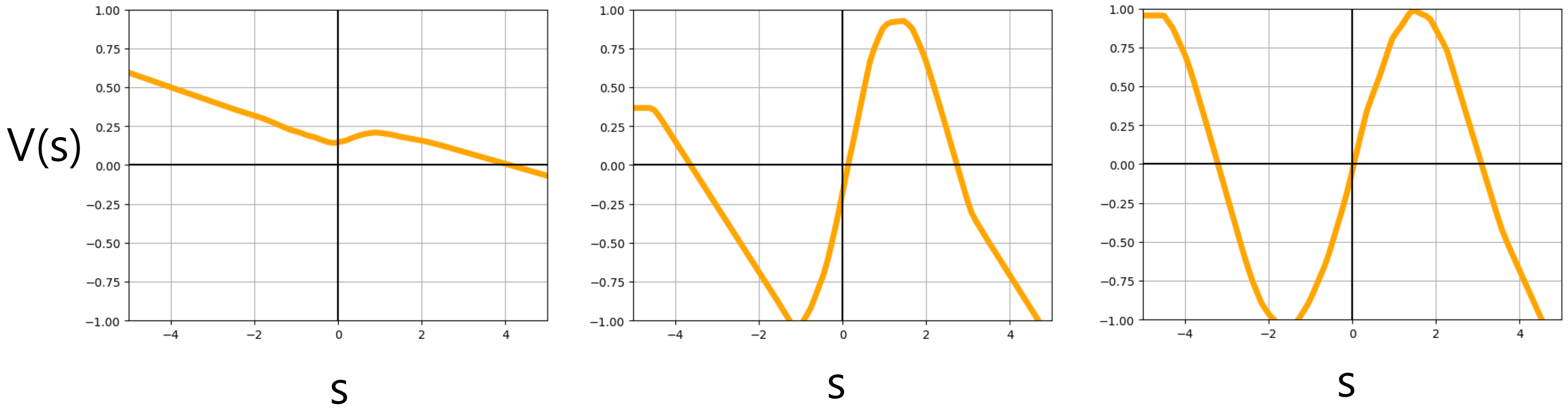




Function approximators

- How do we observe the value function?
  - The agent learns based on experience.
  - The functions v*(s) and q*(s ,a) are not know in advance

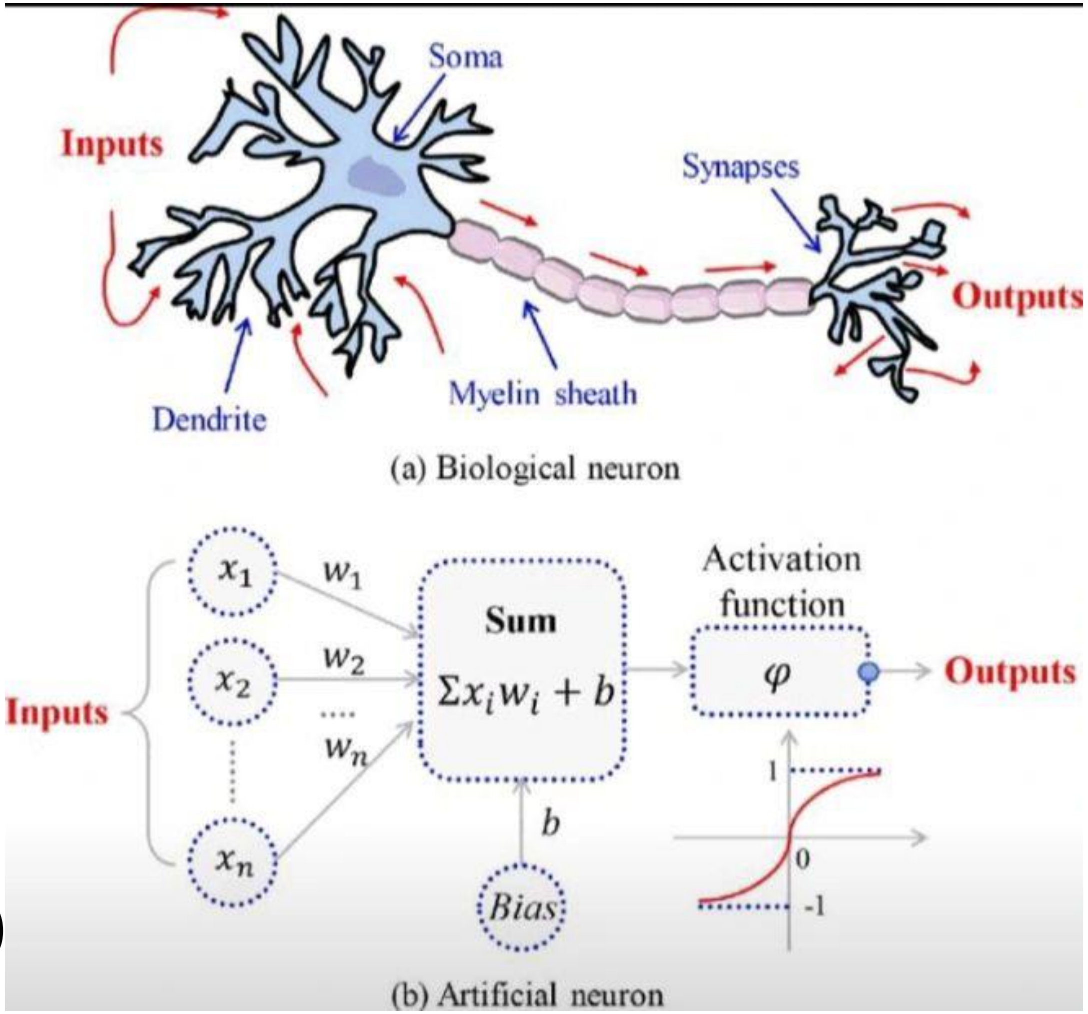




$$f_1(s|w) \rightarrow f_2(s|w) \rightarrow \cdots . \rightarrow f_n(s|w) \approx v^*(s)$$

