CSCI 1470

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Monday
4/14/25

Deep Learning

Day 31: DQNs and Policy Gradient Methods

Lunar Lander, Gymnasium

Terminology Review

MDP <S, A, R, P, γ>
S: States
A: Actions
R: rewards
P: Transition Function
γ: Discount Factor

Returns: $G_t = \sum_{i=0}^{T-t} \gamma^i r^{i+t}$
Value function: $V(s_t) = \mathbb{E}[G_t]$
Q-Function: $Q(s_t, a_t) = \mathbb{E}_{s' \sim T(s_t, a_t)}[V(s')]$

Q-Learning Review

$$Q(s,a) = r + \gamma \max_{a'} Q(s',a')$$

$$0 = [r + \gamma \max_{a'} Q(s',a')] - Q(s,a)$$

Want this relationship to hold

Q-learning:

Maintain estimates of Q(s, a) for all (s, a) pairs

Collect experiences, update Q estimates with:

$$Q(s,a) \leftarrow Q(s,a) + \alpha[r + \gamma \max_{a'} Q(s',a') - Q(s,a)]$$

Current estimate

Learning rate

Error in estimate (Temporal Difference Error)

Deep Q-Learning

- Approximate Q-values with a neural network

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Deep Q-Learning

- Approximate Q-values with a neural network
- Always needed a loss function with neural networks before…
- Can we come up with a loss function here?
- We want this equality to hold: $0 = [r + \gamma \max_{a'} Q(s', a')] - Q(s, a)$
- If we can force $[r + \gamma \max_{a'} Q(s', a')] - Q(s, a)$ to be close to 0, we will have good approximations of Q-values

$$L = \left(\left[r + \gamma \max_{a'} Q(s', a') \right] - Q(s, a) \right)^2$$

Q-Learning

How to update tabular Q-learning to be deep Q-learning

$$L = \left(\left[r + \gamma \max_{a'} Q(s', a')\right] - Q(s, a)\right)^2$$

Algorithm 2 Q-Learning

Initialize $Q(s,a) = 0$ for all $s \in \mathcal{S}$, $a \in \mathcal{A}$
Initialize learning rate $\alpha \in (0,1]$ and discount factor $\gamma \in [0,1)$
Initialize exploration parameter $\epsilon \in (0,1)$
for each episode **do**
  Initialize state s
  repeat
    With probability ϵ: choose a random action $a \in \mathcal{A}$
    Otherwise: choose $a = \arg\max_{a'} Q(s,a')$
    Take action a, observe reward r and next state s'
    $Q(s,a) \leftarrow Q(s,a) + \alpha[r + \gamma \max_{a'} Q(s',a') - Q(s,a)]$
    (Or $Q(s,a) \leftarrow (1-\alpha)Q(s,a) + \alpha(r + \gamma \max_{a'} Q(s',a'))$)
    $s \leftarrow s'$
  until s is terminal
end for
Return Q

