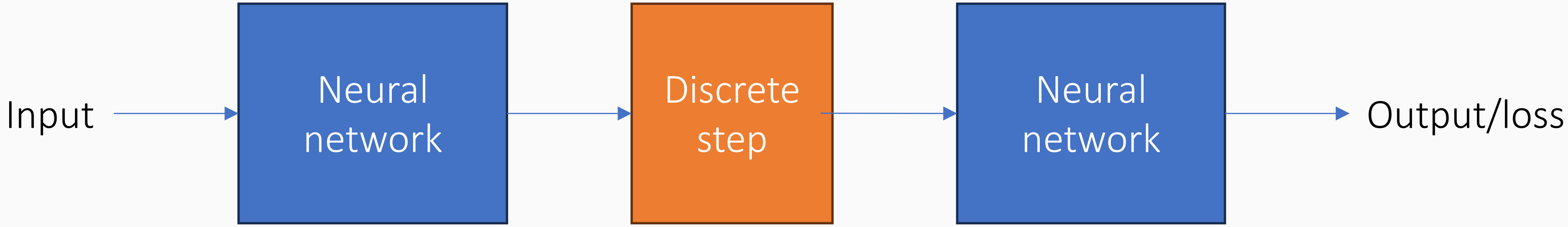
Learning with symbols within neural networks

Neuro-symbolic modeling

THE UNIVERSITY OF UTAH

Neural networks containing discrete elements



Let's see some examples

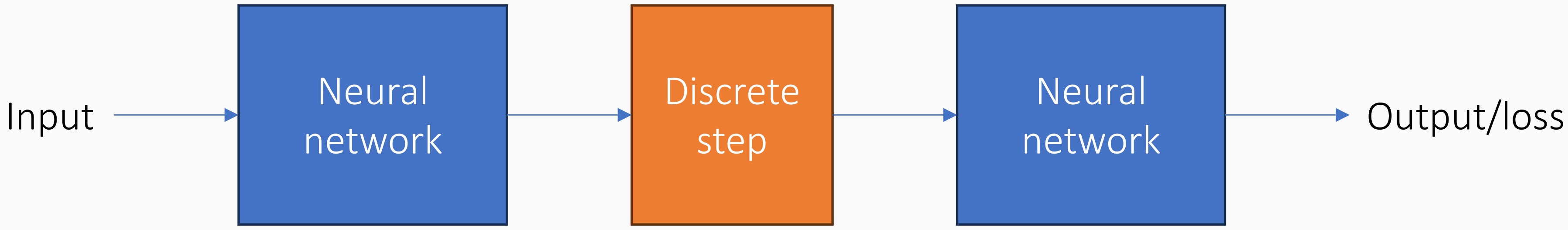
This lecture

- Motivating examples
- The straight-through estimator
- The Gumbel trick
- REINFORCE

(others if time permits)

Not all these approaches are always applicable

Suppose the discrete step is opaque



If we have no idea or control about the inner workings of the discrete step, then we will need to use ideas from reinforcement learning

Reinforcement learning: Some basics

An agent interacts with an environment by taking actions

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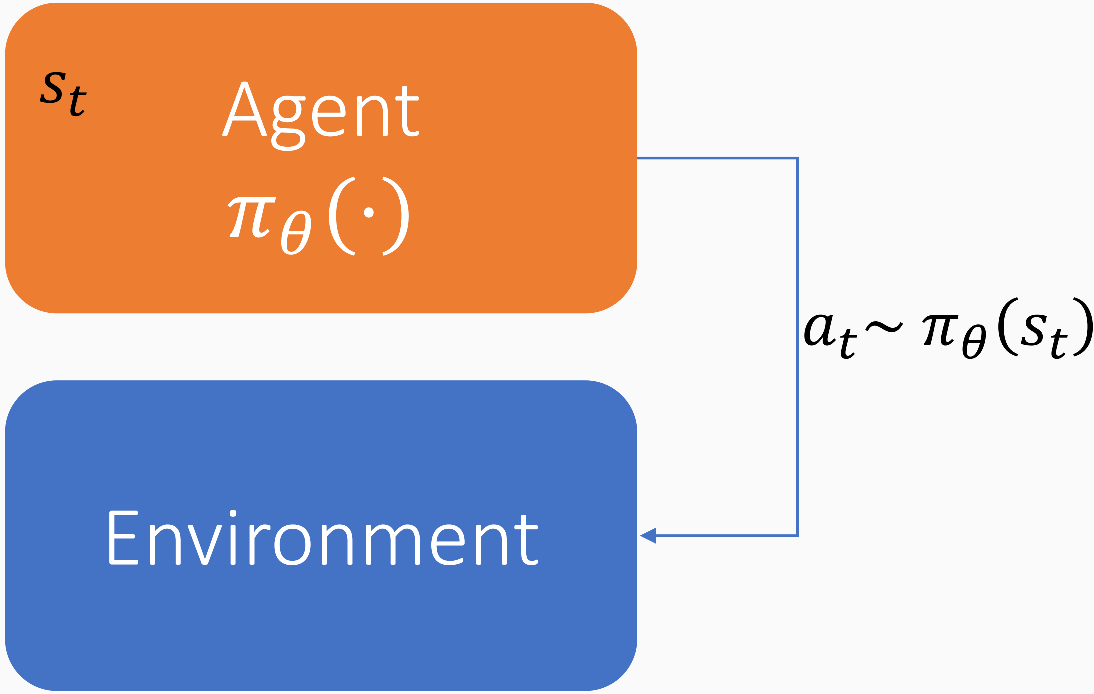