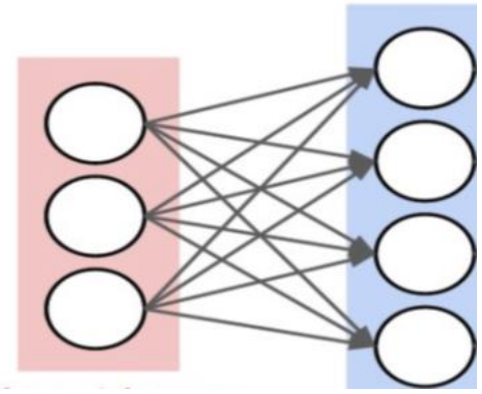
Neural Networks

- Computing system inspired by the biological neural networks that constitute our brain
- They server multiple purposes, including function approximation: $\hat{y} = f(x|w)$
- Mathematical function typically consisting of a weighted sum of inputs and a activation/transfer function $\text{Output} = \varphi(\sum_{i=1}^{n} w_i x_i + b)$



Neural networks

- Input vector x = [x1, x2, x3]



- Connection matrix:

$$W1 = \begin{bmatrix} w11 & w12 & w13 & w14 \\ w21 & w22 & w23 & w24 \\ w31 & w32 & w33 & w34 \end{bmatrix}$$

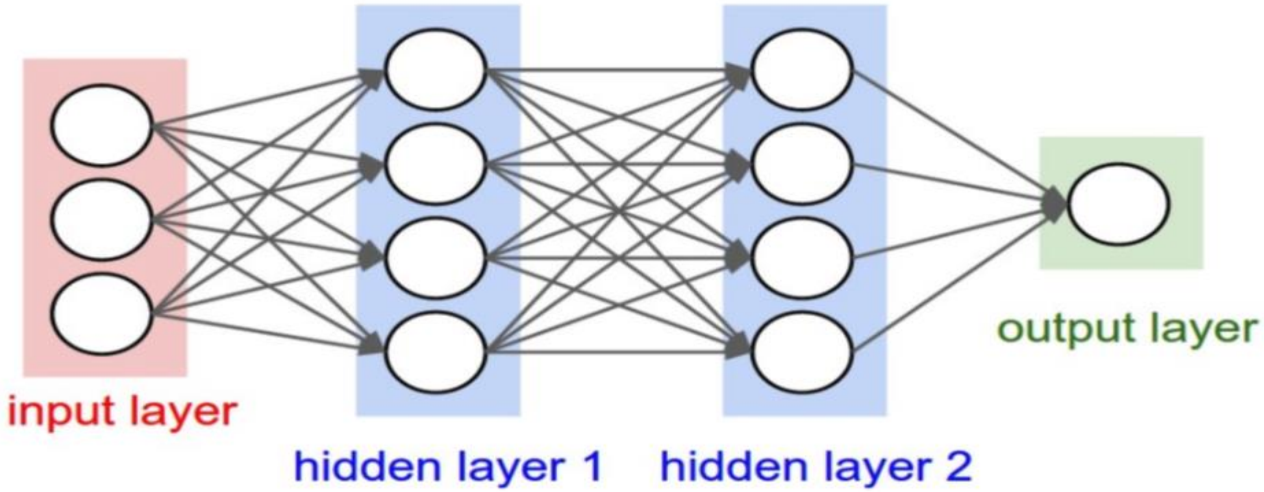
By changing its parameters W1, we can modify it to approximate the function we are interested in

- Output vector:

$$H = [\varphi(\sum_{i=1}^{n} w_i x_i + b), \ldots, \varphi(\sum_{i=1}^{n} w_i x_i + b)]$$

Neural Networks

- Networks that do not have cycles are known as feedforward NN. Signals always propagate forward
- The neuron receives inputs, process & aggregate those inputs, and either inhibits or amplifies before passing the signal to the next layer



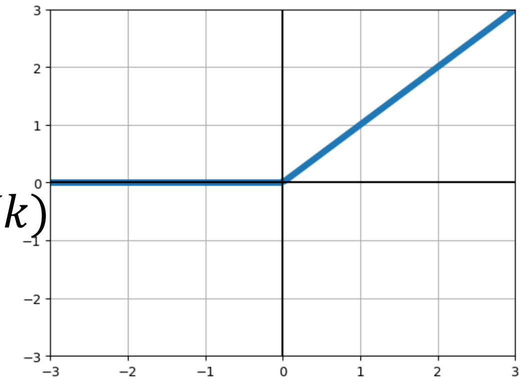
$h_1 = \sigma(W_1 x)$ $h_2 = \sigma(W_2 h_1)$ $y = W_3 h_2$

Neural networks

- Activation functions

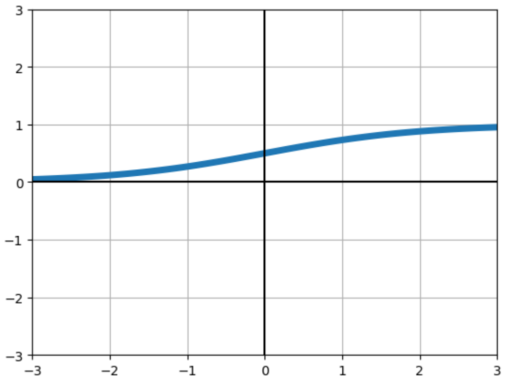
Relu()

$\varphi(Vk)$



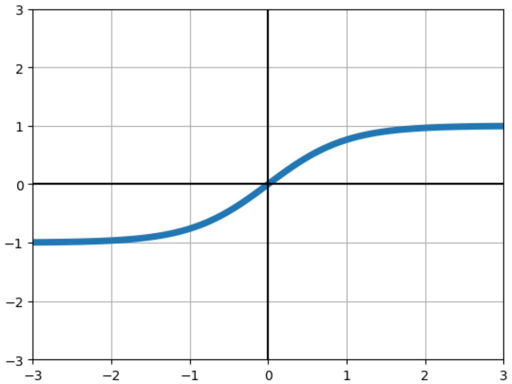
V_k

Sigmoid()