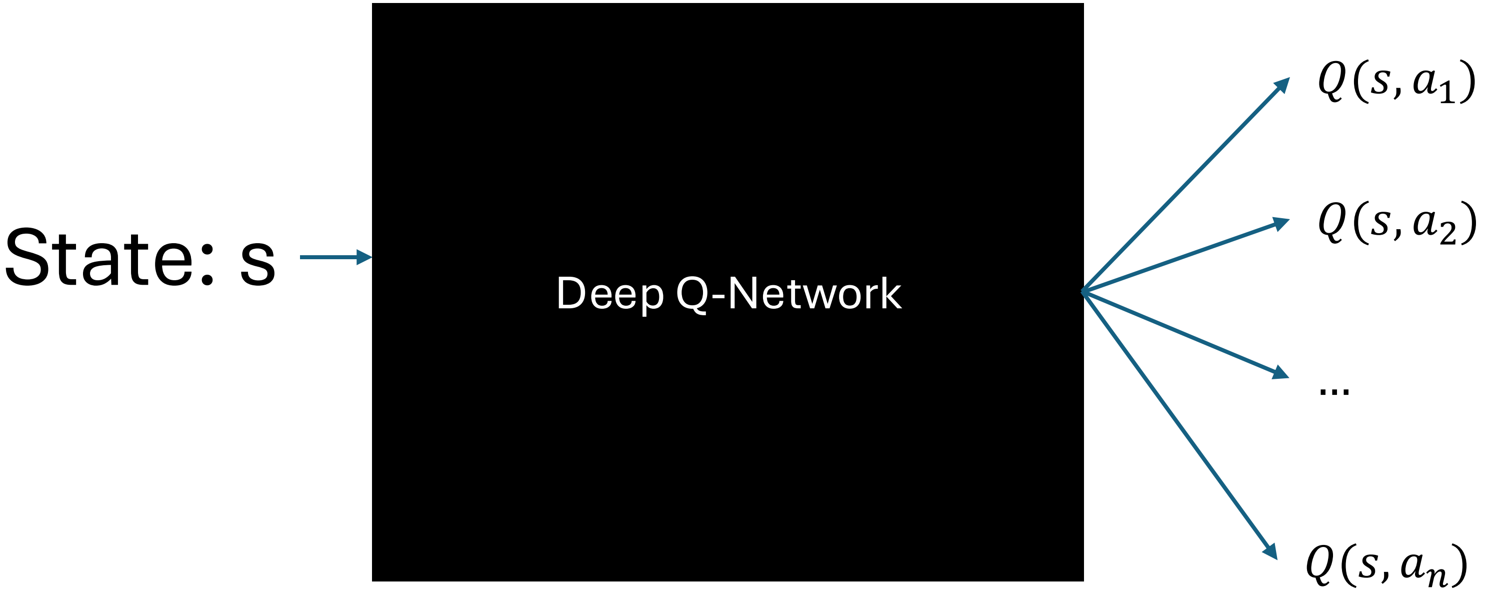
Can't just update outputs of a NN directly...
Instead, compute loss and run a step of SGD

Deep-Q Network

Deep Q-Networks (DQNs):

1. Take in a state
2. Return Q-values for each action

What activation function should the final layer use?



Deep-Q Learning

Initialize DQN to approximate Q

Maintain estimates of Q(s, a) for all (s, a) pairs

Collect experiences, update Q estimates with:

Compute $L_\theta = \left[r + \gamma \max_{a'} Q_\theta(s', a') - Q_\theta(s, a)\right]^2$

update θ with SGD on Loss function

(non-)Stationarity in RL

$$L_\theta = \Big[\overbrace{r + \gamma \max_{a'} Q_\theta(s', a')}^{\text{Target}} - \overbrace{Q_\theta(s, a)}^{\text{Estimate}}\Big]^2$$

We'd like our current estimate $Q_\theta(s, a)$ to be like our estimate for the next timestep $r + \gamma \max_{a'} Q_\theta(s', a')$.

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1. $\max_{a'} Q_\theta(s', a')$ is not differentiable

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1. $\max_{a'} Q_\theta(s', a')$ is not differentiable
2. $\nabla Q_\theta(s', a')$ would tell us how to update the target to match our current estimate (that's backwards)

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Using only the gradient of the estimate helps with *stationarity*

Q-Values to Policy

What do we do after we learn Q? We need to turn them into a policy.

For a given state, take the action associated with the best Q-value.

$$\pi(s) = argmax_a \, Q(s, a)$$

Policies

Why learn Q-values first and turn them into a policy? Why not just learn a policy?

