

Deep Reinforcement Learning IN ACTION

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welcome

Firstly, we want to thank you for giving this book a chance. With so many options available in the machine learning space for tutorials and training, you may be wondering why we chose to join the fray. Well, there are, in fact, a lot of resources out there for learning the basics of machine learning and deep learning (to shamelessly plug another Manning book, we recommend Andrew Trask's *Grokking Deep Learning* to get up to speed there). But once people get a handle on the basics, where do they go from there?

We think a great next step for the newly-minted deep learning aficionado is to apply their new skills to the field of reinforcement learning. Reinforcement learning has seen tremendous success in the past few years and exciting results are happening every day, yet the landscape of truly beginner-level material in this area is comparatively sparse. Unlike deep learning, which has already infiltrated almost every major technology, reinforcement learning has just recently started to take form as a viable solution to practical problems. This means if you learn reinforcement learning now, you'll be walking in on the ground floor of something that is surely going to surge in value in the near future.

While reinforcement learning is a distinct field from deep learning, the marriage of the two into deep reinforcement learning is a natural and powerful combination and is the dominant form of machine learning being developed. This book aims to teach you to use core deep reinforcement learning skills to solve real-world problems in the most approachable and intuitive manner possible.

If you have any questions, comments, or suggestions, please share them in Manning's [liveBook's Discussion Forum](#) for our book. We hope you'll enjoy the ride!

— Alex Zai and Brandon Brown

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1

What is Reinforcement Learning?

“Computer languages of the future will be more concerned with goals and less with procedures specified by the programmer.”

– Marvin Minsky, 1970

1.1 The Journey Here

In 1936 the English mathematician Alan Turing published a paper entitled “*On Computable Numbers, with an Application to the Entscheidungsproblem*,” in which he developed a mathematical description of an algorithm, which later became known as a Turing machine. His conception of the Turing machine became the basis of the development of modern electronic computers. Interestingly, he originally developed the Turing machine as a tool to solve a mathematical problem, not because he wanted to invent a new field of computer science. Nevertheless, he and many others recognized the power of this new idea of computation and it immediately begged the question of whether these new computing systems could become intelligent like humans. Alan Turing himself kicked off the field of artificial intelligence by subsequently publishing the paper “Computing Machinery and Intelligence” in 1950 where he began with the question, “Can machines think?” The board game Chess has always been considered an intellectual sport, and thus it was natural to use it as a testbed for whether machines could be made intelligent. Several attempts at writing Chess-playing algorithms were made over the subsequent years, starting with algorithms that were only described on paper and had to be run by a human following a sequence of rules, up to the landmark defeat of the Chess world champion Gary Kasparov in 1996 by IBM’s DeepBlue algorithm.

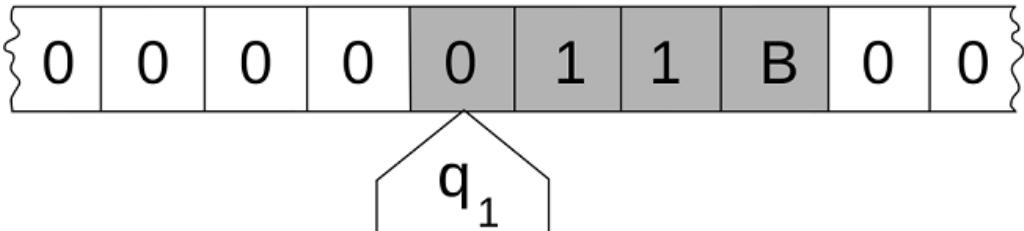


Figure 1.1: This depicts how a single-tape Turing machine works. The shape labeled “q1” is a read and write head that can move left or right across a tape that has printed values in evenly spaced cells. The read/write head follows a predefined set of rules and can read certain values on the tape, erase, and write new values to the tape. This simple model captures the essence of computation and started the field of computer science.

While these Chess playing machines were impressive at the time, they were (and continue to be) mostly based on exhaustive search and pre-programmed logic rather than performing any sort of human-like analysis or strategizing. Indeed, most of what was called artificial intelligence in the early days was just hard-coded logic and heuristics. The first descriptions of artificial neural networks, algorithms that attempted to model biological neural networks, appeared in the 1940s and would become one of many algorithms that fall under the umbrella of machine learning. One particularly influential theory of how neural networks learn was advanced by psychologist Donald Hebb in his 1949 book “Organization of Behavior.” Hebb proposed that learning happens at the level of neurons when two neurons repeatedly fire an electrochemical signal called an action potential in synchrony and in close proximity, then the causal relationship between these two neurons will become enhanced, or reinforced. His theory later became known as Hebbian learning and is still considered relevant with significant empirical evidence backing it.

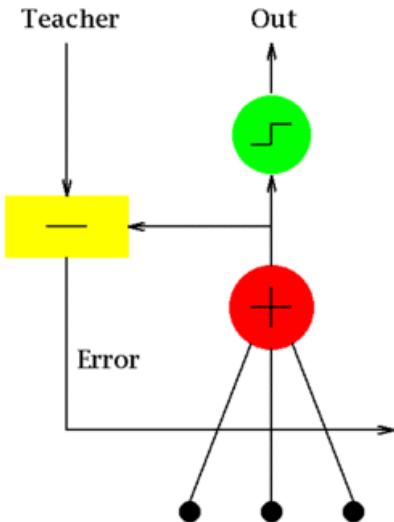


Figure 1.2: A diagram of one of the first neural networks called ADALINE that was used to filter out echoes in telephone lines. The network simply computed a weighted sum of its input variables and if the sum was greater than some threshold parameter, it would return 1, otherwise it returns 0 (called a step function). By defining some error function, you could follow simple rules to modify the threshold parameter in order to reduce the error and improve the performance of the algorithm.

With some theoretical neuroscience to take advantage of, the first artificial neural networks were implemented on some of the earliest computing machines in the 1950s. Remarkably, in 1959, researchers at Stanford created the first commercial application of a neural network, an algorithm called ADALINE, which was designed to filter out echoes in telephone line signals and is still in use today. Any neural network algorithm, and indeed most machine learning algorithms, involve parameters that control their behavior. In order for the neural network to perform whatever task is desired, the network's parameters must be "trained" to be set to the right values. ADALINE and other early neural networks were trained by simple heuristics and searching procedures, although some did employ what would later be rigorously worked out and defined as **backpropagation**. The history of the backpropagation technique is a little uncertain, but it was not widely adopted until the mid 1980s where it was able to train more sophisticated neural networks than ADALINE and remains the standard training procedure for neural networks.

1.2 Supervised and Unsupervised Learning

ADALINE, like most of the neural networks and other types of machine learning algorithms that followed it, was a **supervised learning** algorithm. Supervised learning algorithms are trained in a teacher-student manner. For example, if you want to build an algorithm to classify a dataset of images into certain categories, then a teacher would supply the algorithm with

images to classify, and the algorithm would make a prediction, and then based on the accuracy of the prediction, the teacher would provide corrective feedback such that the algorithm would perform a little better next time. Doing this over many examples of images, the algorithm would eventually perform well enough. More accurately, a learning algorithm is given an input datum and produces an output. The output is then evaluated by some objective function that compares the algorithm's output to the known correct or labeled outputs, and produces a measure of how wrong the algorithm's output was (i.e. an error). Then the parameters of the algorithm are updated to minimize the error produced by the objective function, often using the backpropagation technique. Hence, you need two sets of data for every supervised learning task: the data to be learned and the labeled data (i.e. the correct answers to whatever the problem is). The labeled data must be produced and curated by humans specifically for the purpose of training an algorithm, whereas the data to be learned may be acquired from the "environment", e.g. telephone line signals. Most large-scale commercial applications require at least tens of thousands and often millions and billions of rows of labeled training data to achieve satisfactory accuracy in their task.

In contrast, **unsupervised learning** algorithms attempt to learn something from data without being given explicit feedback by a teacher. The most common form of unsupervised learning would be clustering, in which an algorithm attempts to find clusters of related data points in some data set. More modern and sophisticated unsupervised learning techniques include a kind of neural network called an auto-encoder, which can automatically learn fairly complex patterns in data. Nonetheless, unsupervised methods are limited in utility since it's difficult to operationalize them. A fancy unsupervised algorithm might learn some interesting patterns in your data, but unless you tell it what you want it to do (in effect converting it to supervised learning), then it won't be able to say, classify your images into the categories you care about.

Supervised learning has been the dominant form of machine learning and the most successful commercially, however, it is unsatisfactory in our quest for the intelligent machines that Alan Turing dreamed of. Surely one major reason for wanting to develop intelligent machines is so that they can do things we don't already know how to do. This is the major limitation of supervised learning; there must already exist a teacher that knows how to do the task and can teach the machine. If the machine learns how to do the task, then it is of course very useful since it may be able to do it faster, cheaper and with less error than a human, but it still cannot learn how to do anything we don't already know how to do. These supervised learning algorithms are necessarily extremely domain specific.

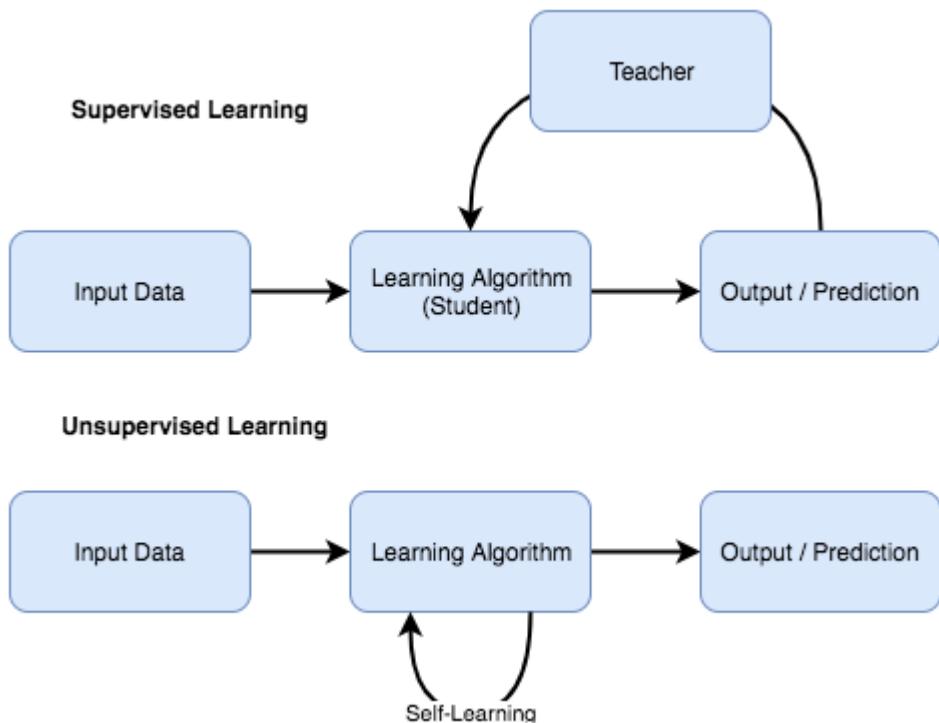


Figure 1.3: Supervised learning is the class of algorithms that exhibit a teacher-student relationship where the algorithm learns by being given explicit feedback by a teacher. Unsupervised learning algorithms are able to self-teach to some extent, and learn something about data on their own.