V_k

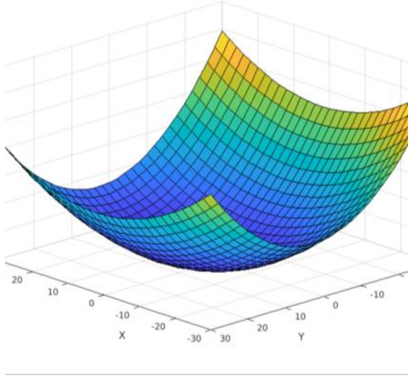
Tanh()

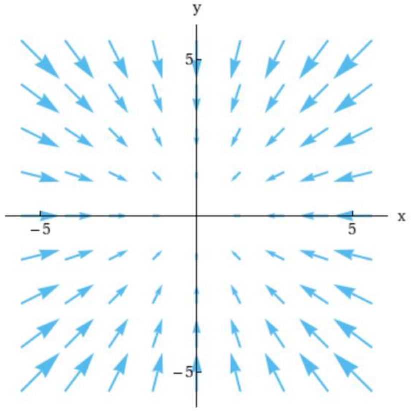


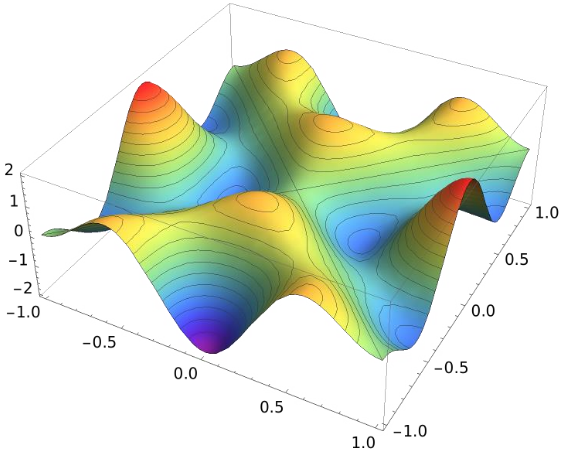
V_k

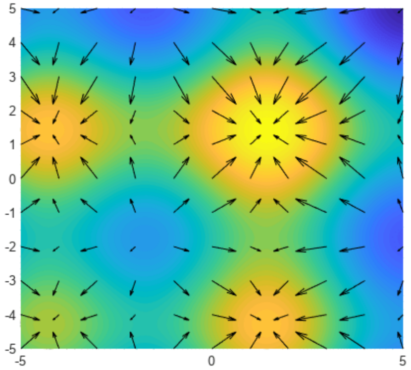
Gradient Descent

- Given some loss function: $L(\vec{x}, \vec{y}) = \ ||2\vec{x} + 2\vec{y}||$
- Update rules for the parameters: $w_{t+1} = w_t - \ \alpha\nabla\hat{L}(w)$
- Gradient vector: $\nabla\hat{L}(w) = \ [\frac{\partial L}{\partial w1}, \frac{\partial L}{\partial w2}, \ldots, \frac{\partial L}{\partial wn}]$
- Computed using the backpropagation algorithm
- $\nabla\hat{L}(w)$ points to the direction of maximum growth of $\nabla\hat{L}(w)$
- α is the size of the step we take in the opposite direction to $\nabla\hat{L}(w)$