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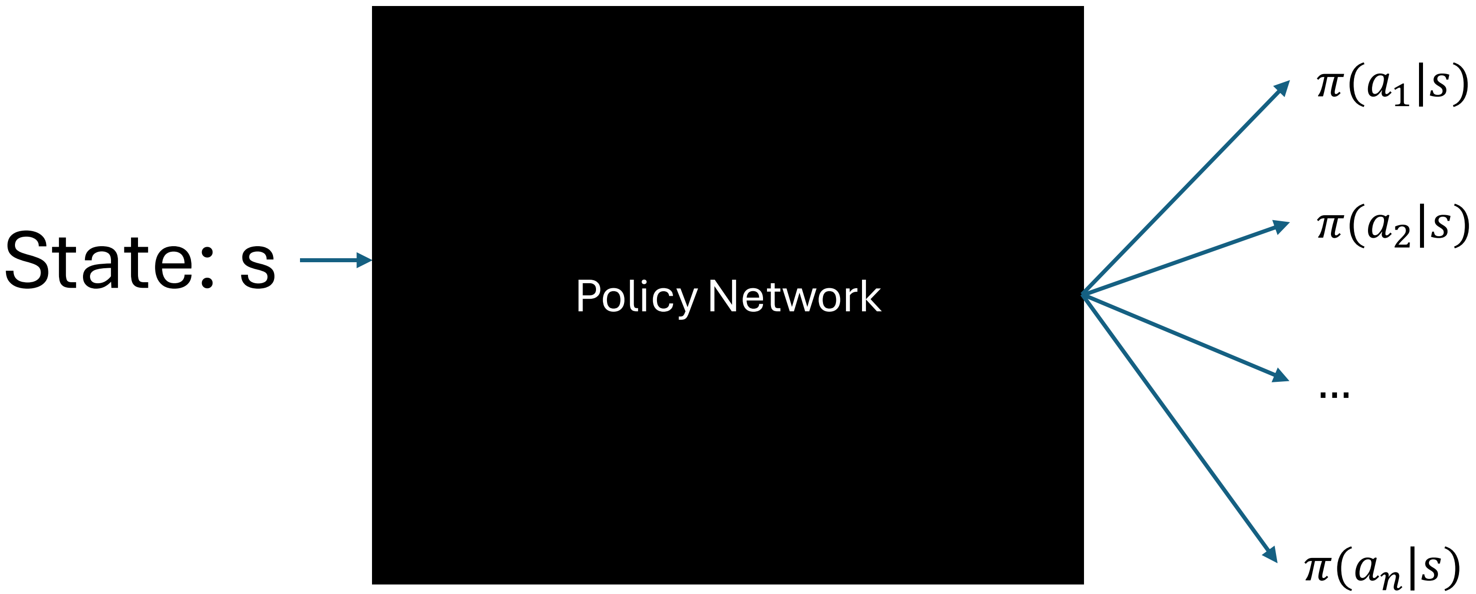

What should the activation function be for the final layer?

How do we train a policy network?

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$$\pi = \text{argmax}_{\pi} \left(V(s_0)\right)$$

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What's our objective?

Find a policy π such that the value of the start state is maximized:

$$\pi = \text{argmax}_{\pi} \left(V(s_0) \right)$$

How can we maximize $V(s_0)$?

Let $J(\theta)$ be our objective function:

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Probability of a trajectory occurring

Returns of a specific trajectory

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$$\Pr(\tau|\theta) = \Pi_{t=0}^{T} P(s_{t+1}|s_t, a_t)\pi_\theta(a_t|s_t)$$

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State transition Probability

Probability of taking an action for a given state

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$$J(\theta) = V(s_0)$$

$$J(\theta) = \mathbb{E}[G_0]$$

$$J(\theta) = \sum_{\tau} \Pr(\tau|\theta)\, G(\tau)$$

Sum over all possible trajectories

Probability of a trajectory occurring

Returns of a specific trajectory

$$\Pr(\tau|\theta) = \Pi_{t=0}^{T} P(s_{t+1}|s_t, a_t)\pi_\theta(a_t|s_t)$$

State transition Probability

Probability of taking an action for a given state

Log-Derivative Trick

We can rewrite the derivative of a function using the derivative of the natural log function:

$$\nabla \ln f(x) = \frac{\nabla \mathrm{f}(x)}{f(x)}$$

$$\nabla f(x) = f(x) \nabla \ln \mathrm{f(x)}$$

When applied to $\Pr(\tau|\theta)$:

$$\nabla_\theta \Pr(\tau|\theta) = \Pr(\tau|\theta)\, \nabla_\theta \ln \Pr(\tau|\theta)$$