Clearly, humans have aspects of both supervised and unsupervised learning. Learning a new subject in school for example, is largely an instance of a teacher-student situation. However, it's unsupervised learning that is responsible for human progress: the creation of new knowledge, new skills, art and creativity. There has to be the first one to learn something on their own before being able to teach it. Supervised learning can help us be more efficient by saving us time and resources, thereby giving us more resources to invest in creation, but it is not going to give us artificial general intelligence (AGI) where machines would become our intellectual peers and not just automation tools. But even if you're entirely practically-minded and have no interest in AGI, supervised learning is still unsatisfactory because it is limited by how much training data we can give it; just like the number of students that can go to school is limited by the number of teachers. Sometimes we just don't have the resources to produce the labeled data set, or doing so outweighs the benefit of using the algorithm.

For example, one of the authors' wife is a neuroscientist who uses fancy microscopes to image neurons in living rodents. The microscopes produce gigabytes of video data that must be painstakingly analyzed by manually identifying and delineating neurons to produce

quantitative data about the neurons' characteristics. A machine learning paper was recently published in which the paper's authors developed a neural network that could automatically identify neurons in these videos. However, it was a supervised neural network that required each user to provide a labeled data set of thousands of manually identified neurons. The authors themselves noted that this process may take more than 10 hours (optimistically). While such a significant time investment might pay off in the long term if you have to do this type of experiment many times, no busy scientist wants to risk spending an entire working day building a training data set for an algorithm that is not guaranteed to work for them.

Perhaps even more illustrative of the inadequacy of supervised learning is teaching an algorithm how to drive a car or operate a robot. Let's say you want a car to learn how to drive just by analyzing video feeds (i.e. no other sensors like radar and lidar); this is in fact the strategy that Tesla is currently using to develop its autopilot software. The car must continuously control the steering wheel and continuously adjust the accelerator or breaks. How are you going to collect training data for this task? This is a **control task** (or decision task) not a prediction or classification task which are the bread-and-butter of supervised learning.

In a traditional supervised learning task, the environment is precisely managed and only the data we curated is accessible to the algorithm, and each piece of data is fully independent (i.e. we could arbitrarily remove or add data without significantly affecting the overall performance of the algorithm). In a control task, the environment is largely unmanaged and produces data "on its own" and may be probabilistic. In our self-driving car example, the data the algorithm is receiving from its cameras is not produced by some human curator, it's produced by the natural evolution of the environment around it as a function of time, which is largely unpredictable. In addition, without a bunch of expensive sensors, the car can only make incomplete observations of the surrounding environment. It would be totally unfeasible to teach the algorithm what it should be doing at every instant of time, such as the exact amount the steering wheel should be rotated given what the cameras are currently recording.

1.3 Problem Structuring in Control Tasks

This takes us back to the quote at the beginning of this chapter by the pioneering artificial intelligence researcher Marvin Minsky. Many early artificial intelligence algorithms were nothing more than hard-coded rules that could be easily followed by a human. The advent of neural networks and other learning algorithms allowed us to teach an algorithm how to do something just by giving it the correct answers, telling it how wrong it was and let it update itself to be less wrong next time. This freed us from having to work out and program a fixed set of rules to solve a problem and gave us greater flexibility. But it's still a very procedural process: feed in some data, get an output, produce an error value based on our knowledge of the correct answer, then update the algorithm using some technique like backpropagation. What if instead we could just give a high-level objective or goal to the algorithm and let it figure out the details? We want to be able to do goal-directed programming like Marvin Minsky suggested would be the future.

The field of **reinforcement learning** is starting to realize that imagined future. In reinforcement learning, we don't need to give the algorithm a bunch of labeled data to learn some task, we just need to be able to define what success looks like in the environment. For example, we might give the high-level goal of "don't hit anything, follow all traffic rules, and navigate from point A to point B along the most efficient route" to our self-driving car algorithm and let it figure out how to work out the details of achieving that goal. This may seem like a remarkable feat, but it's exactly the kind of thing we'll be learning how to do in this book.

All human behavior is fundamentally goal-directed, so it makes sense that this is how we should design our learning algorithms. Biological evolution by natural selection has endowed most species with a set of primitive goals or drives, such as minimizing hunger, avoiding pain, seeking pleasure, reducing uncertainty, and in the case of humans and other social animals, achieving social acceptance. Even in the modern world that is far abstracted away from our ancestral environment, every human behavior can be reduced to some combination of these primitive drives and goals. For example, as awkward as it is to admit, the authors writing this book may think that they are doing it because they are excited about reinforcement learning and want to share it with others, but fundamentally we are motivated by our evolutionary primitive drive to be contributing members of our tribe. It's amazing how much has been accomplished in the world by a bunch of people individually maximizing or minimizing a fairly small set of high-level drives and goals.

Let's run with this idea. If a person is hungry (high-level drive) then she must eat to minimize her hunger. But eating can't be done in a single step; she first must make very low level decisions like which direction to walk in. In this sense, in order to solve a high-level objective we can break it down into small sub-problems that together will contribute to solving the high-level problem.

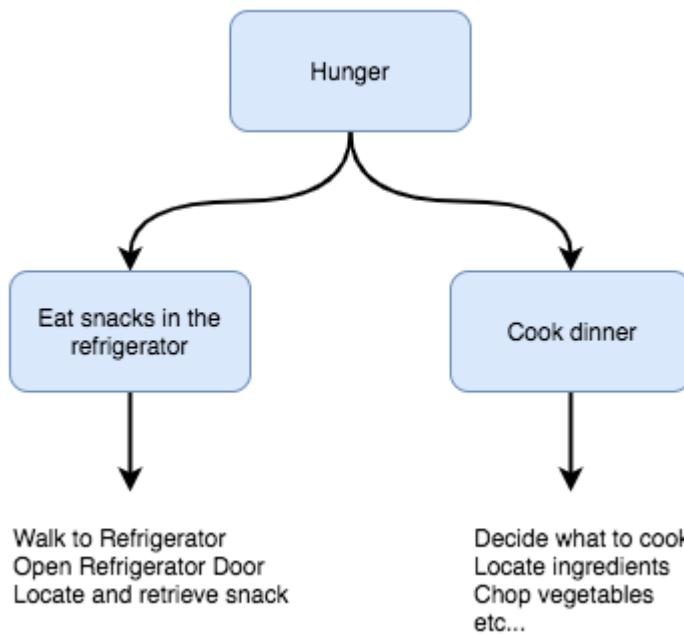


Figure 1.4: A high-level goal like satisfying one's hunger can be broken down into a tree of “local” sub-goals that each must be solved in order to achieve the global goal.

This idea of breaking a high-level goal, in which it is unclear how to solve on its own, into a hierarchy of sub-goals which at the lowest level are all almost trivial decisions was given a rigorous mathematical description by Richard Bellman in 1957. Bellman called this technique **dynamic programming** for reasons that mostly had to do with historical circumstances than for clarity. A more intuitive name might be “goal decomposition.” Bellman’s dynamic programming has one more trick besides goal decomposition; in addition to breaking an objective into a set of easier to solve sub-objectives, we should also store the solutions to all of the solutions of these sub-objectives so that if we need to solve the same sub-objective at a later time point, we can just look up the solution we got last time rather than figuring it out all over again. This technique of storing previously solved sub-problems is called **memoization** (note, it’s not **memorization**, it’s memoization; there’s no “r”).

Dynamic programming (DP) can be used to solve any control task that can be broken down into smaller parts. This has applications from economics to mathematics to computer science and of course to reinforcement learning, as we’ll soon see. But to give a simple example of DP in action (and the example you’ll find most often in textbooks), let’s see how you might use it to improve the efficiency of a computer algorithm that produces the n -th number in the Fibonacci sequence. If you’re not familiar with the Fibonacci sequence, it’s the sequence of positive whole numbers that follows this pattern: 0, 1, 1, 2, 3, 5, 8, 13, 21, ... where the n -th

number is the sum of the previous two numbers. In other words, $n=(n-1)+(n-2)$ where n refers to the n-th number (zero-indexed) in the sequence and the first two numbers are always 0 and 1. Just take our word for it that this sequence of numbers is special and actually has useful applications, hence why we might want to write a computer program to produce it. Using this mathematical definition as our starting point, we might write this function in Python as:

```
def fib(n):
    if n <= 1:
        return n
    else:
        return fib(n - 1) + fib(n - 2)

>>> fib(7)
13
```

It works great. The problem is this function is terribly inefficient; look what happens when we call `fib(4)`:

```
fib(4)
fib(3) + fib(2)
(fib(2) + fib(1)) + (fib(1) + fib(0))
```

We get a tree of recursive function calls where some identical computations are performed multiple times, for example, we can see `fib(2)` is computed twice. If we use the dynamic programming approach of memoizing our computations, we could have a much more efficient algorithm at the cost of a relatively mild memory overhead. Here's what the DP approach looks like in Python:

```
mem = {0:0, 1:1}

def fib_mem(n):
    if n not in mem:
        mem[n] = fib(n-1) + fib(n-2)
    return mem[n]

>>> fib_mem(7)
13
```

We defined a Python dictionary to store any computations we make and we initialized it to the first two numbers in the Fibonacci sequence. If the function is called with an input that it has already encountered, it can just use the Python dictionary to look up that previously computed number and return it, otherwise it will compute it (but just once) and store it in the `mem` dictionary.

As we now know, in order to apply Bellman's dynamic programming we have to be able to break our problem into sub-problems that we know how to solve. But even this seemingly innocuous assumption is difficult to realize in the real world. How do you break the high level goal for a self-driving car of "don't crash" into small non-crashing sub-problems? Does a child learn to walk by first solving easier sub-walking problems? In reinforcement learning where we

often have these kinds of nuanced situations that may include some element of randomness, we can't apply dynamic programming exactly as Bellman laid out. In fact DP can be considered one extreme of a continuum of problem solving techniques where the other end would be random trial and error.

Another way to view this learning continuum is that in some situations we have maximal knowledge of the environment and in others we have minimal knowledge of the environment, hence we need to employ different strategies in each case. If you need to use the bathroom in your own house, then you know exactly (well, unconsciously at least) what sequence of muscle movements will get you to the bathroom from any starting position (i.e. dynamic programming-ish). This is of course because you know your house extremely well, or in other words, you have a more or less perfect *model* of your house in your mind. If you go to a party at someone else's house that you've never been to before, then assuming no one tells you, you would just have to look around until you find the bathroom on your own (i.e. trial and error); since you don't have a good model of that person's house.