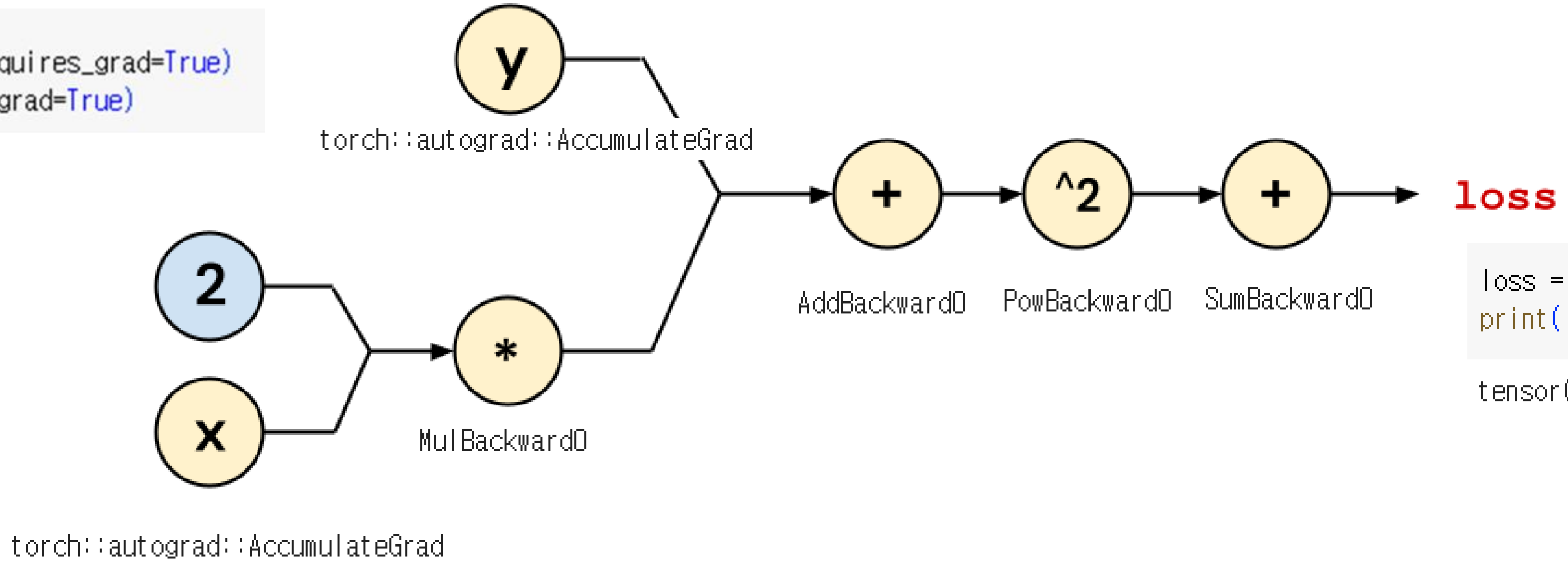
Backpropagation

- Computed using the backpropagation algorithm
- We want to evaluate partial derivative: $\frac{\partial L}{\partial \vec{x}}$ and $\frac{\partial L}{\partial \vec{y}}$

```
shape = (3, )
x = torch.tensor([1., 2, 3], requires_grad=True)
y = torch.ones(shape, requires_grad=True)
```

```
loss = ((2 * x + y)**2).sum()
loss.backward()
print(x.grad)
print(y.grad)
```

```
tensor([24., 40., 56.])
tensor([12., 20., 28.])
```




```
loss = ((2 * x + y)**2).sum()
print(loss)
```

```
tensor(83., grad_fn=<SumBackward0>)
```

Cost function

- Mean squared error:

$$\mathrm{L}(\mathrm{w}) = \frac{1}{\mathrm{N}} \sum_{\mathrm{i}=0}^{\mathrm{N}} [\mathrm{y} - \hat{\mathrm{y}}]^2$$

- For our neural network to estimate q(s, a) as well as possible, we will minimize the observed squared errors

$$\hat{\mathrm{L}}(\mathrm{w}) = \frac{1}{\mathrm{N}} \sum_{\mathrm{i}=0}^{\mathrm{N}} [\mathrm{R}_{\mathrm{t}+1} + \gamma \hat{\mathrm{q}}(\mathrm{S}_{\mathrm{t}+1}, \mathrm{A}_{\mathrm{t}+1}|\mathrm{w}) - \hat{\mathrm{q}}(\mathrm{S}_{\mathrm{t}}, \mathrm{A}_{\mathrm{t}}|\mathrm{w})]^2$$

- Target value:

$$\mathrm{R}_{\mathrm{t}+1} + \gamma \hat{\mathrm{q}}(\mathrm{S}_{\mathrm{t}+1}, \mathrm{A}_{\mathrm{t}+1}|\mathrm{w})$$

Estimated value:

$$\hat{\mathrm{y}} = \hat{\mathrm{q}}(\mathrm{S}_{\mathrm{t}}, \mathrm{A}_{\mathrm{t}}|\mathrm{w})$$

Neural network optimization

- For our neural network to estimate q(s, a) as well as possible, we will minimize the observed squared errors

$$\hat{\mathrm{L}}(\theta) = \frac{1}{\mathrm{N}} \sum_{\mathrm{i}=0}^{\mathrm{N}} [\mathrm{R}_i + \gamma \hat{\mathrm{q}}(\mathrm{S}_i{'}, \mathrm{A}_i{'} | \theta_{targ}) - \hat{\mathrm{q}}(\mathrm{S}_i, \mathrm{A}_i | \theta)]^2$$

- Target value: a value towards which we want to push the estimates

$$\mathrm{R}_i + \gamma \hat{\mathrm{q}}(\mathrm{S}_i{'}, \mathrm{A}_i{'} | \theta_{targ})$$

- Estimate of the q-value of a state-action pair

$$\hat{\mathrm{q}}(\mathrm{S}_i, \mathrm{A}_i | \theta)$$

Pytorch

Pictures from Stanford's CS231n
Pictures from Berkeley CS285

Numpy & PyTorch

NumPy

- Fast CPU implementations
- **CPU-only**
- **No autodiff**
- **Imperative**

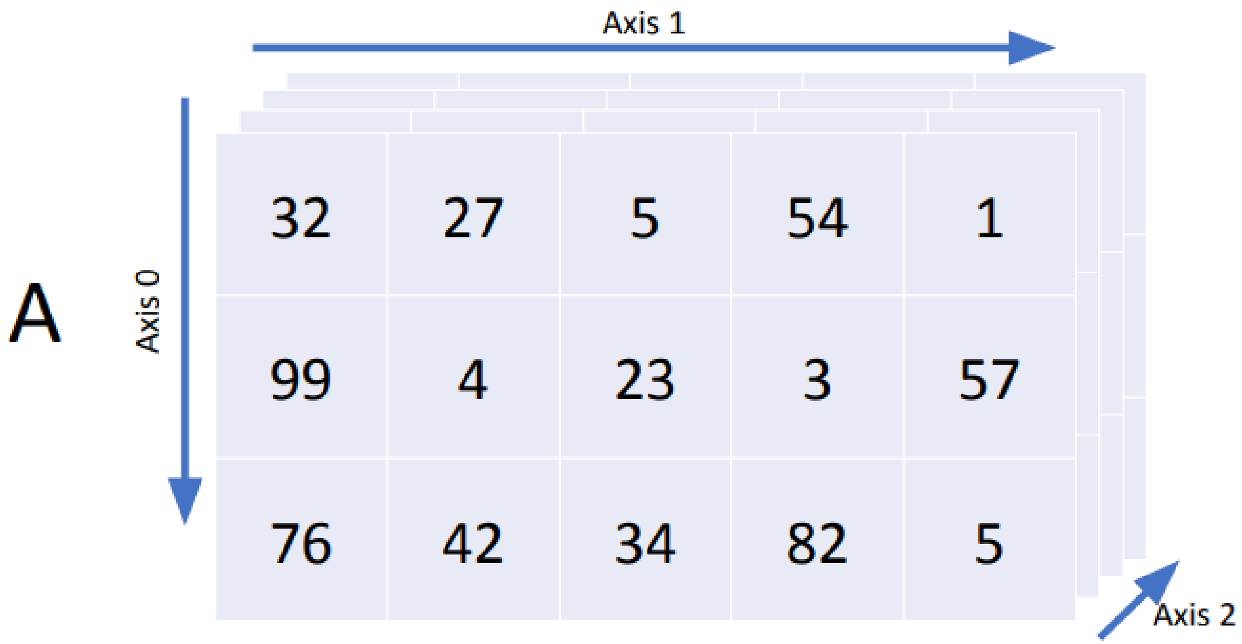
PyTorch

- Fast CPU implementations
- **Allows GPU**
- **Supports autodiff**
- **Imperative**