Log Probability Trick

This gradient term is what we want to calculate

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$$\nabla_\theta \ln \Pr(\tau|\theta) = \nabla_\theta \sum_{t=0}^{T} \ln P(s_{t+1}|s_t, a_t)\pi_\theta(a_t|s_t)$$

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$$\nabla_\theta \ln \Pr(\tau|\theta) = \nabla_\theta \sum_{t=0}^{T} \ln P(s_{t+1}|s_t, a_t) + \ln \pi_\theta(a_t|s_t)$$

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This gradient term is what we want to calculate

Log of product -> sum of logs

$$\nabla_\theta \ln \Pr(\tau|\theta) = \nabla_\theta \sum_{t=0}^{T} \ln P(s_{t+1}|s_t, a_t)\pi_\theta(a_t|s_t)$$

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Derivative of sum -> sum of derivative

$$\nabla_\theta \ln \Pr(\tau|\theta) = \sum_{t=0}^{T} \nabla_\theta \ln P(s_{t+1}|s_t, a_t) + \nabla_\theta \ln \pi_\theta(a_t|s_t)$$

Gradient of a trajectory

$$\nabla_\theta \ln \Pr(\tau|\theta) = \sum_{t=0}^{T} \nabla_\theta \ln P(s_{t+1}|s_t, a_t) + \nabla_\theta \ln \pi_\theta(a_t|s_t)$$

State transition function
does not depend on θ!

$$\nabla_\theta \ln \Pr(\tau|\theta) = \sum_{t=0}^{T} \nabla_\theta \ln \pi_\theta(a_t|s_t)$$

Policy Gradient Derivation

Putting it all back together:

$$J(\theta) = \sum_{\tau} \Pr(\tau|\theta)\, G(\tau)$$

Our Objective

Policy Gradient Derivation

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Log-Derivative Trick

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$$\nabla_\theta J(\theta) = \sum_{\tau} \left[\Pr(\tau|\theta) G(\tau) \sum_{t=0}^{T} \nabla_\theta \ln \pi_\theta(a_t|s_t)\,\right]$$ Gradient of a Trajectory

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Gradient of a Trajectory

$$\nabla_\theta J(\theta) = \mathbb{E}[G_0 \sum_{t=0}^{T} \nabla_\theta \ln \pi_\theta(a_t|s_t)]$$

Convert back to Expectation

Policy Gradient

Bigger step if better returns

Direction to move in to increase probability of trajectory

$$\nabla_\theta J(\theta) = \mathbb{E}[G_0 \sum_{t=0}^{T} \nabla_\theta \ln \pi_\theta(a_t|s_t)]$$

We will never be able to sum over all possible trajectories...

How do we get around this?

Policy Gradient

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Sampling!

1. Collect n trajectories following policy π_θ
2. $\Pr(\tau|\theta) = 1/n$ for each trajectory
3. Calculate the total return for each trajectory $G(\tau)$

Reward-To-Go Policy Gradient

You can also do the policy gradient derivation such that the gradient does not depend on G_0, but on G_t

$$\nabla_\theta J(\theta) = \mathbb{E}[\sum_{t=0}^{T} G_t \, \nabla_\theta \ln \pi_\theta(a_t|s_t)]$$

Or

$$\nabla_\theta J(\theta) = \mathbb{E}[\sum_{t=0}^{T} Q(s_t, a_t) \, \nabla_\theta \ln \pi_\theta(a_t|s_t)]$$

REINFORCE (Policy Gradient Learning)

REINFORCE, A Monte-Carlo Policy-Gradient Method (episodic)