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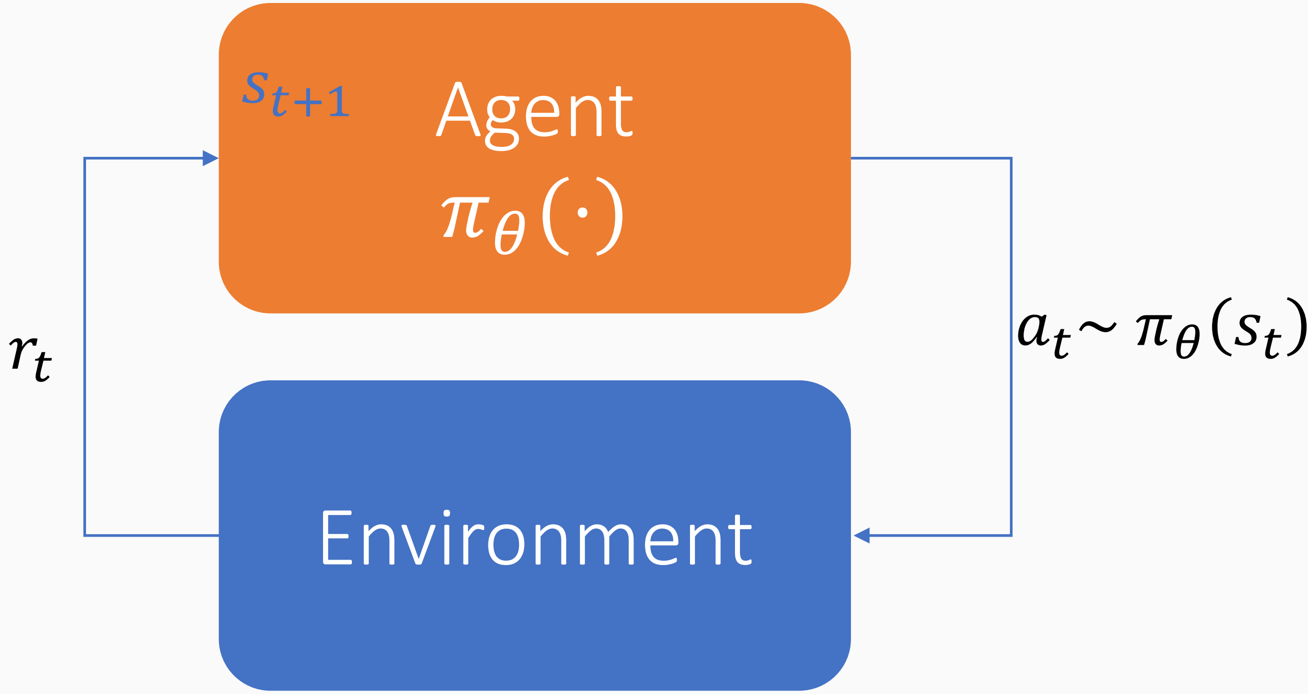