Other features include:

- Datasets and dataloading
- Common neural network operations
- Built-in optimizers (Adam, SGD, …)

Multidimensional Indexing




```
A.shape == (3, 5, 4)
```

Shape Operations

NumPy

```python
A = np.random.normal(size=(10, 15))

# Indexing with newaxis/None
# adds an axis with size 1
A[np.newaxis] # -> shape (1, 10, 15)

# Squeeze removes a axis with size 1
A[np.newaxis].squeeze(0) # -> shape (10, 15)

# Transpose switches out axes.
A.transpose((1, 0)) # -> shape (15, 10)

# !!! BE CAREFUL WITH RESHAPE !!!
A.reshape(15, 10)    # -> shape (15, 10)
A.reshape(3, 25, -1) # -> shape (3, 25, 2)
```

PyTorch

```python
A = torch.randn((10, 15))

# Indexing with None
# adds an axis with size 1
A[None] # -> shape (1, 10, 15)

# Squeeze removes a axis with size 1
A[None].squeeze(0) # -> shape (10, 15)

# Permute switches out axes.
A.permute((1, 0)) # -> shape (15, 10)

# !!! BE CAREFUL WITH VIEW !!!
A.view(15, 10)    # -> shape (15, 10)
A.view(3, 25, -1) # -> shape (3, 25, 2)
```

Device Management

- Numpy: all arrays live on the CPU's RAM
- Torch: tensors can either live on CPU or GPU memory
  - Move to GPU with `.to("cuda")`/`.cuda()`
  - Move to CPU with `.to("cpu")`/`.cpu()`

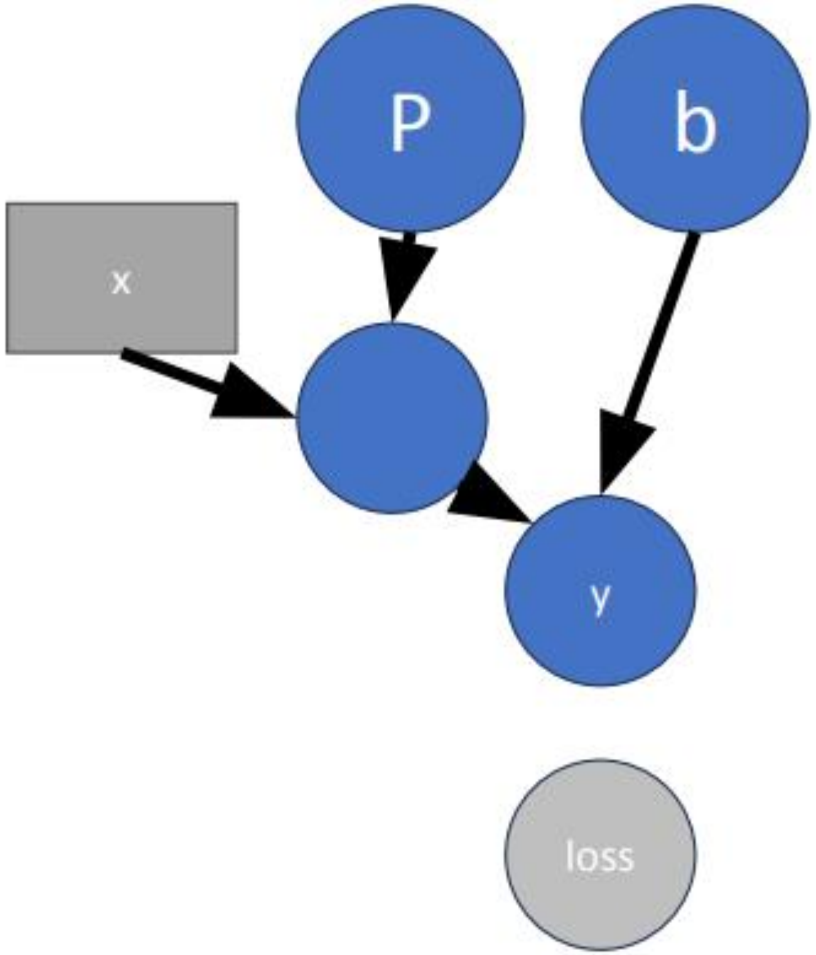
YOU CANNOT PERFORM OPERATIONS BETWEEN TENSORS ON DIFFERENT DEVICES!

Computing Gradients

```
P = torch.randn((1024, 1024))
print(P.requires_grad) # -> False
P = torch.randn((1024, 1024), requires_grad=True)
b = torch.randn((1024,), requires_grad=True)
print(P.grad) # -> None

x = torch.randn((32, 1024))
y = torch.nn.relu(x @ P + b)

target = 3
loss = torch.mean((y - target) ** 2).detach()
```



Training Loop

REMEMBER THIS!

```
net = (...).to("cuda")
dataset = ...
dataloader = ..
optimizer = ...
loss_ fn = ..
for epoch in range(num_epochs):
  # Training..
  net.train()
  for data, target in dataloader:
    data = torch.from_numpy(data).float().cuda()
    target = torch.from_numpy(data).float().cuda()

    prediction = net(data)
    loss = loss_fn(prediction, target)

    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

  net.eval()
  # Do evaluation..
```

Converting Numpy / PyTorch

Numpy -> PyTorch:

```
torch.from_numpy(numpy_array).float()
```

PyTorch -> Numpy:

- (If `requires_grad`) Get a copy without graph with `.detach()`
- (If on GPU) Move to CPU with `.to("cpu")/.cpu()`
- Convert to numpy with `.numpy`

