# 535514: Reinforcement Learning Lecture 7 — Stochastic PG Algorithms

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# Quick Review: Policy Gradient

- What is  $V^{\pi_{\theta}}(\mu)$ ?
- What is  $d_{\mu}^{\pi_{\theta}}$ ?
- Expressions of Policy Gradient (aka Policy Gradient Theorem):

(P1) Total reward: 
$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{\tau \sim P^{\pi_{\theta}}_{\mu}} \left[ G(\tau) \sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \right]$$

(P2) REINFORCE: 
$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[ \sum_{t=0}^{\infty} \gamma^{t} Q^{\pi_{\theta}}(s_{t}, a_{t}) \nabla_{\theta} \log \pi_{\theta}(a_{t} | s_{t}) \right]$$

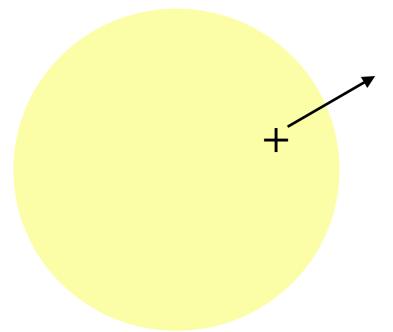
(P3) Q-value and discounted state visitation:

$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi_{\theta}}_{\mu}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot \mid s)} \left[ Q^{\pi_{\theta}}(s, a) \nabla_{\theta} \log \pi_{\theta}(a \mid s) \right]$$

## (P3) Q-Value and Discounted State Visitation

Question: How to interpret this expression?

Sample space of (s, a)



- Q(s, a) > 0:
- Q(s, a) < 0:

Question: Why is this expression useful?

## (P3) Q-Value and Discounted State Visitation (Cont.)

Proof idea: Use the following lemma and (P2)

Lemma (From Trajectories to Visitation):

For any function  $f(s, a) : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ , we have

$$\mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[ \sum_{t=0}^{\infty} \gamma^{t} f(s_{t}, a_{t}) \right] = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d_{\mu}^{\pi_{\theta}}, a \sim \pi_{\theta}(\cdot | s)} [f(s, a)]$$

Proof: Expand RHS and recollect terms to get LHS (HW1)

# Computing $\nabla_{\theta} \log \pi_{\theta}(a \mid s)$ : Linear Softmax Policy

- (P1)-(P3) all involve  $\nabla_{\theta} \log \pi_{\theta}(a \mid s)$
- $\nabla_{\theta} \log \pi_{\theta}(a \mid s)$  is often called the "score function"
- Example: Linear softmax policy
  - Feature vector for each state-action pair  $\phi(s, a)$
  - Probability of action is proportional to exponentiated weight

$$\pi_{\theta}(a \mid s) = \frac{e^{\phi(s,a)^T \theta}}{\sum_{a' \in \mathcal{A}} e^{\phi(s,a')^T \theta}}$$
 on is

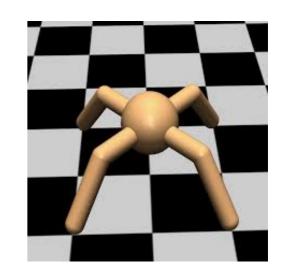
The score function is

$$\nabla_{\theta} \log \pi_{\theta}(a \mid s) = \phi(s, a) - \mathbb{E}_{a \sim \pi_{\theta}(\cdot \mid s)} [\phi(s, a)]$$

# Computing $\nabla_{\theta} \log \pi_{\theta}(a \mid s)$ : Gaussian Policy

- Example: Gaussian policies for continuous actions
  - $a \sim \mathcal{N}(\mu_{\theta}(s), \sigma^2)$ 
    - Mean is a linear combination of state features  $\mu_{\theta}(s) = \phi(s)^T \theta$
    - Variance may be fixed  $\sigma^2$  (or can also be parametrized)
  - The score function is

$$\nabla_{\theta} \log \pi_{\theta}(a \mid s) = \frac{(a - \mu_{\theta}(s))\phi(s)}{\sigma^2}$$



Question: How about an NN-based Gaussian policy?