Input: a differentiable policy parameterization $\pi(a|s, \boldsymbol{\theta})$
Initialize policy parameter $\boldsymbol{\theta} \in \mathbb{R}^{d'}$
Repeat forever:
    Generate an episode $S_0, A_0, R_1, \ldots, S_{T-1}, A_{T-1}, R_T$, following $\pi(\cdot|\cdot, \boldsymbol{\theta})$
    For each step of the episode $t = 0, \ldots, T-1$:
        $G \leftarrow$ return from step t
        $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha\gamma^t G \nabla_{\boldsymbol{\theta}} \ln \pi(A_t|S_t, \boldsymbol{\theta})$

Source: Sutton and Barto, Reinforcement Learning: An Introduction

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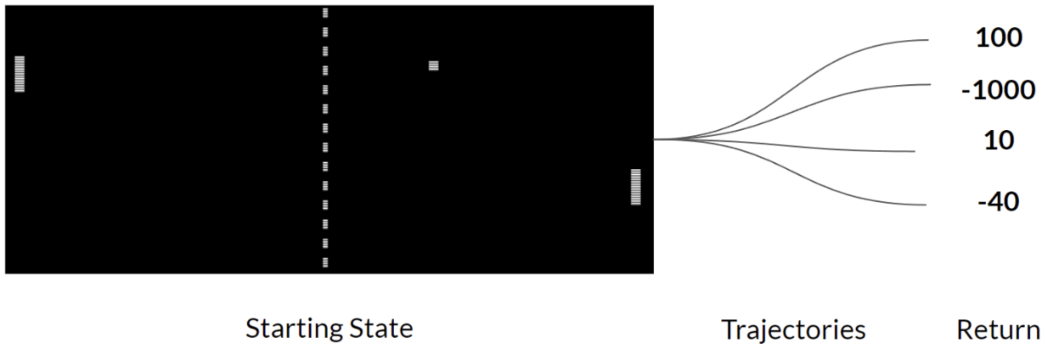
Why is the update adding the gradient instead of subtracting?

When π is based on a softmax, $\nabla_\theta \ln \pi_\theta(a|s)$ is actually easy to compute by hand using log rules and the fact that $\ln e^x = x$

Source: Sutton and Barto, Reinforcement Learning: An Introduction

Variance of REINFORCE



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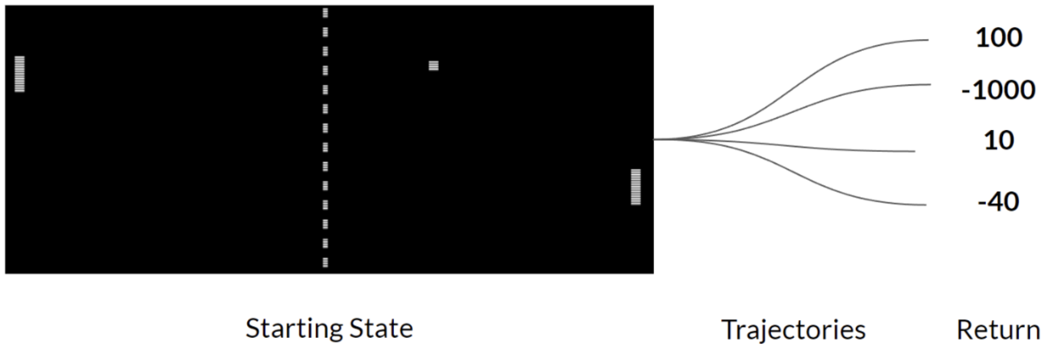