All together:

```
torch_tensor.detach().cpu().numpy()
```

Custom networks

```python
import torch.nn as nn

class SingleLayerNetwork(nn.Module):
  def __init__(self, in_dim: int, out_dim: int, hidden_dim: int):
    super().__init__() # <- Don't forget this!
    self.net = nn.Sequential(
      nn.Module(in_dim, hidden_dim),
      nn.ReLU(),
      nn.Module(hidden_dim, out_dim),
    )

  def forward(self, x: torch.Tensor) -> torch.Tensor:
    return self.net(x)

batch_size = 256
my_net = SingleLayerNetwork(2, 32, 1).to("cuda")
output = my_net(torch.randn(size=(batch_size, 2)).cuda())
```

- nn.Module represents the building blocks of a computation graph.
  - For example, in typical pytorch code, each convolution block is its own module, each fully connected block is a module, and the whole network itself is also a module.
- Modules can contain modules within them. All the classes inside of \`torch.nn\` are instances \`nn.Modules\`.

Custom networks

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    super().__init__() # <- Don't forget this!
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batch_size = 256
my_net = SingleLayerNetwork(2, 32, 1).to("cuda")
output = my_net(torch.randn(size=(batch_size, 2)).cuda())
```

- Prefer `net()` over `net.forward()`
- Everything (network and its inputs) on the same device!!!

Torch Best Practices

- When in doubt, **`assert`** is your friend