(P1) Total reward: 
$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{\tau \sim P^{\pi_{\theta}}_{\mu}} \left[ G(\tau) \sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \right]$$

(P2) REINFORCE: 
$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[ \sum_{t=0}^{\infty} \gamma^{t} Q^{\pi_{\theta}}(s_{t}, a_{t}) \nabla_{\theta} \log \pi_{\theta}(a_{t} | s_{t}) \right]$$

(P3) Q-value and discounted state visitation:

$$\nabla_{\theta} V^{\pi_{\theta}}(\mu) = \frac{1}{1 - \gamma} \mathbb{E}_{s \sim d^{\pi_{\theta}}_{\mu}} \mathbb{E}_{a \sim \pi_{\theta}(\cdot \mid s)} \left[ Q^{\pi_{\theta}}(s, a) \nabla_{\theta} \log \pi_{\theta}(a \mid s) \right]$$

### Next Question: Is it easy to compute PG?

(P1)-(P3) all involve a highly complex expectation!

(This issue is quite common in many ML problems)

# Issues With (Exact) PG

(Exact) PG Update (Use (P1) as an Example):

$$\begin{aligned} \theta_{k+1} &= \theta_k + \eta_k \cdot \nabla_{\theta} V^{\pi_{\theta}}(\mu)|_{\theta = \theta_k} \\ &= \theta_k + \eta_k \cdot \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \Big[ G(\tau) \sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \Big] \end{aligned}$$

- Question: Any issues?
- 1. Distribution / statistics of  $\tau$  is unknown (i.e., model-free setting)
- 2. Expectation usually involves <u>multi-dimensional integral</u>, which is computationally expensive

# "Stochastic" Policy Gradient

Idea: Use sampling to estimate expectation

$$\theta_{k+1} = \theta_k + \eta_k \cdot \mathbb{E}_{\tau \sim P_\mu^{\pi_\theta}} \Big[ G(\tau) \sum_{t=0}^\infty \nabla_\theta \log \pi_\theta(a_t | s_t) \Big] \qquad \text{(Exact PG)}$$
 
$$\theta_{k+1} = \theta_k + \eta_k \cdot G(\tau') \sum_{t=0}^\infty \nabla_\theta \log \pi_\theta(a_t' | s_t') \qquad \text{(Stochastic PG)}$$
 
$$g(\theta_k, \tau') \qquad \text{where } \tau' \equiv (s_0', a_0', r_1', s_1', a_1', r_2' \cdots)$$

- $g(\theta_k, \tau')$  is an **unbiased** estimate of exact PG  $\nabla_{\theta} V^{\pi_{\theta}}(\mu)|_{\theta=\theta_k}$
- An unbiased estimate can be constructed from 1 or multiple trajectories

## Unbiasedness

Definition (Unbiasedness):

Let  $\phi \in \mathbb{R}^d$  be some (unknown) real vector to be estimated, and let X be a random estimator of  $\phi$  with distribution D.

We say that X is an *unbiased* estimator of  $\phi$  if

$$\mathbb{E}_{X \sim D}[X] = \phi$$

- Example: Let  $X_1, \dots, X_n$  be i.i.d. random variables from  $\mathcal{N}(\mu, 1)$ 
  - Define  $\bar{X} := (X_1 + \dots + X_n)/n$ . Then, is  $\bar{X}$  an unbiased estimator of  $\mu$ ?

