

Deep Value

CISC 7404 - Decision Making

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I noticed the last 1 hour of class everyone looks tired and sad

Three hours is a long time to pay attention, especially at night

Would you prefer:

- To have a long break (30 mins) in the middle?
- No breaks, end lecture after 2 or 2.5 hours
- Keep as-is (approximately 3 hours + 10 min break)

HW1 bug:

There was a bug in the update Q TD0 starter code, thanks He Zhe! Before: terminateds = jnp.concatenate([jnp.zeros(states.shape[0], dtype=bool), jnp.array([1], dtype=bool)]) After: terminateds = jnp.concatenate([jnp.zeros(states.shape[0] - 1,

dtype=bool), jnp.array([1], dtype=bool)])

$$Q_{i+1}(s_0,a_0,\theta_\pi) = Q_i(s_0,a_0,\theta_\pi) - \alpha \cdot \eta$$

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$$\eta = Q_i(s_0, a_0, \theta_\pi) - \\ \\ \left(\hat{\mathbb{E}}[\mathcal{R}(s_1) \mid s_0, a_0] + \neg \underset{a \in A}{\operatorname{d}} \gamma \max_{a \in A} Q_i(s_1, a, \theta_\pi) \right)$$

$$Q_{i+1}(s_0,a_0,\theta_\pi) = Q_i(s_0,a_0,\theta_\pi) - \alpha \cdot \eta$$

Predicted value

$$\eta = Q_i(s_0, a_0, \theta_\pi) - \left(\hat{\mathbb{E}}[\mathcal{R}(s_1) \mid s_0, a_0] + \neg d\gamma \max_{a \in A} Q_i(s_1, a, \theta_\pi) \right)$$

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 Empirical value

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If s_1 is a terminal state, future value is 0 ($\neg d = \text{not terminated}$)

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 Empirical value

If s_1 is a terminal state, future value is 0 ($\neg d = \text{not terminated}$)

Without the $\neg d$ term, takes longer to train!

I thought about coding deep Q networks in class today

But I realize if I do this, then you will not learn as much

Learning to debug is the #1 skill to succeed in reinforcement learning

Instead, you will implement deep Q learning for your second homework

Homework 2:

- Deep Q learning
- Deep policy gradient

Will release after homework 1

Next quiz in 2-3 weeks

Focus on

- Returns
- Value functions
- Q learning
- Deep Q learning
- Policy gradient

Review

We model neural networks as parameterized functions

$$f: X \times \Theta \mapsto Y$$

Map an input $x \in X$ and parameters $\theta \in \Theta$ to output space Y

$$f(\boldsymbol{x}, \boldsymbol{\theta})$$

Neural networks consist of artificial neurons

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Or ReLU

$$\sigma(x) = \max(0, x)$$

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 d_y neurons (wide):

$$f: \mathbb{R}^{d_x} \times \Theta \mapsto \mathbb{R}^{d_y}$$

$$\Theta = \mathbb{R}^{(d_x + 1) \times d_y}$$

For a single neuron

For a single neuron

$$f\left(\begin{bmatrix}x_1\\\vdots\\x_{d_x}\end{bmatrix},\begin{bmatrix}\theta_0\\\theta_1\\\vdots\\\theta_{d_x}\end{bmatrix}\right) = \sigma\left(\sum_{i=0}^{d_x}\theta_i\overline{x}_i\right)$$

For a single neuron

For a wide network

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For a wide network

$$f\left(\begin{bmatrix}x_1\\x_2\\\vdots\\x_{d_x}\end{bmatrix},\begin{bmatrix}\theta_{0,1}&\theta_{0,2}&\dots&\theta_{0,d_y}\\\theta_{1,1}&\theta_{1,2}&\dots&\theta_{1,d_y}\\\vdots&\vdots&\ddots&\vdots\\\theta_{d_x,1}&\theta_{d_x,2}&\dots&\theta_{d_x,d_y}\end{bmatrix}\right)=\begin{bmatrix}\sigma\left(\sum_{i=0}^{d_x}\theta_{i,1}\overline{x}_i\right)\\\sigma\left(\sum_{i=0}^{d_x}\theta_{i,2}\overline{x}_i\right)\\\vdots\\\sigma\left(\sum_{i=0}^{d_x}\theta_{i,d_y}\overline{x}_i\right)\end{bmatrix}$$