The trial and error strategy generally falls under the umbrella of Monte Carlo methods. A Monte Carlo method is essentially random sampling from the environment. In many real world problems, we have at least some knowledge of how the environment works, so we end up having to employ a mixed strategy of some amount of random trial and error and some amount of exploiting what we already know about the environment and directly solve the easy sub-objectives.

A silly example of a mixed strategy would be if you were blindfolded, placed in an unknown location in your house and told to find the bathroom by throwing pebbles and listening for the noise. You might start by decomposing the high level goal (find the bathroom) into a more accessible sub-goal, figure out which room you're currently in. To solve this sub-goal, you might throw a few pebbles in random directions and assess the size of the room, which might give you enough information to infer which room you're in, say the bedroom. Then you need to pivot to another sub-goal, navigate to the door so you can enter the hallway. You'd then start throwing pebbles again, but since you memoized (remember) the results of your last random pebble throwing, you could target your throwing to areas of less certainty. Iterating over this process, you might eventually find your bathroom. Hence, in this case, you're applying both the problem structuring (i.e. goal decomposition) of dynamic programming and the random sampling of Monte Carlo methods.

1.4 The Standard Model

We learned how Richard Bellman introduced dynamic programming as a general method of solving certain kinds of control or decision problems, but we also know that it occupies an extreme end of the reinforcement learning continuum. Arguably, Bellman's more important contribution was helping develop what we might call the "standard model" for reinforcement learning-type problems. The standard model is essentially the core set of terms and concepts that every reinforcement learning problem can be phrased in. This not only provides a standardized language in which to communicate to other engineers and researchers, it also

forces us to formulate our problems in a way that is amenable to dynamic programming-like problem decomposition, such that we can iteratively optimize over local sub-problems and yet still make progress toward achieving the global high-level objective. Fortunately, it's actually pretty simple too.

To concretely illustrate the standard model, let's consider the task of building a reinforcement learning algorithm that can learn to minimize the energy usage at a big data center. Computers need to be kept cool to function well, so large data centers can incur significant costs from cooling systems. The naïve approach to keeping a data center cool would be just to keep the air conditioning on all the time at some level that results in no servers ever running too hot. You could probably do better than this since it's unlikely that all servers in the center are running hot at the same times and that the data center usage is always at the same level, so if you could target the cooling to where and when it matters most, you could achieve the same result for less money.

Step one of the standard model is to define your overall objective. In this case our overall objective is minimize dollars spent on cooling with the constraint that no server in our center can surpass some threshold temperature. Although this appears to be two objectives, we can bundle these together into a new composite objective function. This will be a function that returns an error value that indicates how off-target we are at meeting the two objectives, given the current cost and the temperature data for the servers. The actual number that our objective function is not important, we just want to make it as low as possible. Hence, we need our reinforcement learning algorithm to minimize this objective (error) function with respect to some input data which will definitely include the running costs and temperature data, but may also include other useful contextual information that can help the algorithm predict the data center usage.

This input data is data that is generated by the environment, a term we've been loosely using so far. In general, the environment of a reinforcement learning (or control) task is whatever dynamic process produces data that is relevant to achieving our objective. Although we use it as a technical term, it's not too far abstracted from its everyday usage. As an instance of a very advanced reinforcement learning algorithm yourself, you are always in some environment and your eyes and ears are constantly consuming information produced by your environment so you can achieve your daily objectives. Since the environment is a dynamic process (i.e. a function of time), it may be producing a continuous stream of data at every instant of time of varied size and type. To make things algorithm-friendly, we need to take this environment-data and bundle it into discrete packets that we call the *state* (of the environment) and can deliver to our algorithm at each of its discrete time steps. The state reflects our knowledge of the environment at some particular time point; just like a digital camera captures a discrete snapshot of a scene at some time (and produces a consistently formatted PNG image or something).

To summarize so far, we defined an objective function (minimize costs and temperature) that is a function of the state (current costs, current temperature data) of the environment (our data center and any related processes). The last part of our model is the reinforcement

learning algorithm itself. This could be *any* algorithm that can learn from data to minimize or maximize some objective function. It does *not* need to be a deep learning algorithm; we want to make clear that reinforcement learning is a field of its own, separate from the concerns of any particular learning algorithm. We'll lay out our reasons for why this book almost exclusively uses deep learning as our learning algorithm in a few sections.

As we noted before, one of the key differences between reinforcement learning (or control tasks generally) and ordinary supervised learning is that in a control task the algorithm needs to make decisions and take actions. These actions will have a causal effect on what happens in the future. Taking an action is indeed another keyword in the standard model and is more or less what you expect it to mean. However, every decision made or action taken is the result of analyzing the current state of the environment and attempting to make the best decision based on that information. The last concept in the standard model is that after each action taken the algorithm is given a *reward*. The reward is a (local) signal of how well the learning algorithm is performing at achieving the global objective. The reward can be a positive signal (i.e. doing well, keep it up) or a negative signal (i.e. this is not working, try something else) even though we call both situations a reward.

The reward signal is the only cue the learning algorithm has to update itself in hopes of performing better at the next state of the environment. In the case of our data center example, we might grant the algorithm a reward of +10 (an arbitrary value) whenever its action reduces the error value. Or more reasonably, we grant a reward proportional to how much it decreases the error. If it increases the error, then we give it a negative reward. Lastly, we give a fancier name to our learning algorithm by calling it the *agent*. The agent is the action-taking or decision-making learning algorithm in any reinforcement learning problem. Finally, we can put this all together as seen in Figure 1.5.

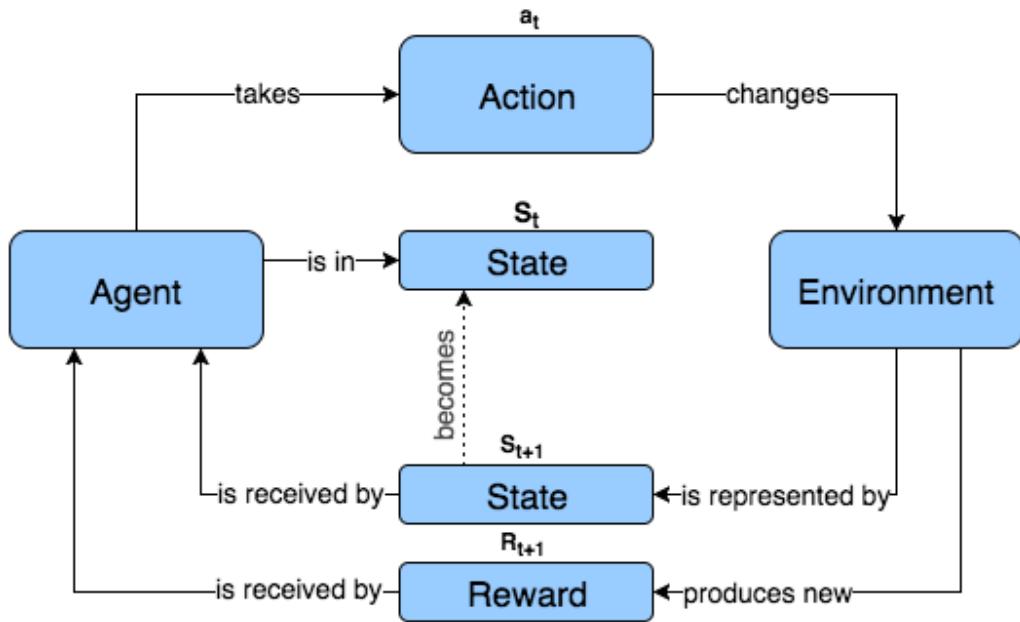


Figure 1.5: The standard model for reinforcement learning algorithms. RL algorithms involve an agent that learns the best way to interact in an environment. The agent takes an action in the environment - such as moving a chess piece - which then updates the state of the environment. For every action we take, we receive a reward (e.g. +1 for winning the game, -1 for losing the game, 0 otherwise). The RL algorithm repeats this process with the objective of maximizing rewards in the long term and eventually learns how the environment works.

In our data center example, we hope that our agent will learn how to decrease our cooling costs. Unless we're able to supply it with complete knowledge of the environment, it will have to employ some degree of trial and error. If we're lucky, the agent might learn so well that it can be used in different environments than the one it was originally trained in. Since the agent is the learner, it is implemented as some sort of learning algorithm. And since this is a book about *deep* reinforcement learning, our agents will be implemented using *deep learning* algorithms (also known as deep neural networks). But remember, reinforcement learning is more about the type of problem and solution than any particular learning algorithm, and one could certainly use alternatives to deep neural networks. In fact, in Chapter 3 we begin using a very simple non-neural network algorithm and then we'll replace it with a neural network by the end of the chapter.

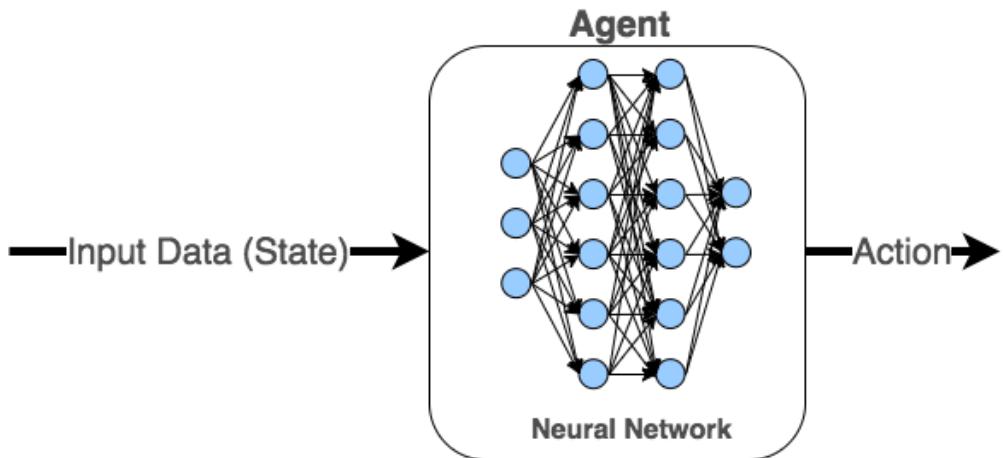


Figure 1.6: The input data (which is the state of the environment at some time point) is fed into the agent, which is implemented as a deep neural network in this book, which then evaluates that data to take an action. This process is a little more involved than shown here, but this captures the essence.