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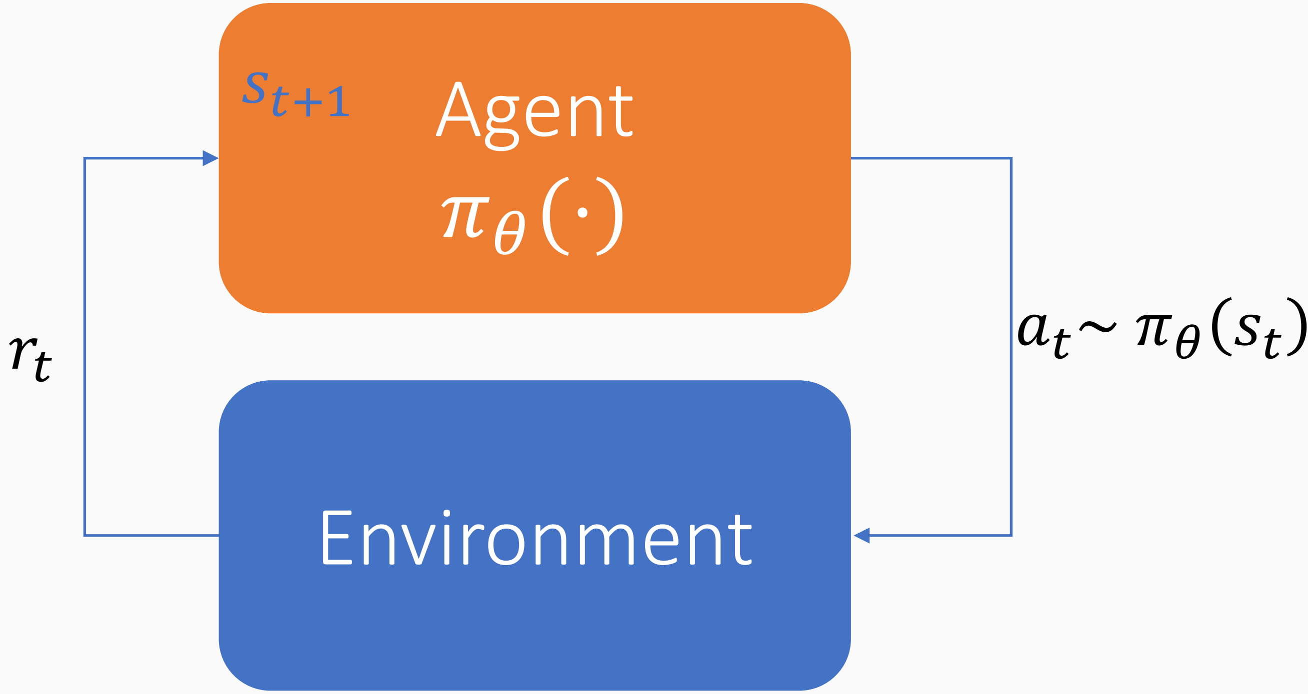

Quite an open-ended learning paradigm

Reinforcement learning: Some basics

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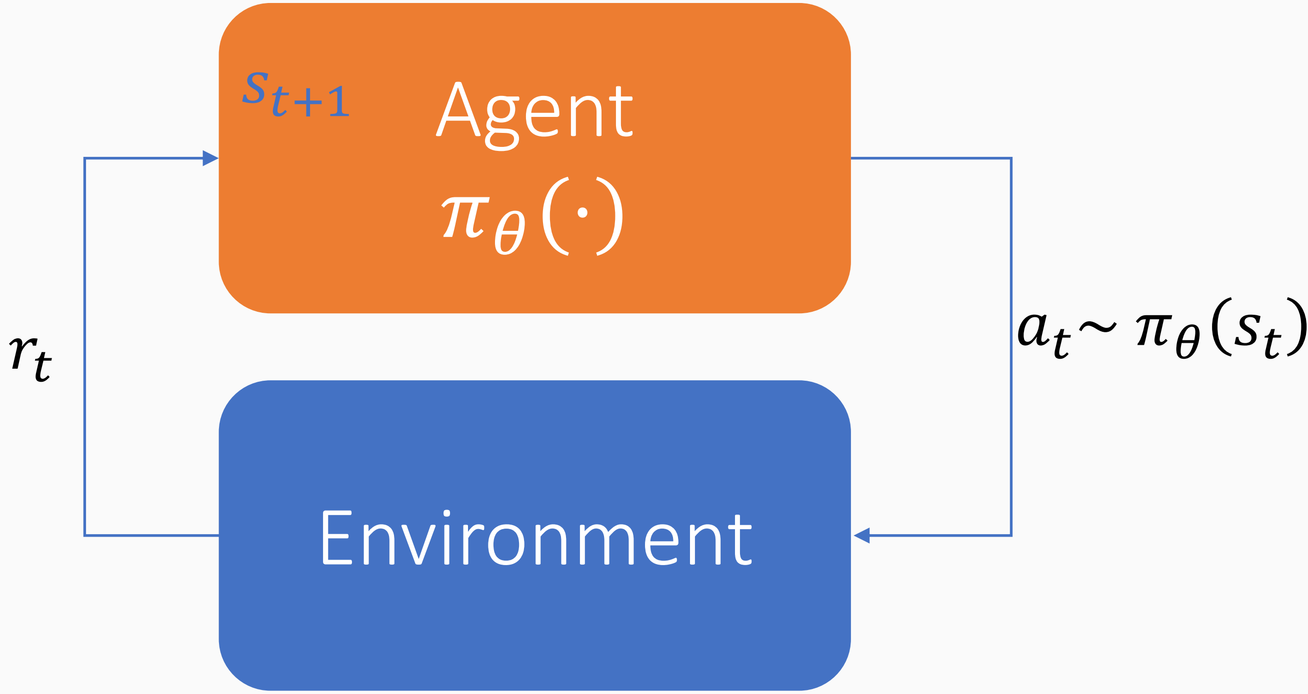
What are some examples of agents and environments?