# More Generally: Stochastic Gradient Descent (SGD) for Stochastic Optimization

### **Stochastic Optimization:**

$$\theta^* = \arg\min_{\theta \in \Theta} \ F(\theta), \text{ where } F(\theta) := \mathbb{E}_{\xi}[f(\theta; \xi)]$$

where  $\xi$  is the randomness in our problem

#### **Stochastic Gradient Descent:**

$$\theta_{k+1} = \theta_k - \eta_k \cdot \mathbb{E}[\nabla_{\theta} f(\theta_k; \xi)] \qquad \theta_{k+1} = \theta_k - \eta_k \cdot g(\theta_k; \xi_k)$$
 (SGD)

- $g(\theta_k; \xi_k)$  is an estimate of the true gradient (constructed from 1 or multiple samples)
- Advantage: SGD has a low computational cost in each iteration
- H. Robbins and S. Monro, "A Stochastic Approximation, Method," The Annals of Mathematical Statistics, 1951

# Almost All ML Problems are Stochastic Optimization Problems!

#### **Policy Optimization in RL:**

$$\max_{\theta} V^{\pi_{\theta}}(\mu)$$

where 
$$V^{\pi_{\theta}}(\mu) = \mathbb{E}_{ au \sim P^{\pi_{\theta}}_{\mu}}[G( au)]$$

#### Regression / Classification:

$$\min_{\theta} \mathbb{E}_{(x,y)\sim D} [\ell(f_{\theta}(x), y)]$$

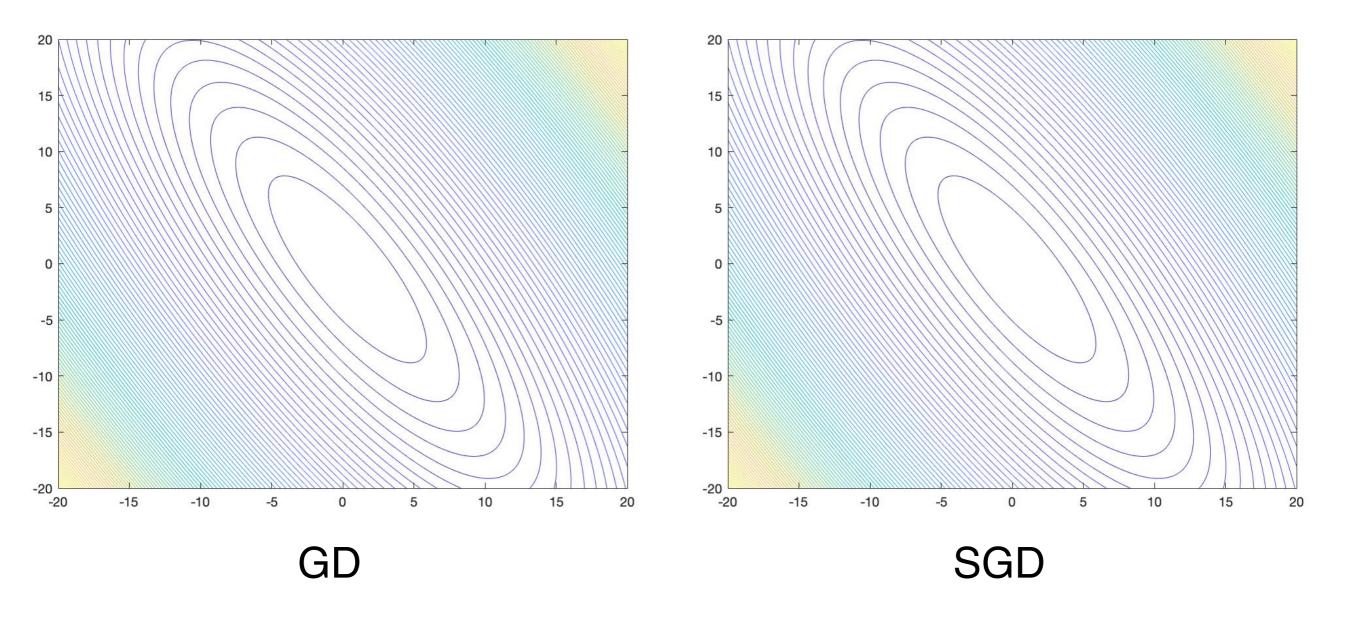
where  $\ell$  is some loss function

#### Fine-Tuning of Language Models:

$$\max_{\theta} \mathbb{E}_{x \sim D} \left[ \mathbb{E}_{y \sim \pi_{\theta}(\cdot \mid x)} \left[ r_{\phi}(x, y) \right] - \beta D_{KL} \left( \pi_{\theta}(\cdot \mid x) || \pi_{ref}(\cdot \mid x) \right) \right]$$