```
assert x.shape == (B, N), \
       f"Expected shape ({B, N}) but got {x.shape}"
```

- Be extra careful with `.reshape/.view`
  - If you use it, assert before and after
  - Only use it to collapse/expand a single dim
  - In Torch, prefer `.flatten()/.permute()/.unflatten()`
- If you do some complicated operation, test it!
  - Compare to a pure Python implementation

Torch Best Practices

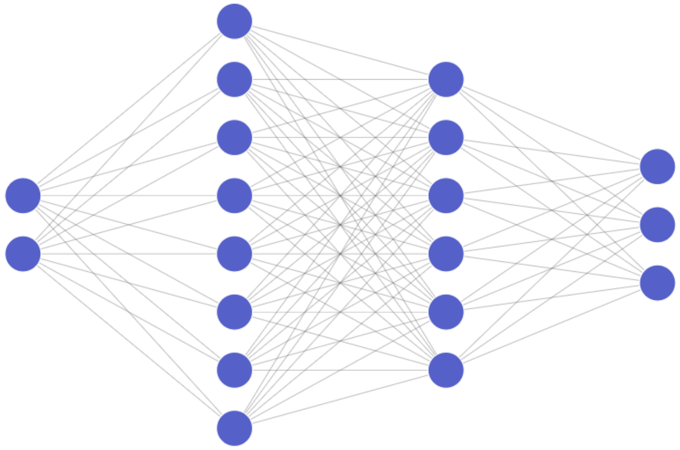
- Don’t mix numpy and Torch code
  - Understand the boundaries between the two
  - Make sure to cast 64-bit numpy arrays to 32 bits
  - `torch.Tensor` only in `nn.Module`!
- Training loop will always look the same
  - Load batch, compute loss
  - `.zero_grad()`, `.backward()`, `.step()`

Deep Q-learning

Deep Q-learning

- Q-learning + Neural Network
- Swap the q-value table for a neural network
- Tackle more difficult problems
- Leverage generalization power of neural networks

S=[s1,s2]



$\hat{q}= [\hat{q}(s,s_1), \hat{q}(s,s_2), \hat{q}(s,s_3)]$

Neural Net. Architecture for V, Q

- St vector input → NN → V scalar output

- St, At vector input → NN → Q scalar output
  - Continuous case

- St vector input → Q vector output
  - Discrete action space only
  - Output size is $|A|$

Neural Net. Architecture for policy, π

- St input → NN → vector output
  - Discrete action space case
  - Output size is $|A|$
  - SOFTMAX turns the output into prob. (sum of prob. is 1)

- St input → NN → $\mu_\theta(S_t), \delta_\theta(St)$ output
  - Continuous action space case
  - Represented with Gaussian Distribution

Neural network optimization

- Mean squared error:

$$L(\theta) = \frac{1}{N}\sum_{i=1}^{N}[y_i - \hat{y}_i]^2$$

- We calculate the gradient vector of the cost function with respect to the θ parameters:

$$\nabla\hat{\mathrm{L}}(\theta) = \left[\frac{\partial L}{\partial \theta 1}, \frac{\partial L}{\partial \theta 2}, \ldots, \frac{\partial L}{\partial \theta \mathrm{n}}\right]$$

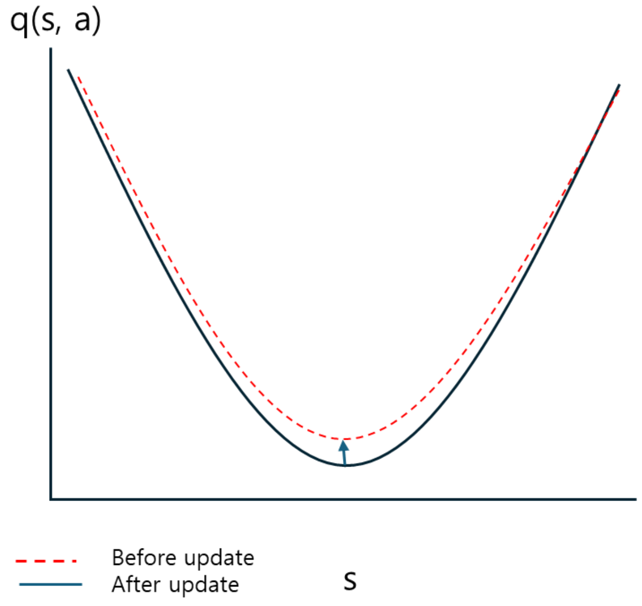
- With the gradient vector, we will make a SGD step:

$$\theta \leftarrow \theta - \alpha\nabla\hat{\mathrm{L}}(\theta)$$

Target network

- Two techniques combined generate an unstable learning process.
- Bootstrapping($y_i = R_i + \gamma\hat{q}(S_i{}', A_i{}'|\theta_{targ})$) + function approximator
- Why? : When a value is changed, nearby values will also be affected.

- When a value is changed, nearby values will also be affected.
- By modifying a $\hat{q}(S_i, Ai|\theta)$ estimate we also modify its $\hat{q}(S_i{}', Ai'|\theta_{targ})$ target
- For the learning process to be stable, the target must also be stable



Target network

- We make a copy of the neural network to calculate the targets.

$$\theta_{targ} \leftarrow \theta$$

- This neural network does not change with SGD. Its θ parameters remain the same
- The estimated value of S_i', A_i' is calculated with the target network:

$$\hat{L}(\theta) = \frac{1}{N}\sum_{i=0}^{N}[R_i + \boxed{\gamma\hat{q}(S_i', A_i'|\theta_{targ})} - \hat{q}(S_i, A_i|\theta)]^2$$

Deep Q-learning

Algorithm 1 Deep Q-Learning

Input: α learning rate, ϵ random action probability,
    γ discount factor,
Initialize q-value parameters θ and target parameters $\theta_{targ} \leftarrow \theta$
$b \leftarrow \epsilon$-greedy policy w.r.t $\hat{q}(s, a|\theta)$
$\pi \leftarrow$ greedy policy w.r.t $\hat{q}(s, a|\theta)$
Initialize replay buffer B
for episode $\in 1..N$ **do**
    Restart environment and observe the initial state S_0
    for $t \in 0..T-1$ **do**
        Select action $A_t \sim b(S_t)$
        Execute action A_t and observe S_{t+1}, R_{t+1}
        Insert transition $(S_t, A_t, R_{t+1}, S_{t+1})$ into the buffer B
        $K = (S, A, R, S') \sim B$
        Select actions $A' \sim \pi(S')$
        Compute loss function over the batch of experiences:

$$L(\theta) = \frac{1}{|K|} \sum_{i=1}^{|K|} \left[\boxed{R_i + \gamma \hat{q}(S'_i, A'_i|\theta_{targ})} - \hat{q}(S_i, A_i|\theta)\right]^2 \tag{1}$$

    end for
    Every k episodes synchronize $\theta_{targ} \leftarrow \theta$
end for
Output: Near optimal policy π and q-value approximations $\hat{q}(s, a|\theta)$

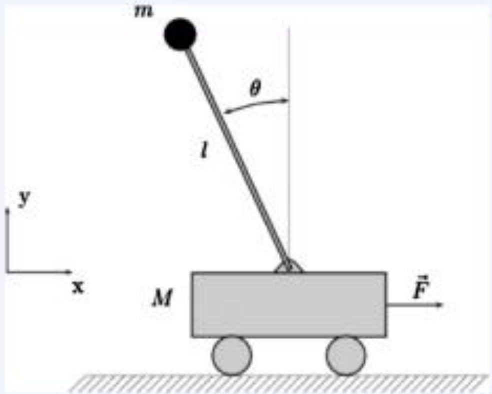
Code Ex.

- Cartpole: Keep the tip of the pole straight

- States: Pole angle and angular velocity
- Actions: Move left, right
- Transition model:

$$\begin{bmatrix} \dot{x} \\ \ddot{x} \\ \dot{\theta} \\ \ddot{\theta} \end{bmatrix} = \begin{bmatrix} \dot{x} \\ \frac{-ml\sin(\theta)\dot{\theta}^2 + F + mg\cos(\theta)\sin(\theta)}{M + m - m\cos(\theta)^2} \\ \dot{\theta} \\ \frac{-ml\cos(\theta))\sin(\theta)\dot{\theta}^2 + F\cos(\theta) + mg\sin(\theta) + Mg\sin(\theta)}{l*(M + m - m\cos(\theta)^2} \end{bmatrix}$$

- Rewards:
  - +1: Survive
  - 0: Fall



https://danielpiedrahita.wordpress.com/portfolio/cart-pole-control/

If we know angle and velocity, we can calculate accelerations (Able to describe the whole dynamics)

Code Ex.

The state

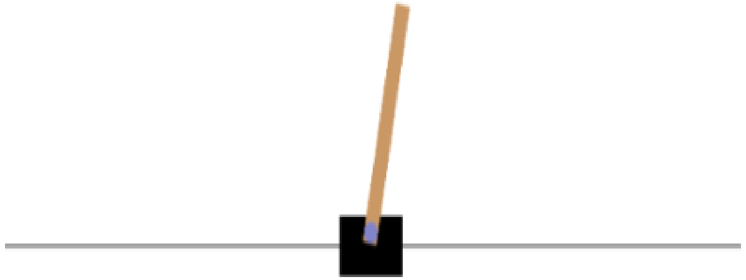
The states of the cartpole task will be represented by a vector of four real numbers:

Num	Observation	Min	Max
0	Cart Position	-4.8	4.8
1	Cart Velocity	-Inf	Inf
2	Pole Angle	-0.418 rad (-24 deg)	0.418 rad (24 deg)
3	Pole Angular Velocity	-Inf	Inf

The actions available

We can perform two actions in this environment:

```
0    Apply +1 torque on the joint between the links.
1    Do nothing
2    Apply -1 torque on the joint between the links.
```



Reward: +1 for every step

Code Ex.