The agent's only objective is to maximize its expected rewards in the long term. The agent just repeats this cycle: process the state information, decide what action to take, see if you get a reward, observe the new state, take another action... and so on. And if we set all this up correctly, the agent will eventually learn to understand its environment and make reliably good decisions at every step. This general mechanism can be applied to autonomous vehicles, chatbots, robotics, automated stock trading, healthcare and much more. We'll be exploring some of these applications in the next section and throughout this book.

In this book, we spend most of the time learning how to structure problems into our standard model and how to implement sufficiently powerful learning algorithms (agents) to solve difficult problems. For our cases, you don't need to do construct environments, you'll just be plugging into existing environments (such as game engines or other APIs). For example, OpenAI has released a Python Gym library that provides us with a plethora of environments and an easy interface for our learning algorithm to interact with them (Figure 1.5). The code on the left shows just how simple it is to setup and use one of these environments, a 9x9 Go game in only 5 lines of code.

```
import gym
env = gym.make('Go9x9-v0')
env.reset()
env.step(action)
env.render()
```

	A	B	C	D	E	F	G	H	J
9		X	.	.	
8		X	
7		
6		
5		
4		
3		.	.	0	.	.	0	.	
2		
1		

Figure 1.7. The OpenAI python library comes with many environments and an easy interface for a learning algorithm to interact with them. With just a few lines of code we've loaded up a 9x9 Go board.

1.5 What can I do with Reinforcement Learning?

We began this chapter by exploring the history of artificial intelligence and how it leads us to believe that, although recent successes in supervised learning are important and useful, supervised learning is not going to get us to artificial general intelligence (AGI). We ultimately seek general purpose learning machines that can be applied to multiple problems with minimal to no supervision and whose repertoire of skills can be transferred across domains. Large data-rich companies can gainfully benefit from supervised approaches, but smaller companies and organizations may not have the resources to exploit the power of machine learning. General purpose learning algorithms would level the playing field for everyone.

Nonetheless, while general purpose learning machines would be more powerful than domain-specific and supervised machines, there are still reasons to consider using current reinforcement learning technology in practice. Reinforcement learning research and applications are still maturing but there have been many exciting developments in recent years. Google's DeepMind research group has showcased some impressive results and garnered international attention. The first was in 2013 with an algorithm that could play a spectrum of Atari games at superhuman levels. Previous attempts at creating agents to solve these games involved fine-tuning the underlying algorithms to understand the specific rules of the game, often called feature engineering. While these feature engineering approaches can work well for a particular game, they are unable to transfer any knowledge or skills to a new game or domain. DeepMind's Deep Q-Network (DQN) algorithm was robust enough to work on seven games without any game-specific tweaks. It had nothing more than the raw pixels from the screen and was merely told to maximize the score, yet the algorithm learned how to play beyond an expert human level.

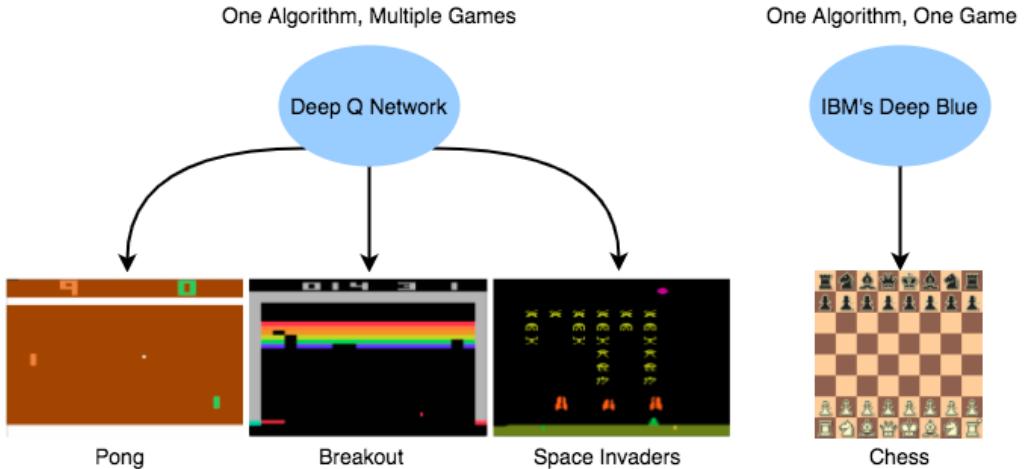


Figure 1.8: DeepMind’s DQN algorithm successfully learned how to play seven Atari games with only the raw pixels as input and the players score as the objective to maximize. Previous algorithms, such as IBM’s Deep Blue, needed to be fine-tuned to play a specific game.

Even more recently is DeepMind’s AlphaGo and AlphaZero algorithms, which beat the world’s best players at the ancient Chinese game Go. Experts believed artificial intelligence (AI) would not be able to play Go competitively for at least another decade. Players do not know the best move to make at any given turn and only receive feedback for their actions at the end of the game. Many high level players saw themselves as artists rather than calculating strategists and described winning moves as being beautiful or elegant. These are characteristics that algorithms typically don’t handle well. With over 10^{170} legal board positions, brute force algorithms (like what IBM’s Deep Blue used to beat Chess) were not feasible. AlphaGo managed this feat largely by playing simulated games of Go millions of times and learning which actions maximized the rewards of playing the game well. Similarly to the Atari case, AlphaGo only had access to the same information a human player would, where the pieces were on the board.

While algorithms that can play games better than humans are remarkable, the promise and potential of RL goes far beyond making better game bots. DeepMind was able to create a model to decrease Google’s data center cooling cost by 40%, something we explored earlier in this chapter as just an example. Autonomous vehicles use RL to learn which series of actions (accelerating, turning, breaking, signaling) leads to passengers reaching their destinations on time and how to avoid accidents. And researchers are training robots to complete tasks, such as learning to run, without needing to explicitly program complex motor skills.

Many of these examples are high-stakes, like driving a car. You of course cannot just let a learning machine learn how to drive a car by trial and error. Fortunately, there are an increasing number of successful examples of letting learning machines loose in some harmless

simulator and then once it has mastered the simulator, try it on real hardware in the real world. One instance of this that we will explore in this book is algorithmic trading. A substantial fraction of all stock trading is actually executed by computers with little to no input from human operators. Most of these algorithmic traders are wielded by huge hedge funds managing billions of dollars. In the last few years, however, we've seen more and more interest by individual traders in building trading algorithms. Indeed, Quantopian is a company that provides a platform where individual users can write trading algorithms in Python and test them in a safe, simulated environment. If their algorithms perform well, they can use them to trade real money. Many traders have achieved relative success with simple heuristics and rule-based algorithms, however, equity markets are dynamic and unpredictable, so a continuously learning reinforcement learning algorithm has the advantage of being able to adapt to changing market conditions in real-time.

One practical problem we tackle early on in this book is advertisement placement. Many web businesses derive significant revenue from advertisements, and the revenue from ads is often tied to the number of clicks those ads can garner. Hence there is a big incentive to place advertisements that maximize clicks. The only way to do this, however, is by utilizing knowledge about the users to place the most appropriate ads. Unfortunately, we generally don't know what characteristics of the user are related to the right ad choices. However, we can employ reinforcement learning techniques to make some headway. If we give an RL algorithm some potentially useful information about the user (what we would call the environment, or state of the environment) and just tell it to maximize ad clicks, then it will learn how to associate its input data to its objective, and will eventually learn which ads will produce the most clicks given a particular user.

1.6 Why Deep Reinforcement Learning?

Okay, so reinforcement learning sounds pretty interesting, but why *deep* reinforcement learning? RL has existed long before the popular rise of deep learning. In fact, some of the earliest methods (which we will introduce for learning purposes) involved nothing more than storing experiences in a lookup table (e.g. a Python dictionary) and updating that table on each iteration of the algorithm.

Game Play Lookup Table

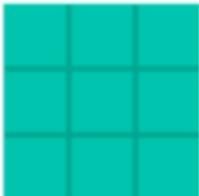
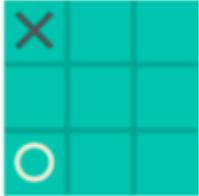
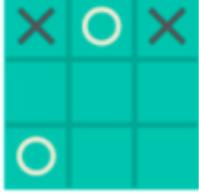
Key	Value
Current State	Action to Take
	Place X in Top Left
	Place X in Top Right
	Place X in Bottom Right

Figure 1.9: An action lookup table for Tic-Tac-Toe with only three entries where the player plays X. When the player is given a board position, the lookup table dictates the move that they should make next. There will be an entry for every possible state in the game.

The idea was to let the agent play around in the environment and just see what happens, but store its experiences of what happens in some sort of database. After awhile, you can look back on your database of knowledge and just observe what worked and what didn't. No neural networks or any other fancy algorithms. For very simple environments this actually works fairly well. For example, in Tic-Tac-Toe there are 255,168 valid board positions. The lookup table (also called a memory table) would have that many entries which mapped from each state to a specific action (Figure 1.5). During training, the algorithm can learn which move leads towards more favorable positions and update that entry in the memory table.

However, once the environment gets more complicated, using a memory table becomes intractable. For example, every screen configuration of a video game can be considered a different state. Imagine trying to store every possible combination of valid pixel values that

may present on screen in a video game! DeepMind's DQN algorithm that played Atari was fed four 84×84 grey-scaled images at each step, which would lead to 256^{28228} unique game states (256 different shades of grey per pixel, $4 \times 84 \times 84 = 28228$ pixels). This number is much larger than the number of atoms in the observable universe and would definitely not fit in computer memory. And this was after the images were scaled down to reduce their size from the original 210×160 pixel color images.

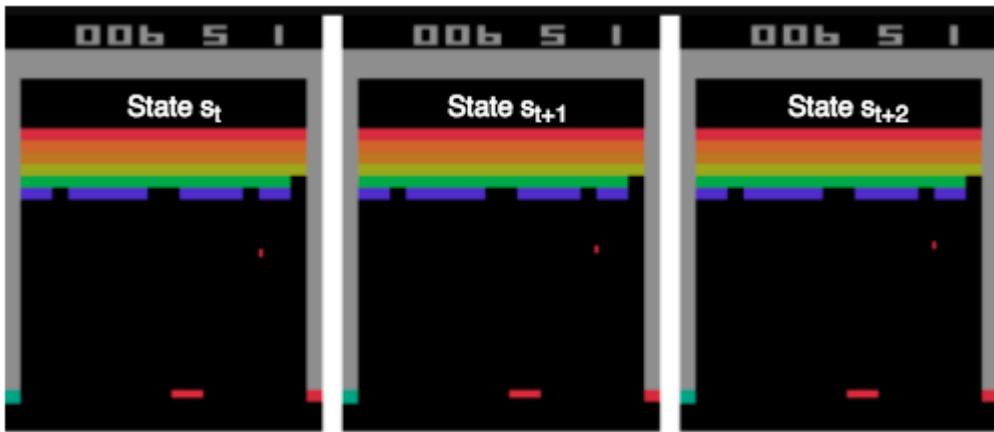


Figure 1.10. A series of three frames of breakout. The placement of the ball is slightly different in each frame. If using a lookup table, this would equate to storing three unique entries in the lookup table. A lookup table would be impractical as there are way too many game states to store.