## Visualization: SGD vs GD

SGD usually exhibits more "random" behavior than GD



## SGD: A Special Case of "Stochastic Approximation"

#### A STOCHASTIC APPROXIMATION METHOD<sup>1</sup>

By Herbert Robbins and Sutton Monro
University of North Carolina

- 1. Summary. Let M(x) denote the expected value at level x of the response to a certain experiment. M(x) is assumed to be a monotone function of x but is unknown to the experimenter, and it is desired to find the solution  $x = \theta$  of the equation  $M(x) = \alpha$ , where  $\alpha$  is a given constant. We give a method for making successive experiments at levels  $x_1, x_2, \cdots$  in such a way that  $x_n$  will tend to  $\theta$  in probability.
- 2. Introduction. Let M(x) be a given function and  $\alpha$  a given constant such that the equation

$$M(x) = \alpha$$

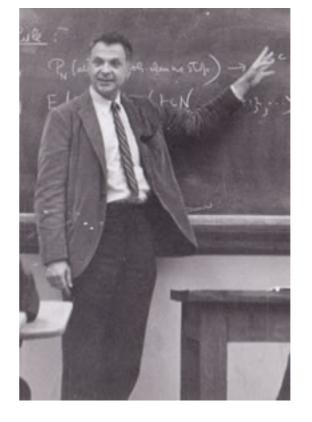
has a unique root  $x = \theta$ . There are many methods for determining the value of  $\theta$  by successive approximation. With any such method we begin by choosing one or more values  $x_1, \dots, x_r$  more or less arbitrarily, and then successively obtain new values  $x_n$  as certain functions of the previously obtained  $x_1, \dots, x_{n-1}$ , the values  $M(x_1), \dots, M(x_{n-1})$ , and possibly those of the derivatives  $M'(x_1), \dots, M'(x_{n-1})$ , etc. If

$$\lim_{n \to \infty} x_n = \theta,$$

irrespective of the arbitrary initial values  $x_1, \dots, x_r$ , then the method is effective for the particular function M(x) and value  $\alpha$ . The speed of the convergence in (2) and the ease with which the  $x_n$  can be computed determine the practical utility of the method.

We consider a stochastic generalization of the above problem in which the nature of the function M(x) is unknown to the experimenter. Instead, we suppose that to each value x corresponds a random variable Y = Y(x) with distribution function  $Pr[Y(x) \le y] = H(y \mid x)$ , such that

(3) 
$$M(x) = \int_{-\infty}^{\infty} y \, dH(y \mid x)$$





**Herbert Robbins** 

**Sutton Monro** 

"Stochastic approximation" is the core of many RL methods, e.g., Q-learning and TD learning

A seminal paper on stochastic approximation in 1951 (Cited for more than 12000 times)

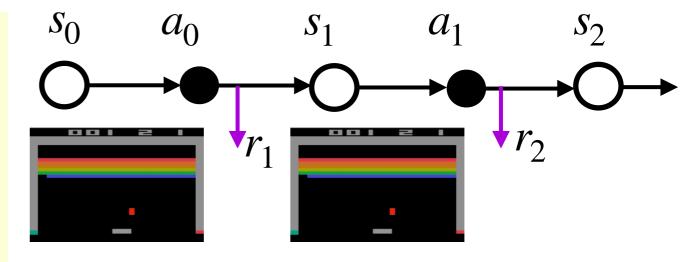
## Let's combine SGD and PG!

# Combining SGD and Policy Gradient

In each iteration, we draw a trajectory  $\tau=(s_0,a_0,r_1,s_1,a_1\cdots)$  under  $\pi_\theta$  and  $\mu$ , and then construct:

$$G_t(\tau) := \sum_{m=t}^{\infty} \gamma^m r_{m+1}$$

$$\hat{\nabla}_{\tau} := \sum_{t=0}^{\infty} \gamma^t G_t(\tau) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$



• Question: Is  $\hat{\nabla}_{\tau}$  an **unbiased** estimate of  $\nabla_{\theta}V^{\pi_{\theta}}(\mu)$ ?