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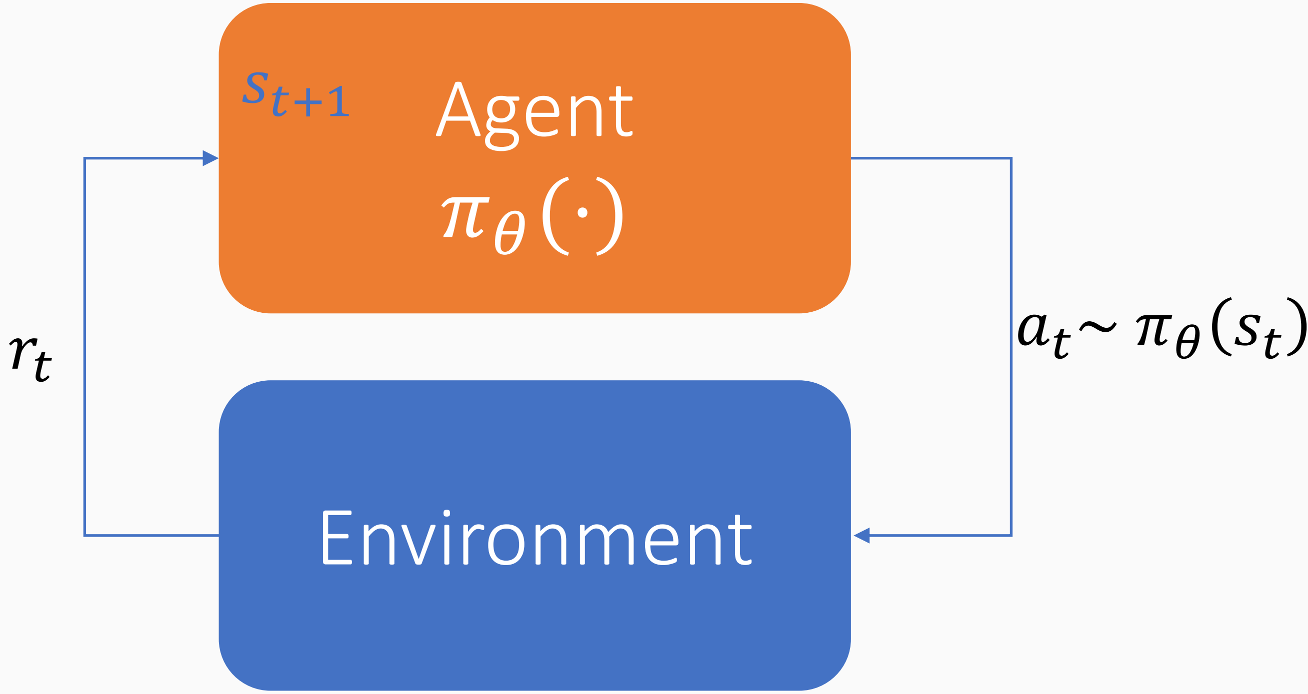
Some examples of agents and environments

Agent: converts a natural language command into a program
Environment: executes the program and returns the output