If one pixel is changed, the game is considered to be in a different state and would require another entry in a lookup table. However, we could try to limit the possibilities. In the game Breakout you control a paddle at the bottom of the screen that can move right or left; the objective of the game is to deflect the ball and break as many blocks located on the top of the screen. In that case we could define constraints - only look at the states as the ball is returning back to the paddle since our actions are not important while we are waiting for the ball at the top of the screen - or provide our own features - instead of providing the raw image, just provide the position of the ball, paddle, and the remaining blocks. However, these methods require the programmer to understand the underlying strategies of the game and would not generalize to other environments.

That's where deep learning comes in. A deep learning algorithm can learn to abstract away the details of specific arrangements of pixels and learn the important features of a state. Since a deep learning algorithm only has a finite number of parameters, we can use it to compress any possible state into something we can efficiently process, and then use that new representation to make our decisions. By using neural networks, the Atari DQN only had 1792 parameters (convolutional neural network with 16 8×8 filters, 32 4×4 filters, 256 node fully

connected hidden layer) as opposed to the 256^{28228} key/values that would be needed to store the entire state space.

In the case of the Breakout game, a deep neural network might learn on its own to recognize the same high level features a programmer would have to hand engineer in a lookup table approach. That is, it might learn how to “see” the ball, the paddle, the blocks and recognize the direction of the ball. That’s pretty amazing given that it’s only being given raw pixel data. And even more interesting is that the learned high level features may be transferable to other games or environments.

Deep learning is the secret sauce that makes all the recent successes in reinforcement learning possible. No other class of algorithms has demonstrated the representational power, efficiency and flexibility as deep neural networks. Moreover, neural networks are actually fairly simple!

1.7 Why this book?

There are a number of resources available that cover reinforcement learning, why choose this book? The fundamental concepts of reinforcement learning have been well-established for decades, but the field is moving very fast, so teaching any particular new result is almost surely going to be short-lived. That’s why this book focuses on teaching skills not details with short half-lives. We do cover some recent advances in the field that will surely be supplanted in the not too distant future, however, we do so only to build new skills, not because the particular topic we’re covering is necessarily a time-tested technique. We’re confident that even if some of our examples become dated, the skills you learn will not and you’ll be prepared to tackle reinforcement learning problems for a long time to come.

Moreover, reinforcement learning is a huge field with a lot to learn. We can’t possibly hope to cover all of it in this book. Rather than be an exhaustive RL reference or comprehensive course, our goal is to teach you the foundations of RL with applications and sample a few of the most exciting recent developments in the field. We expect that you will be able to take what you’ve learned here and easily get up to speed on many other areas of RL that we left out. Plus, we have a section at the end that gives you a roadmap for what areas you might want to check out after finishing this book.

We also aim to write a book that is focused on teaching well, but also rigorously. Reinforcement learning and deep learning are both fundamentally mathematical. If you read any primary research articles in these fields, you will encounter potentially unfamiliar mathematical notation and equations. Mathematics allows us to make precise statements about what’s true, how things are related, and offers rigorous explanations for how and why things work. We could teach reinforcement learning without any math and just use Python, however, that approach would handicap you in understanding future advances.

So we think the math is important, but as our editor noted, there’s a common saying in the publishing world: “for every equation in the book, the readership is halved,” which probably has some truth to it. There’s an unavoidable cognitive overhead in deciphering complex math equations, unless you’re a professional mathematician who reads and writes math all day.

Faced with wanting to present a rigorous exposition of deep reinforcement learning to give our readers a top-rate understanding and yet wanting to reach as many people as possible, we came up with what we think is a very distinguishing feature of this book. As it turns out, even professional mathematicians are becoming tired of traditional math notation with its huge array of symbols, and so within a particular branch of advanced mathematics called category theory, mathematicians have developed a purely graphical language called *string diagrams*. String diagrams look very similar to flow-charts and circuit diagrams and have a fairly intuitive meaning, yet they are just as rigorous and precise as traditional mathematics notation largely based on Greek and Latin symbols.

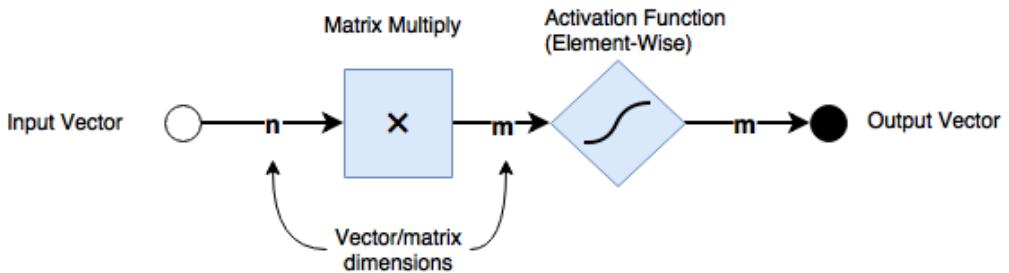


Figure 1.11: A string or flow diagram for a single layer neural network. Reading from left to right, this represents a function that accepts an input vector of dimension n , multiplies it by a matrix of dimensions $n \times m$, returning a vector of dimension m . Then a non-linear (activation) function is applied to each element in the vector and the resulting vector is returned from the function as the output.

Figure 1.11 shows a simple example of the type of diagrams we will frequently use throughout the book to communicate everything from complex mathematical equations to the architectures of deep neural networks. We will describe this graphical syntax in the next chapter and we'll continue to refine and build it up throughout the rest of the book. In some cases this graphical notation is overkill for what we're trying to explain, so we'll use a combination of clear prose and Python or pseudocode. We also include traditional math notation in most cases, so the bottom line is you will be able to learn the underlying mathematical concepts one way or another, whether diagrams, code or normal notation most connect with you.

1.8 What's next?

In the next chapter, we dive right into the real meat of reinforcement learning, covering many of the core concepts such as the tradeoff between exploration and exploitation, Markov Decision Processes, value functions, and policies (these words will make sense soon). But first, in the beginning of the next chapter we'll introduce some of the teaching methods we'll employ for the rest of the book. The rest of the book will cover core deep reinforcement learning algorithms that much of the latest research is built upon starting with Deep Q

Networks, followed by Policy Gradient approaches then to Model-Based algorithms. We will primarily be utilizing OpenAI's Gym (mentioned earlier) to train our algorithms to understand nonlinear dynamics, control robots (Figure 1.7) and play Go.

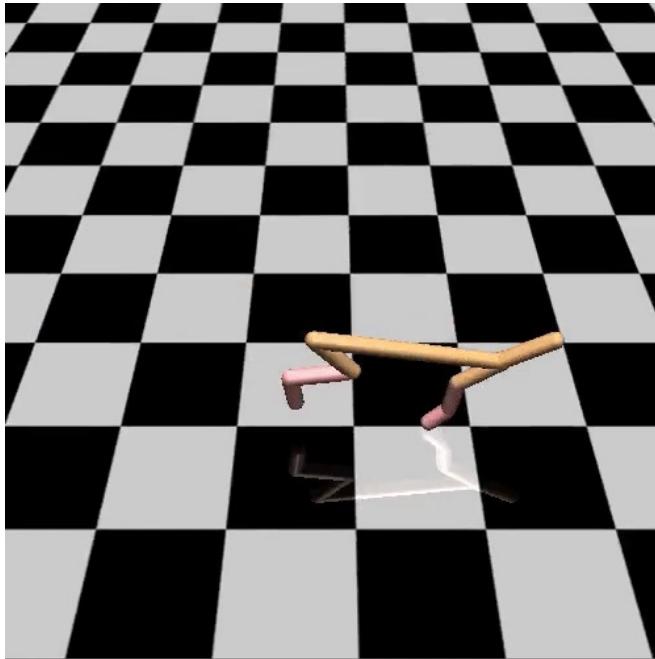


Figure 1.12. The Half-Cheetah Mujoco environment from the OpenAI Gym. We will be implement a Policy Gradient algorithm to solve them in Chapter 6.

In each chapter, we will open with a major problem or project that we will use to illustrate the important concepts and skills for that chapter. As each chapter progresses, we may add complexity or nuance to the starting problem to go deeper into some of the principles. For example, in chapter 2 we start with a problem of maximizing rewards at a casino slot machine and by solving that problem we cover much of foundational reinforcement learning. Later we add some complexity to that problem and change the setting from a casino to a business that needs to maximize advertisement clicks, which allows us to round out a few more of the core concepts.

Although this book is for those who already have experience with the basics of deep learning, we expect to not only teach you fun and useful reinforcement learning techniques but also to hone your deep learning skills. In order to solve some of the more challenging projects, we'll need to employ some of the latest advances in deep learning such as generative adversarial networks, evolutionary methods, meta-learning and transfer learning. Again, this

is all in line with our skills-focused mode of teaching, so the particulars of any of these advances is not what's important.

1.9 Summary

- Reinforcement learning is a subclass of machine learning algorithms that learn by maximizing rewards in some environment. These algorithms are useful when the problem involves making decisions or taking actions. Reinforcement learning algorithms can, in principle, employ any statistical learning model, however, it has become increasingly popular and effective to use deep neural networks.
- The agent is the core of any reinforcement learning problem. It is the part of the reinforcement learning algorithm that processes input information to take an action. In this book we are primarily focused on agents implemented as deep neural networks.
- The environment is the potentially dynamic conditions in which the agent operates. More generally, the environment is whatever process generates the input data for the agent. For example, we might have an agent flying a plane in a flight simulator, so the simulator is the environment.
- The state is a snapshot of the environment that an agent has access to and uses to make decisions. The environment is often a set of constantly changing conditions, however, we can sample from the environment and these samples at particular time points are the state information of the environment we give to the agent.
- An action is a decision made by an agent that produces a change in its environment. Moving a particular chess piece is an action and so is pressing the gas pedal in a car.
- A reward is a positive signal given to an agent by the environment after taking a "good" action. The rewards are the only learning signal the agent is given. The objective of a reinforcement learning algorithm (i.e. the agent) is to maximize rewards.
- The general pipeline for an RL algorithm is a loop in which the agent receives input data (the state of the environment), the agent evaluates that data and takes an action among a set of possible actions given its current state, the action changes the environment, the environment then sends a reward signal and new state information to the agent and the cycle repeats. When the agent is implemented as a deep neural network, then at each iteration we are evaluating a loss function based on the reward signal and backpropagating to improve the performance of the agent.