- $(P2): \nabla_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{\tau \sim P_{\mu}^{\pi_{\theta}}} \left[ \sum_{t=0}^{\infty} \gamma^{t} Q^{\pi_{\theta}}(s_{t}, a_{t}) \nabla_{\theta} \log \pi_{\theta}(a_{t} | s_{t}) \right]$
- Show that  $\hat{\nabla}_{\tau}$  is an **unbiased** estimate of  $\nabla_{\theta}V^{\pi_{\theta}}(\mu)$

$$G_t(\tau) := \sum_{m=t}^{\infty} \gamma^m r_{m+1}$$

$$\hat{\nabla}_{\tau} := \sum_{t=0}^{\infty} \gamma^t G_t(\tau) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t)$$

# The REINFORCE Algorithm (Formally)

REINFORCE algorithm (aka Monte Carlo policy gradient)

Step 1: Initialize  $\theta_0$  and step size  $\eta$ 

Step 2: Sample a trajectory  $au \sim P_{\mu}^{\pi_{\theta}}$  and make the update as

$$\theta_{k+1} = \theta_k + \eta \cdot \hat{\nabla}_{\tau}$$

$$= \theta_k + \eta \left( \sum_{t=0}^{\infty} \gamma^t G_t(\tau) \nabla_{\theta} \log \pi_{\theta}(a_t | s_t) \right)$$

(Repeat Step 2 until termination)

Ronald J. Williams, "Simple Statistical Gradient-Following Algorithms for Connectionist Reinforcement Learning," ML 1992

Can we design RL algorithms by (P1) and (P3)?

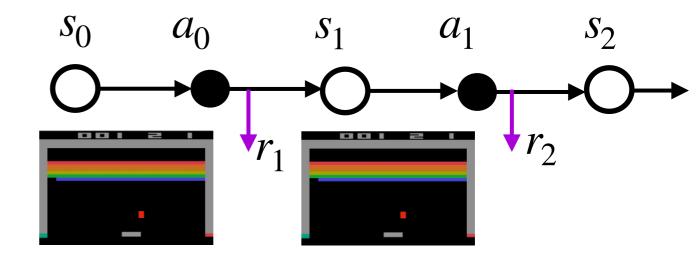
## An Alternative Monte-Carlo Policy Gradient Algorithm

$$\quad \text{Recall (P1):} \quad \nabla_{\theta} V^{\pi_{\theta}}(\mu) = \mathbb{E}_{\tau \sim P^{\pi_{\theta}}_{\mu}} \Big[ G(\tau) \sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_t \,|\, s_t) \Big]$$

Step 1: In each iteration k, draw a trajectory  $\tau = (s_0, a_0, r_1, s_1, a_1 \cdots)$  under  $\pi_{\theta}$  and  $\mu$ , and then construct:

$$G(\tau) := \sum_{t=0}^{\infty} \gamma^{t} r_{t}$$

$$\bar{\nabla}_{\tau} := R(\tau) \sum_{t=0}^{\infty} \nabla_{\theta} \log \pi_{\theta}(a_{t} | s_{t})$$



Step 2: Apply 
$$\theta_{k+1} = \theta_k + \eta \cdot \bar{\nabla}_{\tau}$$

- Question: Is  $\bar{\nabla}_{\tau}$  an unbiased estimate of  $\nabla_{\theta}V^{\pi_{\theta}}(\mu)$ ?
- Question: Any difference from REINFORCE?