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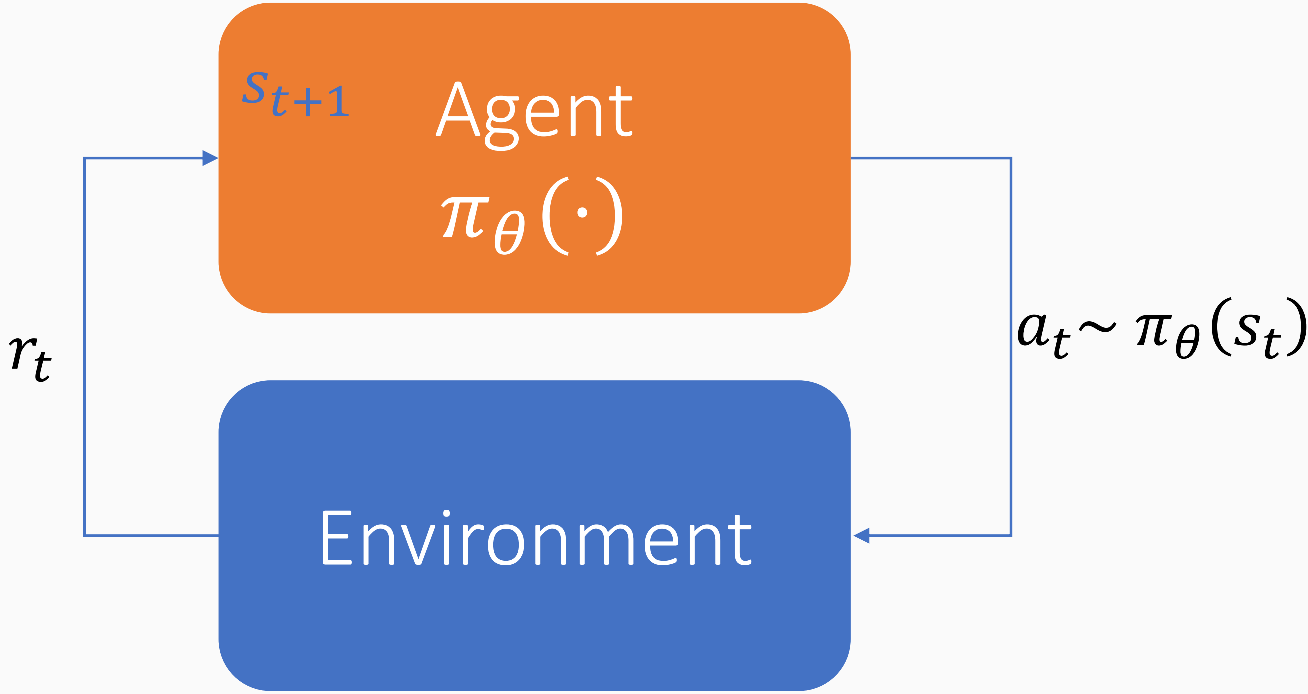

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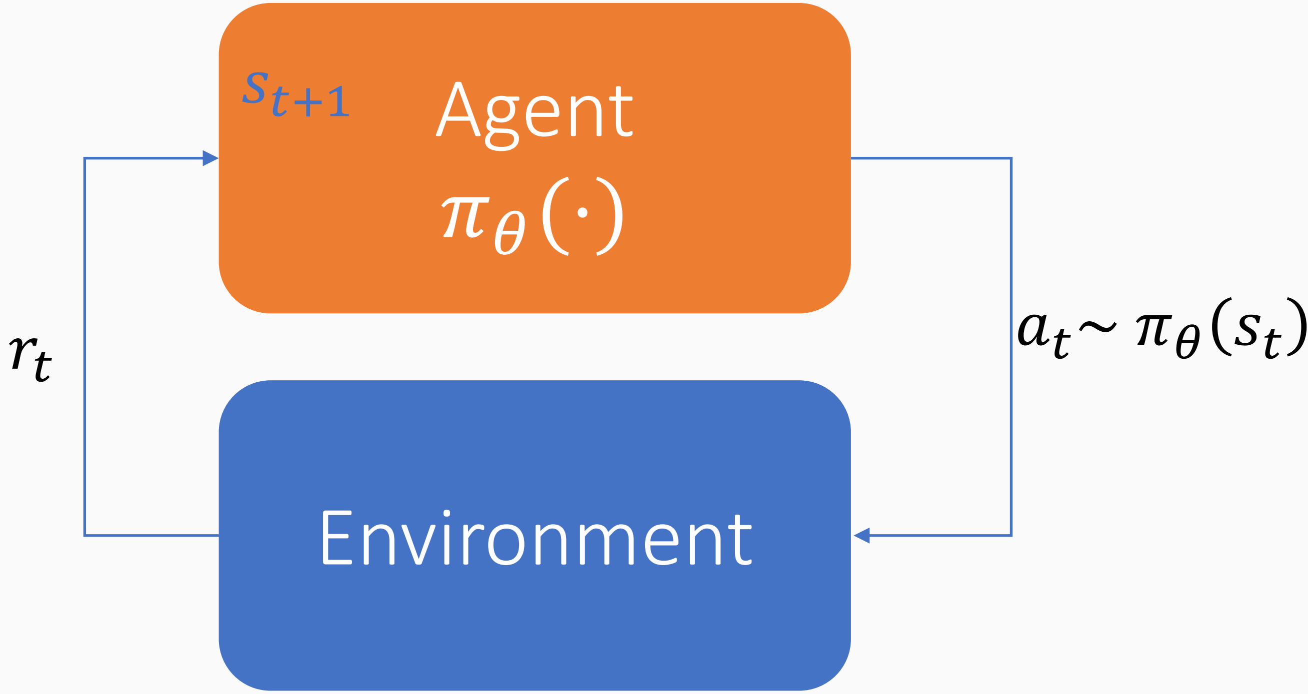

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Environment: A game engine with more real or simulated players