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2

Modeling Reinforcement Learning Problems: Markov Decision Processes

This chapter covers:

- String diagrams and our teaching methods
- The PyTorch deep learning framework
- Solving N-armed bandit problems
- Balancing exploration versus exploitation
- Modeling a problem as a Markov decision process (MDP)
- Implementing a neural network to solve an advertisement selection problem

2.1 String Diagrams and our teaching methods

This chapter covers some of the most fundamental concepts in all of reinforcement learning and will be the basis for the rest of the book. But before we get into that, we want to first go over some of the recurring teaching methods we'll employ in this book, most notably, the string diagrams we mentioned last chapter.

From our experience, when most people try to teach something complicated they tend to teach it in the reverse order in which the topic itself was developed. They'll give you a bunch of definitions, terms, descriptions and perhaps theorems and then they'll say, "great, now that we've covered all the theory, let's go over some practice problems." In our opinion, that's exactly the opposite order in which things should be presented. Most good ideas arise as solutions to real problems in the world, or at least imagined problems. The problem-solver

stumbles across a potential solution, tests it, improves it, and then eventually it gets formalized and possibly mathematized. All the terms and definitions come *after* the solution to the problem was thought of.

We think learning something is most motivating and effective when you take the place of that original idea-maker, who was thinking of how to solve a particular problem. Only once the intuition of the solution crystalizes does it warrant formalization, which is indeed necessary to establish its correctness and to faithfully communicate it to others in the field. There is a powerful urge to engage in this reverse chronological mode of teaching, but we will do our best to resist it and develop the topic as we go. In that spirit, we will introduce new terms, definitions, and mathematical notation as we need them. For example, we will use “callout” boxes like this:

DEFINITION (NEURAL NETWORK):

A neural network is a kind of machine learning model composed of multiple “layers” that perform a matrix-vector multiplication followed by the application of a non-linear “activation” function. The matrices of the neural network are the model’s learnable parameters and are often called “weights” of the neural network.

You will only see these callout boxes once per term, but we will often repeat the definition in different ways in the text to make sure you really understand it and remember it. This is a course on reinforcement learning, not a textbook or reference, so we won’t shy away from repeating ourselves when we think it’s something important to remember.

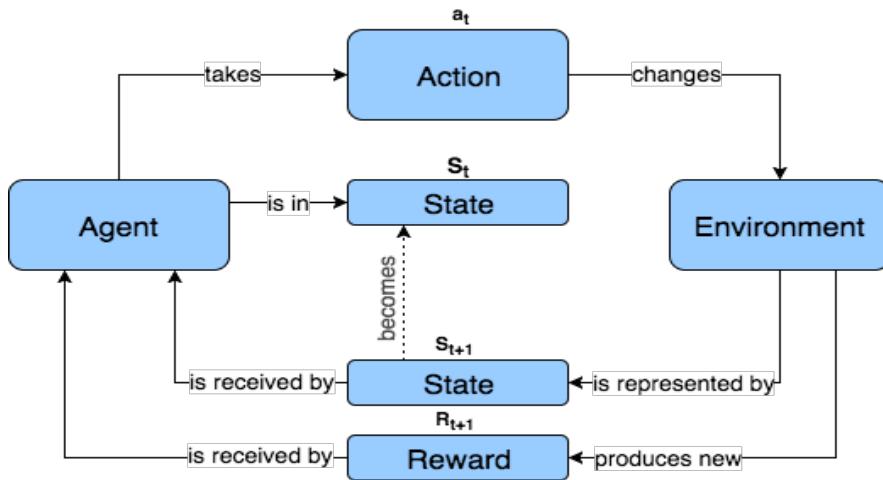
Whenever we need to introduce some math, we typically use a box showing the math and a pseudo-Python version of the same underlying concept. Sometimes it’s easier to think in terms of code or the math, and in any case, we think it’s good to get familiarized with both. As a super simple example, if we were introducing the equation of a line, we would do it like this:

Math	Pseudocode
$y=mx+b$	<pre>def line(x,m,b): return m*x + b</pre>

We also include plenty of inline code (short snippets) and code-listings (longer code examples) and the code for complete projects. All of the code in the book is provided in Jupyter Notebooks categorized by chapter on the book’s GitHub repository <<http://github.com/DeepReinforcementLearning/>>.

Since reinforcement learning involves a lot of interconnecting concepts that can become confusing when left just in words, we include a lot of diagrams and figures of varying sorts. The two more important kinds of figures we use are **string diagrams** and ologs (“oh-log”). They perhaps have odd names, but they’re both really simple ideas and are adapted from category theory, that branch of math we mentioned in the first chapter where they tend to use a lot of diagrams to supplement or replace traditional symbolic notation.

We've already come across an olog when we introduced the general framework for reinforcement learning in chapter 1:

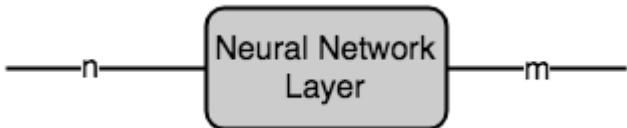


The idea is that the boxes contain nouns or noun-phrases while the arrows are labeled with verbs or verb-phrases. It's a small difference from typical flow-diagrams, but it makes it easy to translate the olog diagram into English prose and vice versa and also makes very clear what exactly the arrows are *doing* functionally.

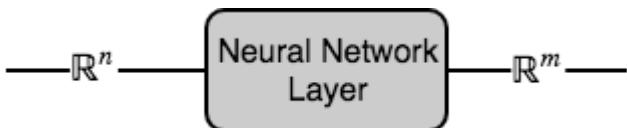
Lastly, string diagrams (sometimes referred to as wiring diagrams in other sources) are also a flow-like diagrams that represent the flow of typed data along strings (i.e. directed or undirected arrows) into processes (computations, functions, transformations, etc.) represented as boxes. The important difference between string diagrams and similar looking flow diagrams is that all data on the wires is explicitly typed (e.g. a numpy array with shape or simply a floating point number) and that they are fully compositional. By compositional, we mean that we can "zoom in" or out on the diagram in a principled way, to see the bigger more abstract picture or drill down to the computational details.

If we're showing a more high-level depiction, the process boxes may just be labelled with a word or short phrase indicating the kind of process that happens, but we can also show a zoomed-in view of that process box that reveals all its internal details, composed of its own set of sub-strings and sub-processes. The compositional nature of these diagrams also means that we can plug parts of diagrams into other diagrams, forming more complex diagrams, as long as all the strings' types are compatible.

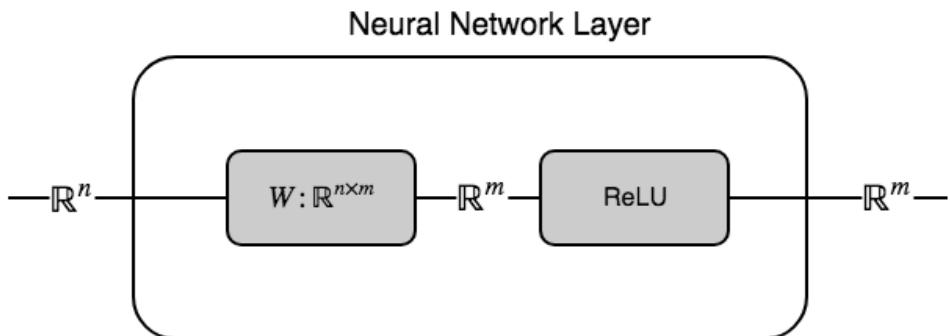
For example, here's a single layer of a neural network as a string diagram:



Reading from left to right, we see some data of type "n" flows into a process box called "Neural Network Layer" and produces an output of type "m." Since neural networks typically take vectors as inputs and produce vectors as outputs, these types refer to the dimensions of the input and output vectors, respectively. That is, this neural network layer accepts a vector of length or dimension n and produces a vector of dimension m . It's possible that $n=m$ for some neural network layers. This manner of "typing" the strings is simplified and we do it only when it's clear what the types mean from the context. In other cases, we may employ mathematical notation such as \mathbb{R} for the set of all real numbers, which in programming languages basically translates to floating point numbers. So for a vector of floating point numbers with dimension n we could type the strings like this:



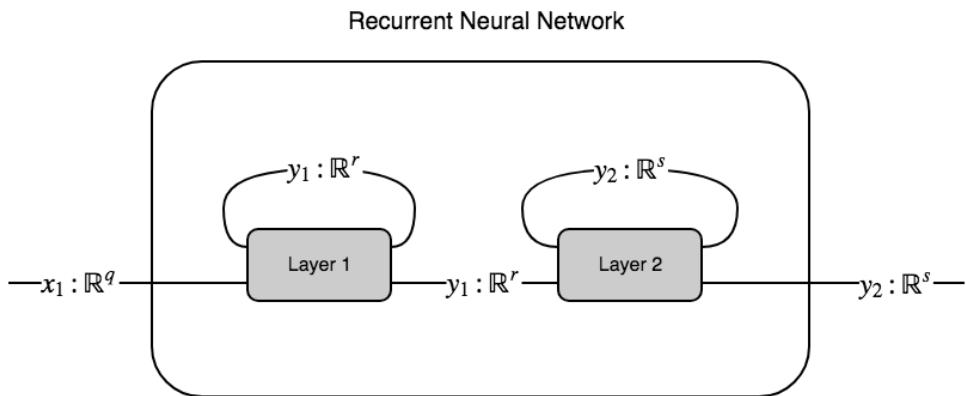
Now the typing is richer, we not only know the dimensions of the input and output vectors, we know that they're real/floating point numbers. While this is almost always the case, sometimes we may be dealing with integers or binary numbers. In any case, our process box "Neural Network Layer" is left as a black-box, we don't know exactly what's going on in there other than the fact that it transforms a vector into another vector of possibly different dimensions. We can decide to zoom-in on this process to see what specifically is happening:



Now we can see the inside of the original process box, and it is composed of its own set of sub-processes. We can see that our n -dimensional vector gets multiplied by a matrix of dimension $n \times m$, which produces an m -dimensional vector product. This vector then passes

through some process called “ReLU,” which you may recognize as the standard neural network activation function, the rectified linear unit. We could continue to zoom-in on the ReLU sub-sub-process if we wanted. Hence, anything that deserves the name string diagram must be able to be scrutinized at any level of abstraction and remain well-typed (meaning the types of data entering and exiting processes are compatible and make sense, e.g. a process that is supposed to produce sorted lists should not be hooked up to another process that expects integers) at any level.

As long as the strings are well-typed, then we can string together a bunch of processes into a complex system. This allows us to build components once and re-use them wherever they’re type matched. At a somewhat high level, we might depict a simple two-layer recurrent neural network (RNN) like this:



So this RNN takes in a q -vector and produces an s -vector. However, we can see the inside processes. There are two layers, each one looks identical in its function. They each take in a vector and produce a vector, except that the output vector gets copied and fed back into the layer process as part of the input, hence the recurrence.