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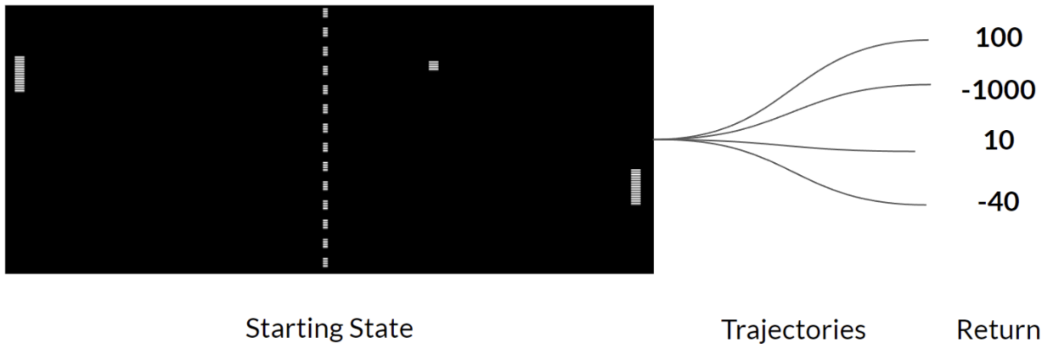

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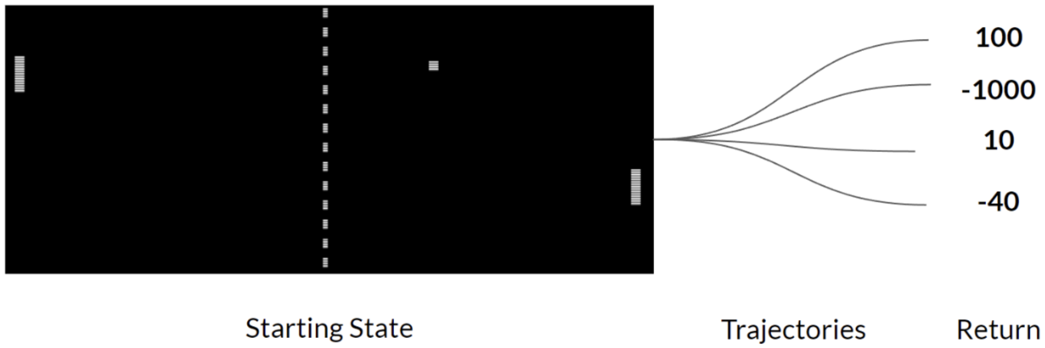

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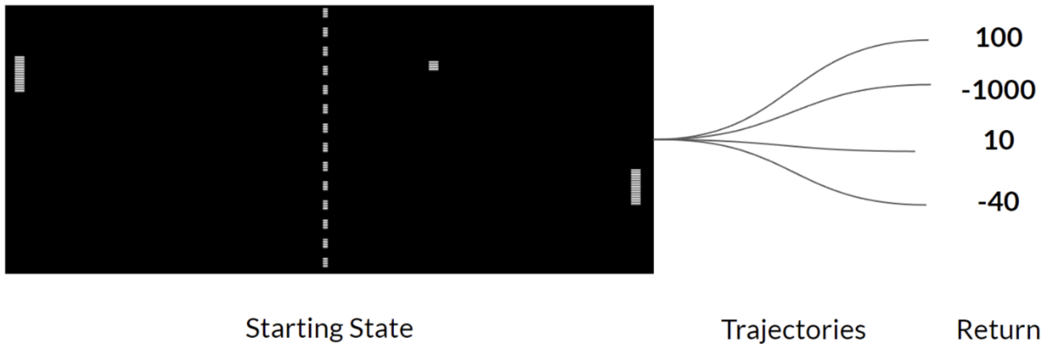

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Or...

Baseline Functions

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Subtracting a baseline function from G_t does not change the expected gradient

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Subtracting a *baseline* function from G_t does not change the expected gradient

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The value function V(s) is the ideal baseline function

REINFORCE with Baseline

REINFORCE with Baseline (episodic), for estimating $\pi_{\boldsymbol{\theta}} \approx \pi_*$