```
env = gym.make('CartPole-v0')
#seed_everything(env)
env.reset()
plt.imshow(env.render(mode='rgb_array'))
```

```
state_dims = env.observation_space.shape[0]
num_actions = env.action_space.n
print(f"CartPole env: State dimensions: {state_dims}, Number of actions: {num_actions}")
```

```
CartPole env: State dimensions: 4, Number of actions: 2
```

Code Ex.

Create the Q-Network: $\hat{q}(s, a|\theta)$

```
q_network = nn.Sequential(
    nn.Linear(state_dims, 128),
    nn.ReLU(),
    nn.Linear(128, 64),
    nn.ReLU(),
    nn.Linear(64, num_actions))
```

액션의 개수만큼 output이 나옴

Create the target Q-Network: $\hat{q}(s, a|\theta_{targ})$

```
target_q_network = copy.deepcopy(q_network).eval()
```

Code Ex.

Unsqueeze(dim=0) put a extra. dim. in front.
View(1,-1) put a extra. dim. in front.

For every step,

- **Sample state:**
  tensor([[-0.0220, -0.0468, 0.0114, -0.0126]])
- **Next state:**
  tensor([[-0.0230, -0.2421, 0.0112, 0.2836]])
- **Reward:**
  tensor([[1.]])
- **Done:**
  tensor([[False]])

```
class PreprocessEnv(gym.Wrapper):

    def __init__(self, env):
        gym.Wrapper.__init__(self, env)

    def reset(self):
        obs = self.env.reset()
        return torch.from_numpy(obs).unsqueeze(dim=0).float()

    def step(self, action):
        action = action.item()
        next_state, reward, done, info = self.env.step(action)
        next_state = torch.from_numpy(next_state).unsqueeze(dim=0).float()
        reward = torch.tensor(reward).view(1, -1).float()
        done = torch.tensor(done).view(1, -1)
        return next_state, reward, done, info
```

Experience Replay

$[[S_1, A_1, R_2, S_2], [S_2, A_2, R_3, S_3]]$

$[[S_1, S_2], [A_1, A_2], [R_2, R_3], [S_2, S_3]]$

$[[[S_1], [S_2]], [[A_1], [A_2]], [[R_2], [R_3]], [[S_2], [S_3]]]$
A batch shape : N x D for each

Torch.cat은 default가 행(0) 방향으로 붙임
S, A, R, 에 대해 각각 batch(N x D) 로 바꿔 줌

```
class ReplayMemory:

    def __init__(self, capacity=1000000):
        self.capacity = capacity
        self.memory = []
        self.position = 0

    def insert(self, transition):
        if len(self.memory) < self.capacity:
            self.memory.append(None)
        self.memory[self.position] = transition
        self.position = (self.position + 1) % self.capacity

    def sample(self, batch_size):
        assert self.can_sample(batch_size)

        batch = random.sample(self.memory, batch_size)
        batch = zip(*batch)
        return [torch.cat(items) for items in batch]

    def can_sample(self, batch_size):
        return len(self.memory) >= batch_size * 10

    def __len__(self):
        return len(self.memory)
```

Deep Q-learning

$\pi \leftarrow$ greedy policy w.r.t $\hat{q}(s, a|\theta)$

A batch shape : N x D.

$[[[S_1], [S_2]], [[A_1], [A_2]], [[R_2], [R_3]],[[S_2], [S_3]]]$
A batch shape : N x D for each

각 state당 액션의 개수만큼 output이 나옴.
예를들어 $\hat{q}(S_i|\theta)$ 는 $[[(\hat{q}(si)\ for\ A_1)], [\hat{q}(si)\ for\ A_2]]$

$\hat{q}(S_i,' Ai'|\theta_{targ})$, where $A_i' \sim \pi(S')$

$$\hat{L}(\theta) = \frac{1}{N}\sum_{i=0}^{N}[R_i + \gamma\hat{q}(S_i{'}, A_i'|\theta_{targ}) - \hat{q}(S_i, A_i|\theta)]^2$$

$$\nabla\hat{L}(\theta) = [\frac{\partial L}{\partial\theta 1}, \frac{\partial L}{\partial\theta 2}, \ldots, \frac{\partial L}{\partial\theta n}]$$

$$\theta \leftarrow \theta - \alpha\nabla\hat{L}(\theta)$$

```python
def deep_q_learning(q_network, policy, episodes,
                    alpha=0.0001, batch_size=32, gamma=0.99, epsilon=0.2):

    optim = AdamW(q_network.parameters(), lr=alpha)
    memory = ReplayMemory()
    stats = {'MSE Loss': [], 'Returns': []}

    for episode in tqdm(range(1, episodes + 1)):
        state = env.reset()
        done = False
        ep_return = 0
        while not done:
            action = policy(state, epsilon)
            next_state, reward, done, _ = env.step(action)

            memory.insert([state, action, reward, done, next_state])

            if memory.can_sample(batch_size):
                state_b, action_b, reward_b, done_b, next_state_b = memory.sample(batch_size)
                qsa_b = q_network(state_b).gather(1, action_b)

                next_qsa_b = target_q_network(next_state_b)
                next_qsa_b = torch.max(next_qsa_b, dim=-1, keepdim=True)[0]

                target_b = reward_b + ~done_b * gamma * next_qsa_b
                loss = F.mse_loss(qsa_b, target_b)
                q_network.zero_grad()
                loss.backward()
                optim.step()

                stats['MSE Loss'].append(loss)

            state = next_state
            ep_return += reward.item()


        stats['Returns'].append(ep_return)

        if episode % 10 == 0:
            target_q_network.load_state_dict(q_network.state_dict())

    return stats
```

Deep Q-learning

- You can cut a gradient by calling `y.detach()`, which will return a new tensor with `required_grad=False`. Note that `detach` is not an in-place operation! You would want this during evaluation.
- You also can't convert a tensor with `requires_grad=True` to numpy (for the same reason as above). Instead, you need to detach it first, e.g. `y.detach().numpy()`

- y.clone() vs. y.detach():
- If y change, y.clone() not change.
- If y change y.detach() change

Create the exploratory policy: $b(s)$

```
def policy(state, epsilon=0.):
    if torch.rand(1) < epsilon:
        return torch.randint(num_actions, (1, 1))
    else:
        av = q_network(state).detach()
        return torch.argmax(av, dim=-1, keepdim=True)
```

Code Ex.

- Open deep_q_learning_colab.ipynb