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A wide network:

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A deep network has many internal functions

$$\begin{split} f_1(\boldsymbol{x}, \boldsymbol{\varphi}) &= \sigma(\boldsymbol{\varphi}^\top \overline{\boldsymbol{x}}) \quad f_2(\boldsymbol{x}, \boldsymbol{\psi}) = \sigma(\boldsymbol{\psi}^\top \overline{\boldsymbol{x}}) \quad ... \quad f_\ell(\boldsymbol{x}, \boldsymbol{\xi}) = \sigma(\boldsymbol{\xi}^\top \overline{\boldsymbol{x}}) \\ & f(\boldsymbol{x}, \boldsymbol{\theta}) = f_\ell(...f_2(f_1(\boldsymbol{x}, \boldsymbol{\varphi}), \boldsymbol{\psi})...\boldsymbol{\xi}) \end{split}$$

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We call each function a **layer**

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A deep neural network is made of many layers

We can create different models for different tasks

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Standard tasks:

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Standard tasks: Multi-layer perceptron (MLP)

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Image tasks:

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Image tasks: Convolutional neural network (CNN)

Temporal tasks: Recurrent neural network (RNN)

Image, temporal tasks: Transformer

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Very powerful finding! The basis of deep learning.

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Although such θ exists, it can be hard to find

Finding $oldsymbol{ heta}$ is an optimization problem

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$$\operatorname*{arg\;min}_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\theta})$$

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Loss function measures the error between $f(x, \theta)$ and desired g(x) = y

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$$\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{x},\boldsymbol{y},\boldsymbol{\theta})$$

Loss function measures the error between $f(\boldsymbol{x}, \boldsymbol{\theta})$ and desired $g(\boldsymbol{x}) = \boldsymbol{y}$

In this class, we will build loss functions from two error functions

Square error: The squared distance over a dataset of size n

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$$\sum_{i=1}^{n} \sum_{j=1}^{d_y} \left(f(\boldsymbol{x}_{[i]}, \boldsymbol{\theta})_j - g(\boldsymbol{x})_j \right)^2 = \sum_{i=1}^{n} \sum_{j=1}^{d_y} \left(f(\boldsymbol{x}_{[i]}, \boldsymbol{\theta})_j - y_{[i],j} \right)^2$$

Square error: The squared distance over a dataset of size n

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Cross entropy error: The probabilistic error over a dataset of size n

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Cross entropy error: The probabilistic error over a dataset of size n

$$-\sum_{i=1}^{n}\sum_{j=1}^{d_{y}}P\Big(g\Big(\bm{x}_{[i]}\Big)_{j}\mid \bm{x}_{[i]}\Big)\log f\Big(\bm{x}_{[i]},\bm{\theta}\Big)_{j}=-\sum_{i=1}^{n}\sum_{j=1}^{d_{y}}P\Big(y_{[i],j}\mid \bm{x}_{[i]}\Big)\log f\Big(\bm{x}_{[i]},\bm{\theta}\Big)_{j}$$

Deep Learning Review Square error:

$$\sum_{i=1}^n \sum_{j=1}^{d_y} \left(fig(oldsymbol{x}_{[i]}, oldsymbol{ heta}ig)_j - y_{[i],j}
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Cross entropy error:

$$-\sum_{i=1}^n \sum_{j=1}^{d_y} Pig(y_{[i],j} \mid oldsymbol{x}_{[i]}ig) \log fig(oldsymbol{x}_{[i]}, oldsymbol{ heta}ig)_j$$

Question: Which one will we use for Q learning?

Answer: Predict a scalar (expected return), so square error (regression)

We can use these errors in a loss function

$$\mathcal{L}(\boldsymbol{X},\boldsymbol{Y},\boldsymbol{\theta}) = \sum_{i=1}^{n} \sum_{j=1}^{d_y} \left(f \! \left(\boldsymbol{x}_{[i]},\boldsymbol{\theta} \right)_j - y_{[i],j} \right)^2$$

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$$\arg\min_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta}) = \arg\min_{\boldsymbol{\theta}} - \sum_{i=1}^{n} \sum_{j=1}^{a_y} P\big(y_{[i],j} \mid \boldsymbol{x}_{[i]}\big) \log f\big(\boldsymbol{x}_{[i]}, \boldsymbol{\theta}\big)_j$$

Question: Which search method do we use?