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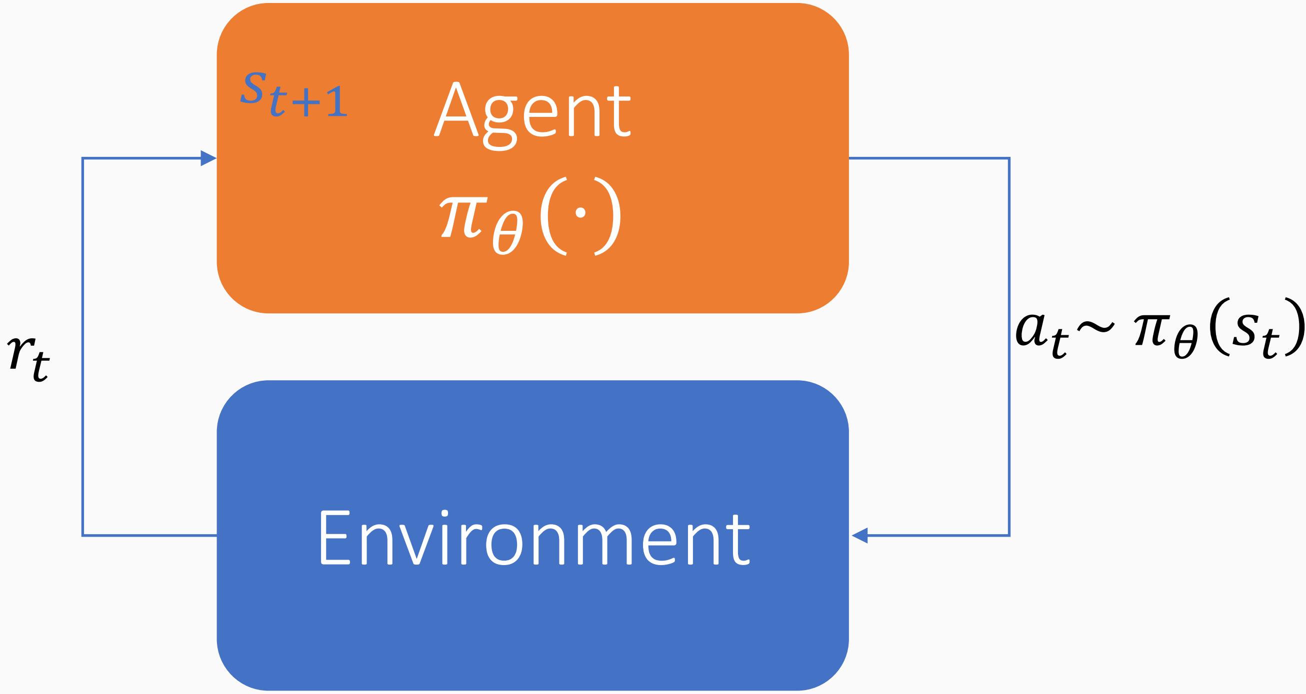

What are the states, actions and rewards in each case?

Reinforcement Learning

The field of reinforcement learning (RL) has studied the problem of learning by interacting with an environment for many years now [Williams, 1992; Sutton and Barto, 1998]

Circa 2013: resurgence of interest in RL applied to deep learning, game-playing [Mnih et al., 2013]

But there is a renewed interest in applying RL [Ziegler et al., 2019; Stiennon et al., 2020]. Why?

- RL w/ LMs has commonly been viewed as very hard to get right (still is!)
- RL algorithms that work for large neural models, including language models (e.g. PPO; [Schulman et al., 2017])

Caveats about this lecture

RL is a rich field with a diverse collection of algorithms and ideas

We will look at one popular approach: REINFORCE

The general setting allows for rewards being harvested over multiple steps corresponding to multiple actions. For this lecture, we will assume that there is only one action and one step that gets a reward

Learning to maximize reward

The goal of learning: Discover a policy that allows the agent to accure high rewards

Formally: Prefer models which maximize expected reward

$$\max_{\theta} \mathbb{E}_{a \sim p_\theta}[R(s, a)]$$

How do we solve this optimization problem?

Learning the policy function

We want $\max_{\theta} \mathbb{E}_{a \sim p_{\theta}}[R(s,a)]$

Gradient ascent:

$$\theta_{t+1} \leftarrow \theta_t + \text{learning rate} \times \text{gradient of the objective}$$

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$$\theta_{t+1} \leftarrow \theta_t + \alpha \nabla_{\theta_t} \mathbb{E}_{a \sim p_{\theta_t}}[R(s, a)]$$

But how do we estimate this gradient?

(Why doesn't the usual approach for derivatives not work?)

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But how do we estimate this gradient?