Input: a differentiable policy parameterization $\pi(a|s, \boldsymbol{\theta})$
Input: a differentiable state-value function parameterization $\hat{v}(s,\mathbf{w})$
Algorithm parameters: step sizes $\alpha^{\boldsymbol{\theta}} > 0$, $\alpha^{\mathbf{w}} > 0$
Initialize policy parameter $\boldsymbol{\theta} \in \mathbb{R}^{d'}$ and state-value weights $\mathbf{w} \in \mathbb{R}^d$ (e.g., to $\mathbf{0}$)

Loop forever (for each episode):
 Generate an episode $S_0, A_0, R_1, \ldots, S_{T-1}, A_{T-1}, R_T$, following $\pi(\cdot|\cdot, \boldsymbol{\theta})$
 Loop for each step of the episode $t = 0, 1, \ldots, T-1$:
  $G \leftarrow \sum_{k=t+1}^{T} \gamma^{k-t-1} R_k$ (G_t)
  $\delta \leftarrow G - \hat{v}(S_t,\mathbf{w})$
  $\mathbf{w} \leftarrow \mathbf{w} + \alpha^{\mathbf{w}} \delta \nabla \hat{v}(S_t,\mathbf{w})$
  $\boldsymbol{\theta} \leftarrow \boldsymbol{\theta} + \alpha^{\boldsymbol{\theta}} \gamma^t \delta \nabla \ln \pi(A_t|S_t, \boldsymbol{\theta})$

Pseudocode uses SGD, but you can just as easily use any other optimizer (e.g., Adam)

Source: Sutton and Barto Chapter 13

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    $\mathbf{w} \leftarrow \mathbf{w} + \alpha^{\mathbf{w}} \delta \nabla \hat{v}(S_t,\mathbf{w})$ ← Gradient of $L = \frac{1}{2}\delta^2$
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Extra Material

Sutton and Barto: Policy Gradient methods chapter 13
http://www.incompleteideas.net/book/RLbook2020.pdf

Spinning up policy gradient:
https://spinningup.openai.com/en/latest/spinningup/rl_intro3.html

Derivation of REINFORCE w/ Baseline Function

First, let's show that the gradient estimate is unbiased. We see that with the baseline, we can distribute and rearrange and get:

$$\nabla_\theta \mathbb{E}_{\tau\sim\pi_\theta}[R(\tau)] = \mathbb{E}_{\tau\sim\pi_\theta}\left[\sum_{t=0}^{T-1} \nabla_\theta \log \pi_\theta(a_t|s_t)\left(\sum_{t'=t}^{T-1} r_{t'}\right) - \sum_{t=0}^{T-1} \nabla_\theta \log \pi_\theta(a_t|s_t) b(s_t)\right]$$

Due to linearity of expectation, all we need to show is that for any single time t, the gradient of $\log \pi_\theta(a_t|s_t)$ multiplied with $b(s_t)$ is zero. This is true because

$$\begin{aligned}
\mathbb{E}_{\tau\sim\pi_\theta}\Big[\nabla_\theta \log \pi_\theta(a_t|s_t) b(s_t)\Big] &= \mathbb{E}_{s_{0:t},a_{0:t-1}}\Big[\mathbb{E}_{s_{t+1:T},a_{t:T-1}}[\nabla_\theta \log \pi_\theta(a_t|s_t) b(s_t)]\Big] \\
&= \mathbb{E}_{s_{0:t},a_{0:t-1}}\Big[b(s_t)\cdot \underbrace{\mathbb{E}_{s_{t+1:T},a_{t:T-1}}[\nabla_\theta \log \pi_\theta(a_t|s_t)]}_{E}\Big] \\
&= \mathbb{E}_{s_{0:t},a_{0:t-1}}\Big[b(s_t)\cdot \mathbb{E}_{a_t}[\nabla_\theta \log \pi_\theta(a_t|s_t)]\Big] \\
&= \mathbb{E}_{s_{0:t},a_{0:t-1}}\Big[b(s_t)\cdot 0\Big] = 0
\end{aligned}$$

Derivation: https://danieltakeshi.github.io/2017/03/28/going-deeper-into-reinforcement-learning-fundamentals-of-policy-gradients/