String diagrams are a very general type of diagram; in addition to diagramming neural networks, we could use them to diagram how to bake a cake. A special kind of string diagram is a **computational graph**. A computational graph is a string diagram where all the processes represent concrete computations that a computer can perform, or that can be described in some programming language like Python. If you’ve ever visualized a computational graph in TensorFlow’s TensorBoard, then that’s what we mean.

2.2 Solving the Multi-Arm Bandit

Okay, we’re ready to get started with a real reinforcement learning problem and learn the relevant concepts and skills needed to solve this problem as we go. But before we get too fancy building AlphaGo, let’s first consider a simple problem (that is easily translated into a practical problem). Let’s say you’re at a casino and in a section with some slot machines. In

front of you are 10 slot machines in a row with a flashy sign that says "Play for free! Max payout is \$10!" Wow, not bad right! Intrigued, you ask one of the employees what's going on here, it seems too good to be true, and she says "It's really true, play as much as you want, it's free. Each slot machine is guaranteed to give you a reward between \$0 and \$10. Oh, by the way, keep this to yourself, but those 10 slot machines each have a different average payout, so try to figure out which one gives out the most rewards on average and you'll be making tons of cash!"

What kind of casino is this?! Who cares, let's just figure out how to make the most money! Oh by the way, here's a joke: What's another name for a slot machine? A one-armed bandit! Get it? It has one arm (a lever) and it generally steals your money! Huh, well I guess we could call our situation a 10-armed bandit problem, or an n -armed bandit problem more generally, where n is the number of slot machines. While this problem sounds pretty fanciful so far, later we'll see that these so-called n -armed bandit (or multi-armed bandit) problems do have some very practical applications.

Let me restate our problem more formally. We have n possible actions (here $n = 10$) where an action means pulling the arm/lever of a particular slot machine and at each play (k) of this game we can choose a single lever to pull. After taking an action a we will receive a reward R_k (reward at play k). Each lever has a unique probability distribution of payouts (rewards). For example, if we have 10 slot machines and play many games, slot machine #3 may give out an average reward of \$9 whereas slot machine #1 only gives out an average reward of \$4. Of course, since the reward at each play is probabilistic, it is possible that lever #1 will by chance give us a reward of \$9 on a single play. But if we play many games, we expect on average slot machine #1 is associated with a lower reward than #3.

In words, our strategy should be to play a few times, choosing different levers and observing our rewards for each action. Then we want to only choose the lever with the largest observed average reward. Thus we need a concept of expected reward for taking an action a based on our previous plays. We'll call this expected reward $Q_k(a)$ mathematically; you give the function an action (given we're at play k) and it returns the expected reward for taking that action. Formally,

Math	Pseudocode
$Q_k(a) = \frac{R_1 + R_2 + \dots + R_k}{k_a}$	<pre>def exp_reward(action, history): rewards_for_action = history[action] return sum(rewards_for_action) / len(rewards_for_action)</pre>

That is, the expected reward at play k for action a is the arithmetic mean of all the previous rewards we've received for taking action a . Thus our previous actions and observations influence our future actions, we might even say some of our previous actions reinforce our current and future actions. We'll come back to this later. The function $Q_k(a)$ is called a value function because it tells us the value of something. In particular, it is an actionvalue function

because it tells us the value of taking a particular action. Since we typically denote this function with the symbol Q , it also often called a Q function. We'll come back to value functions later and give a more sophisticated definition, but this will suffice for now.

That is, the expected reward at play for action a is the arithmetic mean of all the previous rewards we've received for taking action a . Thus our previous actions and observations influence our future actions, we might even say some of our previous actions *reinforce* our current and future actions. We'll come back to this later. The function Q is called a *value function* because it tells us the value of something. In particular, it is an *action value function* because it tells us the value of taking a particular action. Since we typically denote this function with the symbol Q , it also often called a Q function. We'll come back to value functions later and give a more sophisticated definition, but this will suffice for now.

EXPLORATION AND EXPLOITATION. When we first start playing, we need to play the game and observe the rewards we get for the various machines, we can call this strategy *exploration*, since we're just exploring the results of our actions essentially randomly. This is in contrast to a different strategy we could employ called *exploitation*, which means we use our current knowledge about which machine seems to produce the most rewards and just keep playing that machine. So our overall strategy needs to include some amount of exploitation (simply choosing the best lever based on what we know so far) and some amount of exploration (choosing random levers so we can learn more). The proper balance of exploitation and exploration will be important to maximizing our rewards.

So how can we come up with an algorithm to figure out which slot machine has the largest average payout? Well, the simplest algorithm would be to select action a for which this equation is true:

Math	Pseudocode
$a = \arg\max_a (Q_k(a))$ $\forall a \in A_k$	<pre>def get_best_action(actions, history): exp_rewards = [exp_reward(action, history) for action in actions] return argmax(exp_rewards)</pre>

Or as legitimate Python 3 code:

```
def get_best_action(actions):
    best_action = 0
    max_action_value = 0
    for i in range(len(actions)): #loop through all possible actions
        cur_action_value = get_action_value(actions[i]) #get the value of the current
        action
        if cur_action_value > max_action_value:
            best_action = i
            max_action_value = cur_action_value
    return best_action
```

This equation states that the expected reward for the current play k for taking action a is equal to the maximum average reward of all previous actions taken. In other words, we use our above reward function $Q_k(a)$ on all the possible actions and select the action that returns the maximum average reward. Since $Q_k(a)$ depends on a record of our previous actions and their associated rewards, this method will not evaluate actions that we haven't already explored. Thus we might have previously tried lever 1 and lever 3, and noticed that lever 3 gives us a higher reward, but with this method, we'll never think to try another lever, say #6, which, unbeknownst to us, actually gives out the highest average reward. This method of simply choosing the best lever that we know of so far is called a "greedy" method (or as we discussed, exploitation).

ϵ - GREEDY STRATEGY. Obviously, we need to have some exploration of other levers (slot machines) going on to discover the true best action. One simple modification to our above algorithm is to change it to an ϵ (epsilon)-greedy algorithm, such that, with a probability ϵ , we will choose an action a at random, and the rest of the time (probability $1-\epsilon$) we will choose the best lever based on what we currently know from past plays. So most of the time we play greedy, but sometimes we take some risks and choose a random lever and see what happens. This will of course influence our future greedy actions.

Let's see if we can solve this in code with Python.

```
import numpy as np
from scipy import stats
import random
import matplotlib.pyplot as plt

n = 10
arms = np.random.rand(n) #hidden probs associated with each arm
eps = 0.1
```

Per our casino example, we will be solving a 10-armed bandit problem, hence $n = 10$. We've also defined a numpy array of length n filled with random floats that can be understood as probabilities. The way we've chosen to implement our reward probability distributions for each arm/lever/slot machine is this: Each arm will have a probability, e.g. 0.7. The maximum reward is \$10. We will setup a `for` loop to 10 and at each step, it will add +1 to the reward if a random float is less than the arm's probability. Thus on the first loop, it makes up a random float (e.g. 0.4). 0.4 is less than 0.7, so `reward += 1`. On the next iteration, it makes up another random float (e.g. 0.6) which is also less than 0.7, thus `reward += 1`. This continues until we complete 10 iterations and then we return the final total reward, which could be anything between 0 and 10. With an arm probability of 0.7, the *average* reward of doing this to infinity would be 7, but on any single play, it could be more or less.

```
def reward(prob, n=10):
    reward = 0;
    for i in range(n):
        if random.random() < prob:
            reward += 1
```

```
    return reward
```

The next function we define is our greedy strategy of choosing the best arm so far. This function will accept a list of tuples that contains a history of actions and rewards.

```
[(1,8), (2,4), (1,7)]
```

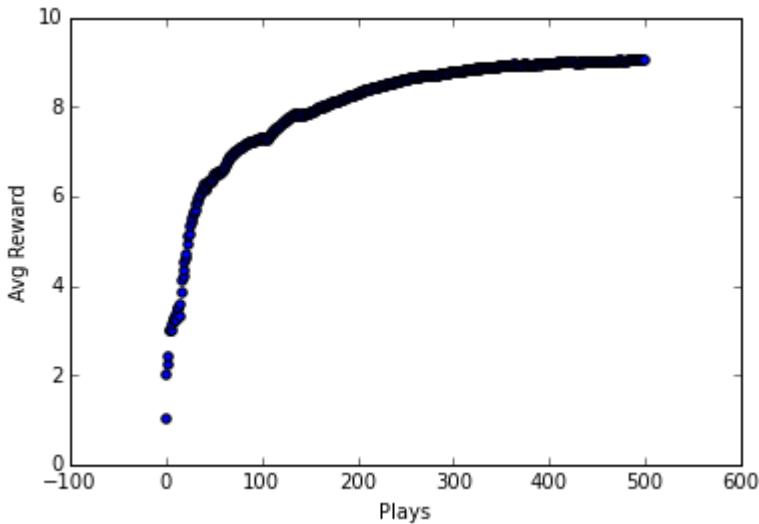
In the above example, there are 3 samples (we have pulled three arms). We first pulled arm 1 and received \$8. We then pulled arm 2 and received \$4. For our last action we decided to pull arm 1 again and we received \$7 this time.

Provided this experience array, we can now create a function that will determine the arm that has provided us the highest average return and thus should be pulled again. In the above case, arm 1 has provided us the highest average return $(8 + 7) / 2 = 7.5$.

```
def get_best_arm(pastRewards, actions):
    bestArm = 0 #just default to 0
    bestMean = 0
    for action in actions:
        avg = np.mean(pastRewards[np.where(pastRewards[:,0] == action)][:, 1])
        if avg > bestMean:
            bestMean = avg
            bestArm = action
    return bestArm
```

And here is the main loop for each play. If a random number is greater than epsilon parameter, then we just calculate the best action using the `get_best_arm` function and take that action, otherwise we take a random action. I've set it to play 500 times and display a matplotlib scatter plot of the mean reward against plays. Hopefully we'll see that the mean reward increases as we play more times.

```
plt.xlabel("Plays")
plt.ylabel("Avg Reward")
for i in range(500):
    if random.random() > eps:
        choice = get_best_arm(pastRewards, actions)
    else:
        choice = np.where(arms == np.random.choice(arms))[0][0]
    thisAV = np.array([[choice, reward(arms[choice])]])
    av = np.vstack((av, thisAV))
    percCorrect = 100*(len(av[np.where(av[:,0] == np.argmax(arms))])/len(av))
    runningMean = np.mean(av[:,1])
    plt.scatter(i, runningMean)
```



As you can see, the average reward does indeed improve after many plays. Our algorithm is *learning*, it is getting reinforced by previous good plays! And yet it is such a simple algorithm.