Let us look at a simple version of policy gradients

Two useful tricks

1. Monte Carlo estimates for approximating expectations

Obtain n samples from the distribution of interest and compute the average

$$E_{x \sim P}[f(x)] \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

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No θ_t in this expression!

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Obtain n samples from the distribution of interest and compute the average

$$E_{x\sim P}\left[f(x)\right] \approx \frac{1}{n}\sum_{i=1}^{n} f(x_i)$$

2. The REINFORCE trick [Williams 1992]

$$\frac{\partial}{\partial x} f(x) = f(x)\frac{\partial}{\partial x}\log f(x)$$

Let us reformulate the gradient

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$$\nabla_\theta \mathbb{E}_{a\sim \mathrm{P}_\theta}[R(s,a)] = \nabla_\theta \sum_a R(s,a) P_\theta(a \mid s)$$

Definition of expectation. Also works with integrals, but let's keep things simple

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Rewrite as an expectation

$$\approx \frac{1}{n} \sum_{i=1}^{n} R(s,a_i) \nabla_\theta \log P_\theta(a_i \mid s)$$

Approximate with n samples

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Approximate with n samples

How do we compute the derivative of the log probability? Autodiff

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We want $\max_{\theta} \mathbb{E}_{a \sim p_\theta}[R(s, a\ )]$

Gradient ascent:

$$\theta_{t+1} \leftarrow \theta_t + \alpha \nabla_{\theta_t} \mathbb{E}_{a \sim p_{\theta_t}}[R(s, a)]$$

But how do we estimate this gradient?

Answer: We use a neat trick to estimate the gradient of the expectation

Policy gradient

We want $\max_{\theta} \mathbb{E}_{a \sim p_\theta}[R(s,a)]$

Gradient ascent with n samples from p_θ:

$$\theta_{t+1} \leftarrow \theta_t + \alpha \cdot \frac{1}{n} \sum_{i=1}^{n} R(s, a_i) \nabla_\theta \log p_\theta(a_i \mid s)$$

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This is a simplified version

There are many variants of this idea

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Note that we have no restriction on the reward $R(s,a)$. It could be non-differentiable, provided by the environment somehow, or provided by humans.

REINFORCE algorithm

Repeat:

1. Sample n actions $a_1, a_2, \cdots, a_n$ at state s
2. Compute all rewards $\mathrm{R}(a_i, s)$
3. Update parameters as:

$$\theta_{t+1} \leftarrow \theta_t + \alpha \cdot \frac{1}{n} \sum_{i=1}^{n} R(s, a_i) \nabla_\theta \log p_\theta(a_i \mid s)$$

For our purposes, the states could represent examples in our data and actions could be predictions of the discrete part of our neuro-symbolic system

Compare to supervised maximum likelihood learning

Suppose we have a dataset of states paired with ground truth actions: $\mathrm{D} = \{(s, a)\}$ whose probability we wish to maximize:

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Similar terms in both cases

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We do not know which action is good. So we sample actions and weight the gradients associated with them by the reward

Problems with policy gradient

Does it always work?

- Vanilla policy gradient tends to have high variance in gradient estimates
  - There may be sudden jumps in performance, but training may be slow overall

- In practice: combine with variance reduction techniques
  - Several approaches exist in the literature
  - Let's look at one: *baselines*

Baselines

Our original update:

$$\theta_{t+1} \leftarrow \theta_t + \alpha \cdot \frac{1}{n} \sum_{i=1}^{n} R(s, a_i) \nabla_\theta \log p_\theta(a_i \mid s)$$

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Modify to:

$$\theta_{t+1} \leftarrow \theta_t + \alpha \cdot \frac{1}{n} \sum_{i=1}^{n} [R(s, a_i) - b(s)] \nabla_\theta \log p_\theta(a_i \mid s)$$

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Subtract a baseline from the reward

- Doing so reduces variance
- But does not introduce any additional bias

In practice: a good choice of $b(s)$ is

$$b(s) = \frac{1}{n}\sum_{i=1}^{n} R(s, a_i)$$

Not theoretically the best, but often good

Introducing a baseline is unbiased

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Consider the expected reward:

$$\mathbb{E}_{a\sim p_\theta}[R(s,a)] = \mathbb{E}_{a\sim p_\theta}[R(s,a)\nabla_\theta \log p_\theta(a \mid s)]$$

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This works by the linearity of expectations

Introducing a baseline is unbiased

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The first term is the same as the original expectation $\mathbb{E}_{a\sim p_\theta}[R(s,a)]$

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Let us focus on the second term

Introducing a baseline is unbiased (2)

Let us look at the second term

$$\mathbb{E}_{a \sim p_\theta}[b(s) \nabla_\theta \log p_\theta(a \mid s)]$$

Introducing a baseline is unbiased (2)