# How About Using (P3)?

Step 1: In each iteration k, draw a batch B of n state-action pairs by following  $\pi_{\theta}$  and construct

$$\tilde{\nabla}_{\tau} := \frac{1}{1 - \gamma} \cdot \left( \frac{1}{n} \sum_{(s,a) \in B} Q^{\pi_{\theta}}(s,a) \nabla_{\theta} \log \pi_{\theta}(a \mid s) \right)$$

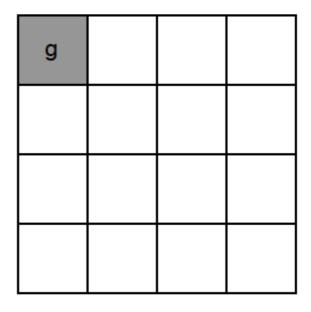
Step 2: Apply 
$$\theta_{k+1} = \theta_k + \eta \cdot \tilde{\nabla}_{\tau}$$

• Question: What does "draw samples by following  $\pi_{\theta}$ " mean? Are the samples i.i.d.?

## One Untold Secret in RL Community...

 $\tilde{\nabla}_{\tau}$  for (P3) is actually NOT an unbiased estimator of the true PG!

• But for large n,  $\tilde{\nabla}_{\tau}$  can still nicely approximate the true PG (Why?)



#### **A Fundamental Property:**

Empirical distribution uniformly approximates the true distribution!

(This is known as Gilvenko-Cantelli Theorem)

## Gilvenko-Cantelli Theorem (Formally)

### Empirical distribution uniformly approximates the true distribution

- Let  $\{X_n, n \geq 1\}$  be a sequence of i.i.d. random variables with a common CDF F
- Define the empirical CDF as  $\hat{F}_n(x) := \frac{1}{n} \sum_{i=1}^n I\{X_i \le x\}$
- Define  $D_n := \sup_{x \in \mathbb{R}} |\hat{F}_n(x) F(x)|$
- Gilvenko-Cantelli Theorem:

$$D_n \to 0$$
, as  $n \to \infty$ 

This result could be directly extended to Markov chains

Stute and Schmann, "A General Gilvenko-Cantelli Theorem for Stationary Sequences of Random Observations," 1980

## Yet Another Untold Secret in RL Community...

. RL people usually ignore the effect of  $\gamma$  on  $d_{\mu}^{\pi_{\theta}}$  (which is not theoretically justified)

#### Is the Policy Gradient a Gradient?

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#### ABSTRACT

The policy gradient theorem describes the gradient of the expected discounted return with respect to an agent's policy parameters. However, most policy gradient methods drop the discount factor from the state distribution and therefore do not optimize the discounted objective. What do they optimize instead? This has been an open question for several years, and this lack of theoretical clarity has lead to an abundance of misstatements in the literature. We answer this question by proving that the update direction approximated by most methods is not the gradient of any function. Further, we argue that algorithms that follow this direction are not guaranteed to converge to a "reasonable" fixed point by constructing a counterexample wherein the fixed point is globally pessimal with respect to both the discounted and undiscounted objectives. We motivate this work by surveying the literature and showing that there remains a widespread misunderstanding regarding discounted policy gradient methods, with errors present even in highly-cited papers published at top conferences.

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is pessimal, regardless of whether the discounted or undiscounted objective is considered.

The analysis in this paper applies to nearly all state-of-the-art policy gradient methods. In Section 6, we review all of the policy gradient algorithms included in the popular stable-baselines repository [9] and their associated papers, including A2C/A3C [13], ACER [28], ACKTR [30], DDPG [11], PPO [18], TD3 [6], TRPO [16], and SAC [8]. We motivate this choice in Section 6, but we note that all of these papers were published at top conferences and have received hundreds or thousands of citations. We found that all of the implementations of the algorithms used the "incorrect" policy gradient that we discuss in this paper. While this is a valid algorithmic choice if properly acknowledged, we found that only one of the eight papers acknowledged this choice, while three of the papers made erroneous claims regarding the discounted policy gradient and others made claims that were misleading. The purpose of identifying these errors is not to criticize the authors or the algorithms, but to draw attention to the fact that confusion regarding the behavior of policy gradient algorithm exists at the very core of the RL community and has gone largely unnoticed by reviewers.



Philip Thomas