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Answer: Gradient-based methods (gradient descent, Adam, etc)

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Answer: Gradient-based methods (gradient descent, Adam, etc)



```
1:function Gradient Descent(\boldsymbol{X}, \boldsymbol{Y}, \mathcal{L}, t, \alpha)
```

- 3: $\theta \leftarrow \text{Glorot}()$
- 4: **for** $i \in 1...t$ **do**
- 5: Compute the gradient of the loss
- 6: $J \leftarrow \nabla_{\boldsymbol{\theta}} \mathcal{L}(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{\theta})$
- 7: b Update the parameters using the negative gradient
- 8: $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} \alpha \cdot \boldsymbol{J}$
- 9: return θ

```
1: function Gradient Descent(X, Y, \mathcal{L}, t, \alpha)
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Gradient descent computes $\nabla \mathcal{L}$ over all X

We can put it all together in jax and equinox

```
from jax import random
from equinox import nn
seed = random.key(0)
key, *net keys= random.split(seed, 4)
net = nn.Sequential([
  nn.Linear(d x, d h, key=net keys[0]),
  nn.Lambda(jax.nn.leaky relu),
  nn.Linear(d h, d h, key=net keys[1]),
  nn.Lambda(jax.nn.leaky relu),
  nn.Linear(d h, d y, key=net keys[2]),
```

We can extract parameters using eqx.partition

```
import equinox as eqx
# Get all arrays (parameters) in the network
theta, model = eqx.partition(net, eqx.is_array)
# Add one to every parameter
theta = jax.tree.map(theta, lambda x: x + 1)
# Put the new parameters back into network
net = eqx.combine(theta, model)
```

We can define loss functions

```
import equinox as eqx
def L square(net, x, y):
 # vmap applies network to batch of data
  prediction = eqx.filter vmap(net)(x)
  return ((prediction - y) ** 2).mean()
def L cross entropy(net, x, y):
 # Net outputs probabilities
 # And y is one-hot, e.g. [0, 0, 1, 0]
  prediction = eqx.filter vmap(model)(x)
  return -(y * jnp.log(prediction)).sum(-1).mean()
```

```
import optax
import equinox as eqx
opt = optimizer.adam(learning rate=3e-4)
# Adam needs to track momentum and variance
opt state = opt.init(eqx.filter(net, eqx.is array))
# Gradient of loss function is a function
grad L = eqx.filter grad(L square)
# Evaluate grad L at x, y, theta to find J
J = grad L(net, x, y)
# Compute parameter update using J (adam)
updates, opt state = opt.update(
    grads, opt state, params=eqx.filter(net, eqx.is array)
net = eqx.apply updates(net, updates) # Update params
```