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We can expand the expectation to write:

$$\sum_a b(s) p_\theta(a \mid s) \nabla_\theta \log p_\theta(a \mid s)$$

We could have written this as an integral, but let's keep things simple

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$$\mathbb{E}_{a\sim p_\theta}[b(s)\nabla_\theta \log p_\theta(a \mid s)]$$

We can expand the expectation to write:

$$\sum_a b(s) p_\theta(a \mid s)\, \nabla_\theta \log p_\theta(a \mid s)$$

Apply the REINFORCE trick to simplify:

$$\sum_a b(s) \nabla_\theta p_\theta(a \mid s)$$

Introducing a baseline is unbiased (2)

Let us look at the second term

$$\mathbb{E}_{a\sim p_\theta}[b(s)\nabla_\theta \log p_\theta(a \mid s)]$$

We can expand the expectation to write:

$$\sum_a b(s)p_\theta(a \mid s)\,\nabla_\theta \log p_\theta(a \mid s)$$

Apply the REINFORCE trick to simplify:

$$\sum_a b(s)\nabla_\theta p_\theta(a \mid s) = b(s)\nabla_\theta \sum_a p_\theta(a \mid s)$$

The baseline $b(s)$ doesn't depend on the action a, so we can pull it out of the summation

And the sum of gradients is the gradient of the sum

Introducing a baseline is unbiased (2)

Let us look at the second term

$$\mathbb{E}_{a \sim p_\theta}[b(s) \nabla_\theta \log p_\theta(a \mid s)]$$

We can expand the expectation to write:

$$\sum_a b(s) p_\theta(a \mid s) \nabla_\theta \log p_\theta(a \mid s)$$

Apply the REINFORCE trick to simplify:

$$\sum_a b(s) \nabla_\theta p_\theta(a \mid s) = b(s) \nabla_\theta \boxed{\sum_a p_\theta(a \mid s)} = 0$$

This quantity is equal to 1 because it accumulates the entire support for the probability p_θ. Its derivative is zero

Introducing a baseline is unbiased (2)

Let us look at the second term

$$\mathbb{E}_{a\sim p_\theta}[b(s)\nabla_\theta \log p_\theta(a \mid s)]$$

We can expand the expectation to write:

$$\sum_a b(s) p_\theta(a \mid s)\, \nabla_\theta \log p_\theta(a \mid s)$$

Apply the REINFORCE trick to simplify:

$$\sum_a b(s)\nabla_\theta p_\theta(a \mid s) = b(s)\nabla_\theta \sum_a p_\theta(a \mid s) = 0$$

$$\mathbb{E}_{a\sim p_\theta}[(R(s,a) - b(s))\nabla_\theta \log p_\theta(a \mid s)] = \mathbb{E}_{a\sim p_\theta}[R(s,a)] - \mathbb{E}_{a\sim p_\theta}[b(s)\nabla_\theta \log p_\theta(a \mid s)]$$

The entire second term vanishes

Introducing a baseline is unbiased (2)

Let us look at the second term

$$\mathbb{E}_{a\sim p_\theta}[b(s)\nabla_\theta \log p_\theta(a \mid s)]$$

We can expand the expectation to write:

$$\sum_a b(s)p_\theta(a \mid s)\, \nabla_\theta \log p_\theta(a \mid s)$$

Apply the REINFORCE trick to simplify:

$$\sum_a b(s)\nabla_\theta p_\theta(a \mid s) = b(s)\nabla_\theta \sum_a p_\theta(a \mid s) = 0$$

What have we done:

$$\mathbb{E}_{a\sim p_\theta}[(R(s,a) - b(s))\nabla_\theta \log p_\theta(a \mid s)] = \mathbb{E}_{a\sim p_\theta}[R(s,a)]$$

REINFORCE algorithm with baselines

Repeat:

1. Sample n actions $a_1, a_2, \cdots, a_n$ at state s
2. Compute all rewards $\mathrm{R}(a_i, s)$
3. Compute baseline $b(s) = \frac{1}{n}\sum_{i=1}^{n} R(s, a_i)$
4. Update parameters as:

$$\theta_{t+1} \leftarrow \theta_t + \alpha \cdot \frac{1}{n}\sum_{i=1}^{n}[R(s, a_i) - b(s)]\nabla_\theta \log p_\theta(a_i \mid s)$$

For our purposes, the states could represent examples in our data and actions could be predictions of the discrete part of our neuro-symbolic system

REINFORCE: Summary

A useful tool when we have a black box system within a neural network

Caveats:

- Gradients will have high variance
- Variance control methods could help a little, but the gradients are still going to be noisy

In practice: this means that experiments will be tricky

- Use much larger batches than you may be used to
- Learning rates will matter, ADAM may be good
  - There are learning rate adjustment strategies designed for policy gradient too