```
def train one batch(net, dataset):
  x, y = batch
  grads = eqx.filter grad(L square)(net, x, y)
  updates, opt state = opt.update(
    grads, opt state, params=eqx.filter(net, eqx.is array)
  net = eqx.apply updates(net, updates) # Update params
  return net, opt state
for epoch in range(num epochs):
  for batch in dataset:
    # Can use eqx.filter jit(f) for speedup
    net, opt state = train one batch(net, batch, opt state)
```

Deep Learning Review Dirty secret of deep learning:

Dirty secret of deep learning: We do not understand deep learning

Biological inspiration, theoretical bounds and mathematical guarantees

Dirty secret of deep learning: We do not understand deep learning

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For complex neural networks, deep learning is a **science** not **math**

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No accepted theory for why deep neural networks are so effective

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In modern deep learning, we progress using trial and error

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Biological inspiration, theoretical bounds and mathematical guarantees

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In modern deep learning, we progress using trial and error

Today we experiment, and maybe tomorrow we discover the theory

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Consider an example problem

Example: Learn a policy to pick up trash and put it in the bin

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Question: What is S?

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$$S \times A$$

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Answer: Discretize the space

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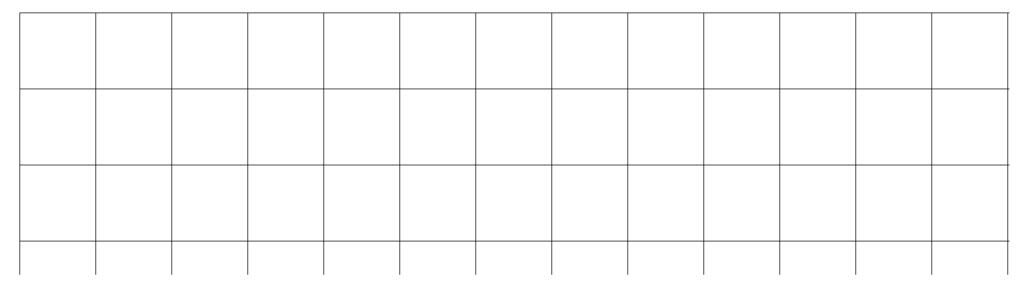
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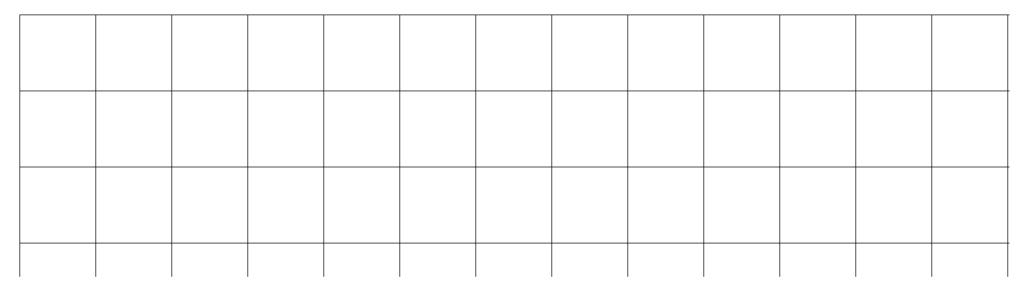
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Very large but not infinite



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This is the **minimum** number of samples to learn Q

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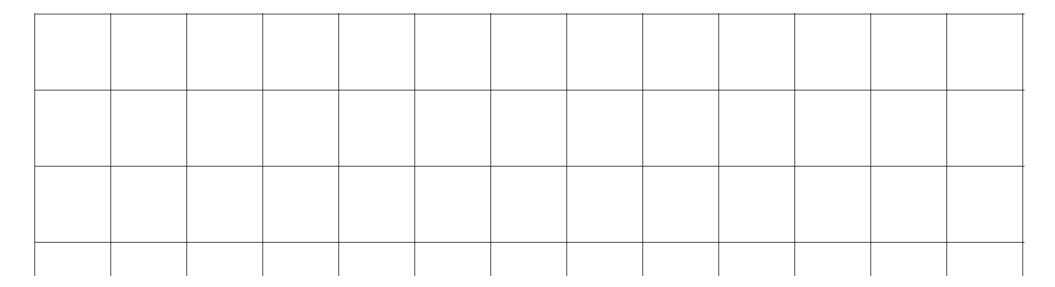
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But we will try!

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The Q function estimates the policy-conditioned discounted return

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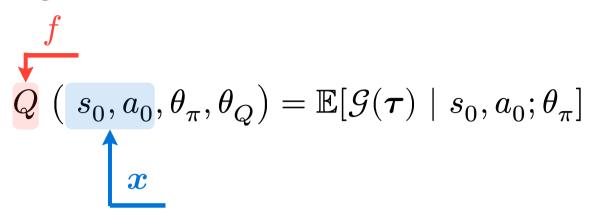
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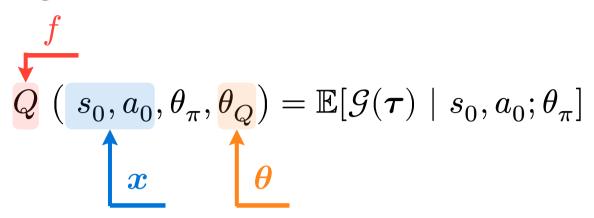
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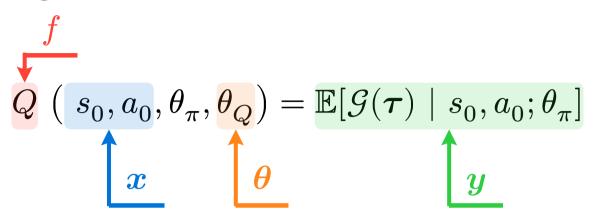
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Answer: Monte Carlo and Temporal Difference

Monte Carlo Objective:

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Temporal Difference Objective:

$$\mathop{\arg\min}_{\theta_Q} \left[\sum_{s_0 \in S} \sum_{a_0 \in A} \right.$$

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$$\underset{\boldsymbol{\theta}_{Q}}{\arg\min}\,\mathcal{L}\big(\boldsymbol{x},\boldsymbol{\theta}_{Q}\big) = \underset{\boldsymbol{\theta}_{Q}}{\arg\min}\left[\sum_{s_{i},a_{i},r_{i}\in\boldsymbol{x}}\left(Q\big(s_{i},a_{i},\theta_{\pi},\theta_{Q}\big) - \sum_{t=i}^{\infty}\gamma^{t}r_{t}\right)^{2}\right]$$

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Can train over batch or dataset containing many episodes

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$$\sum_{\substack{s_i, a_i, r_i, s_{i+1} \\ \subset \sigma}} \left(Q\big(s_i, a_i, \theta_\pi, \theta_Q\big) - \left(r_t + \neg d\gamma \argmax_{a \in A} Q\big(s_i, a, \theta_\pi, \theta_Q\big) \right) \right)^2$$

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Can optimize both loss functions using gradient descent

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RL optimization is more difficult than supervised learning

Can optimize both loss functions using gradient descent

RL optimization is more difficult than supervised learning

Supervised Learning:

- Static inputs
- Static labels
- Limited dataset
 - Human can clean
 - ▶ Bad to overfit

Reinforcement Learning:

- Inputs change as θ_{π} changes
 - Visit new/different states
- Labels change as θ_{π} changes
 - $ightharpoonup \mathbb{E}[\mathcal{G}(oldsymbol{ au}) \mid heta_{\pi}]$
- Infinite dataset
 - Can always collect from env
 - Bad θ_{π} means bad dataset
 - Overfitting no problem

Optimization is difficult in RL

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Most RL papers train for 10M-10B environment steps

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It takes a long time to train a deep Q function

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Let us see if we can improve training speed

```
for epoch in range(num epochs):
  terminated = False
 s = env.reset()
 episode = []
 # Step between 1 and infinity times to get one episode
 while not terminated:
    a = policy(s, theta Q)
    next s, r, d = env.step(action)
    episode.append([s, a, r, d, next s])
 # Compute gradient over episode
 J = grad(L)(theta Q, episode)
 theta Q = update(theta Q, grad)
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Question: Which part is slowest? Answer: Collecting episodes

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Collect episode, train, throw away episode, start again

What if we reuse episodes?

What if we reuse episodes? episodes = [] for epoch in range(num epochs): terminated = False s = env.reset() episode = [] while not terminated: a = policy(s, theta Q)next s, r, d = env.step(action) episode.append([s, a, r, d, next s]) episodes.append(episode) J = grad(L)(theta Q, episodes) # Train over ALL episodes theta Q = update(theta Q, grad)

When we reuse episodes, we call it **experience replay**

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Store episodes in a **replay buffer** (list)

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Train on the dataset

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Humans do experience replay when they dream!

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Question: Which is Q learning?

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Question: Which is Q learning?

Let us find out!

Start with the Monte Carlo return

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$$\underset{\theta_Q}{\arg\min} \left[\sum_{s_0 \in S} \sum_{a_0 \in A} \left(Q\big(s_0, a_0, \theta_\pi, \theta_Q\big) - \sum_{t=0}^\infty \gamma^t \mathbb{E} \big[\mathcal{R}(s_{t+1}) \mid s_0, a_0; \theta_\pi \big] \right)^2 \right]$$

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Do we know arg $\max_{a \in A} Q(s_1, a, \theta_{\pi}, \theta_Q)$? Yes! Just plug in s_1

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MC needs more training data, but TD has harder optimization

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$$Q\big(s_0,a_0,\theta_\pi,\theta_Q\big)=\infty$$

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Question: Can you see why?

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$$Q_{i+1} = 1 + Q_i$$

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$$Q\big(s_0,a_0,\theta_\pi,\theta_Q\big)=\infty$$

$$\left(Q\big(s_0, a_0, \theta_\pi, \theta_Q\big) - \left(\mathbb{E}[\mathcal{R}(s_1) \mid s_0, a_0] + \neg d\gamma \max_{a \in A} Q\big(s_1, a, \theta_\pi, \theta_Q\big)\right)\right)^2$$

Question: Can you see why? Hint: What if $s_0 \approx s_1$?

$$Q(s_0, a_0, \theta_{\pi}, \theta_Q) = r_0 + \max_{a \in A} Q(s_0, a_0, \theta_{\pi}, \theta_Q)$$

Question: If $r_0 = 1$, what happens?

$$Q_{i+1} = 1 + Q_i \qquad \lim_{i \to \infty}?$$

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Usually, the target parameters are older parameters

```
theta Q = ... # Initialize parameters
theta T = theta Q.copy()
for epoch in range(num epochs):
 grad = grad(L)(theta Q, theta T, X)
 theta Q = optimizer.update(theta Q, grad)
  if epoch % 200 == 0:
   # Update target parameters
    theta T = theta Q.copy()
```

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¹Human-level control through deep reinforcement learning. *Nature*. 2014.

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You have all the tools you need to implement DQN, except for one

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For each action, we must execute Q network |A| times. Not efficient!

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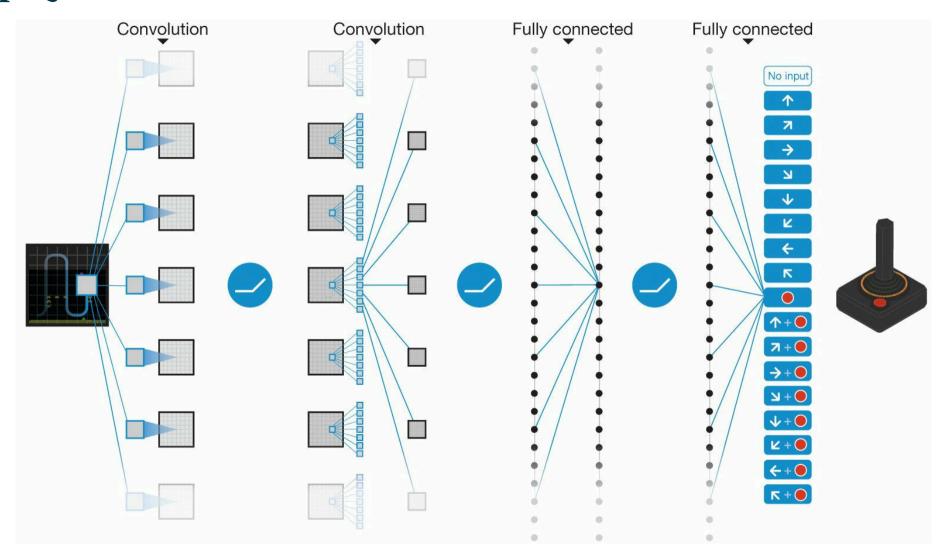
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This is |A| times faster!



```
Q = nn.Sequential([...])
theta T = partition(Q, is array)[0]
replay buffer = deque(maxsize=50 000)
for epoch in range(num epochs):
  while not terminated:
    a = random action if epoch < k else epsilon greedy(Q)</pre>
    s, r, d, next s = env.step(a)
    replay buffer.insert((s, a, r, d, next s))
    X = random.sample(replay buffer, batch size)
    theta Q, model = eqx.partition(Q, is array)
    theta Q = td update(theta Q, theta T, Q, X)
    theta T = copy(theta Q) if epoch % j == 0 else theta T
    Q = eqx.combine(theta Q, model)
```

Finally, let us look at some successes of deep Q learning

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Super Smash Bros: https://www.youtube.com/watch?v=7rDfIcdszxQ

Pokemon https://youtu.be/DcYLT37ImBY?si=AeR2WkQg4X-tWa5v