The problem we've considered here is a *stationary* problem because the underlying reward probability distributions for each arm do not change over time. We certainly could consider a variant of this problem where this is not true, a non-stationary problem. In this case, a simple modification would be to weight more recent action-value pairs greater than distant ones, thus if things change over time, we will be able to track them. Beyond this brief mention, we will not implement this slightly more complex variant here.

SOFTMAX SELECTION POLICY. Imagine another type of bandit problem: A newly minted doctor specializes in treating patients with heart attacks. She has 10 treatment options of which she can choose only one to treat each patient she sees. For some reason, all she knows is that these 10 treatments have different efficacies and risk-profiles for treating heart attacks, and she doesn't know which one is the best yet. We could still use our same ϵ -greedy algorithm from above, however, we might want to reconsider our ϵ policy of completely randomly choosing a treatment once in awhile. In this new problem, randomly choosing a treatment could result in patient death, not just losing some money. So we really want to make sure to not choose the worst treatment but still have some ability to explore our options to find the best one.

This is where a softmax selection might be the most appropriate. Instead of just choosing an action at random during exploration, softmax gives us a probability distribution across our options. The option with the largest probability would be equivalent to our best arm action from above, but then we have some idea about what are the 2nd and 3rd best actions for example. This way, we can randomly choose to explore other options while avoiding the very worst options. Here's the softmax equation:

Math

$$\Pr(A) = \frac{e^{Q_k(A)/\tau}}{\sum_{i=1}^n e^{Q_k(i)/\tau}}$$

Pseudocode

```
def softmax(vals, tau):
    softm = pow(e, vals / tau) / sum( pow(e,
    vals / tau))
    return softm
```

$\Pr(A)$ is a function that accepts an action-value vector (array) and returns a probability distribution over the actions, such that higher value actions have higher probabilities. For example, if your action-value array has 4 possible actions and they all currently have the same value, say $A = [10, 10, 10, 10]$, then $\Pr(A) = [0.25, 0.25, 0.25, 0.25]$, i.e. all the probabilities are the same and must sum to 1.

The numerator of the fraction just exponentiates the action-value array divided by a parameter τ , yielding a vector of the same size as the input. The denominator sums over the exponentiation of each individual action-value divided by τ , yielding a single number.

τ is a parameter called temperature the scales the probability distribution of actions. A high temperature will tend the probabilities to be very similar, whereas a low temperature will exaggerate differences in probabilities between actions. Selecting this parameter requires an educated guess and some trial and error.

When we implement the slot machine 10-armed bandit problem from above using softmax, we don't need our `get_best_arm` function anymore. Since softmax produces a weighted probability distribution across our possible actions, we will just randomly (but weighted) select actions according to their relative probabilities. That is, our best action will get chosen more often because it will have the highest softmax probability, but other actions will be chosen at lesser frequency.

To implement this, we need to create a new numpy array that stores the softmax probabilities of our actions. We'll initialize all the actions to have a uniform small probability of $1/n$ (since we have 10 actions, each action will be assigned a probability of 0.1). Hence, on our first play of the game, all the actions have an equal probability of being chosen, but from then onward the initial uniform probability distribution will become highly skewed toward actions that yielded the highest rewards.

```
n = 10
arms = np.random.rand(n)
av = np.ones(n)
counts = np.zeros(n)
av_softmax = np.zeros(n)
av_softmax[:] = 1.0/n
```

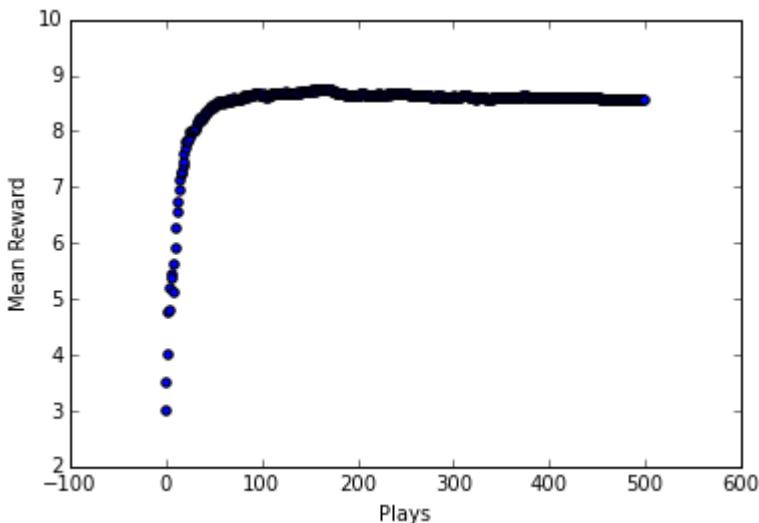
The mathematical exponential is a function call to `np.exp(...)` in numpy. It will apply the function element-wise across the input vector.

```
def softmax(av, tau=1.12):
    softm = ( np.exp(av / tau) / np.sum( np.exp(av / tau) ) )
```

```
    return softmax
```

Our main for loop is a bit different now. In order to choose an action randomly from our softmax probability distribution, we use numpy's `random.choice` function. `random.choice(arr, p=None)` accepts an array (e.g. `arr`) of values and another array of probabilities (e.g. `p`) for each of those values, then it will randomly select a value in `arr` using the probability distribution in `p`. We will give it `arr = arms`, so it will randomly select an index value corresponding to a particular action, given the probability distribution in `av_softmax`. The update rule we developed in the previous sections remains the same, but we need to recalculate the softmax probabilities stored in the `av_softmax` array after we have a new running mean value for the action we just took.

```
for i in range(500):
    choice = np.random.choice(arms, p=av_softmax)
    counts[choice] += 1
    k = counts[choice]
    rwd = reward(arms[choice])
    old_avg = av[choice]
    new_avg = old_avg + (1/k)*(rwd - old_avg)
    av[choice] = new_avg
    av_softmax = softmax(av)
```



Softmax action selection seems to do better than the epsilon-greedy method; it looks like it converges on an optimal policy faster. The downside to softmax is having to manually select the τ parameter. Softmax here was pretty sensitive to τ and it takes awhile of playing with it to find a good value for it. Obviously with epsilon-greedy we had the parameter `epsilon` to set, but choosing that parameter was much more intuitive.

2.3 Applying Bandits to Optimize Ad Placements

The slot machine example doesn't seem to be a particularly real-world problem, but if we just add in one additional element to it, then it does become a practical business problem, one big example being advertisement placement. Whenever you visit a website with ads, the company placing the ads would like to maximize the probability that you will click them.

Let's say we manage 10 e-commerce websites, each focuses on selling a different broad category of retail items such as computers, shoes, jewelry, etc. We would like to increase sales by referring customers who shop on one of our sites to another site that they might be interested in. When a customer checks out on a particular site in our network, we will display an advertisement to one of our other sites in hopes they'll go there and buy something too. Alternatively, we can also place an ad to another product on the same site. Our problem is that we don't know which sites we should refer users to. We could try placing random ads, but we suspect there's a more targeted approach.

CONTEXTUAL BANDITS. Perhaps you can see how this is just a new layer of complexity to the N-armed bandit problem we considered at the beginning. At each "play of the game" (each time a customer checks out on a particular website) we have $N = 10$ possible actions we can take, corresponding to the 10 different types of advertisements we could place. The twist is that the best ad to place may depend on which site in the network the current customer is on. For example, a customer checking out on our jewelry site may be more in the mood to buy a new pair of shoes to go with their new diamond necklace than they would be to buy a new laptop. Thus our problem is to figure out how a particular site relates to a particular advertisement.

This leads us to the introduction of state-spaces. The N-armed bandit problem we started with had an N-element action space (the space or set of all possible actions), but there was no concept of state. That is, there was no information we could use "in the environment" that would help us choose a good arm. The only way we could figure out which arms were good is by trial-and-error. In the ad problem, we know the user is buying something on a particular site, which may give us some information about that user's preferences that we could use to help guide our decision of which ad to place. We call this contextual information a state, and this new class of problems *contextual* bandits.

KEY POINT: A state in a game (or reinforcement learning problem more generally) is the set of information available in the environment that can be used to make decisions.

STATES, ACTIONS, REWARDS. Before we move on, let's consolidate some of the terms and concepts we've introduced so far. Reinforcement learning algorithms attempt to model the world in a way that computers can understand and calculate. In particular, RL algorithms model the world as if it merely involved a set of **states S** ("**state-space**"), which are a set of features about the environment, a set of **actions A** ("**action-space**") than can be taken in a

given state, and **rewards** r given for taking an action in a given state. When we speak of taking a particular action in a particular state, we often call it a **state-action pair** (s, a) .

KEY POINT: The objective of any RL algorithm is to maximize the rewards over the course of an entire episode.

Since our original N-armed bandit problem did not have a state space, only an action space, we just needed to learn the relationship between actions and rewards. We learned the relationship by using a lookup table to store our experience of receiving rewards with particular actions, i.e. we stored action-reward pairs (a_k, r_k) where the reward at play k was an average over all past plays associated with taking action a_k .

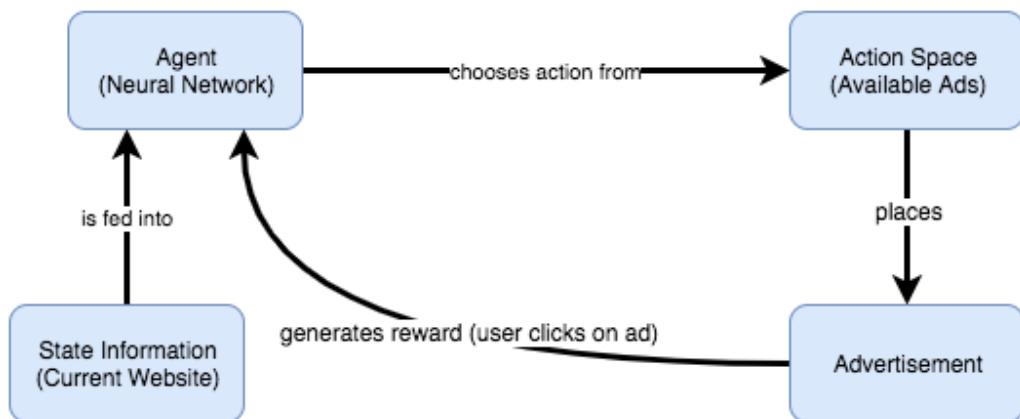


Figure 2.1: Overview of contextual bandit for advertisement placement. The agent (which is a neural network algorithm) receives state information, in this case, the current website the user is on, which it uses to decide which of several advertisements it should place at the checkout step. The users will click on the advertisement or not, resulting in reward signals that get relayed back to the agent for learning.

In our N-armed bandit problem, since we only had 10 actions, a lookup table of 10 rows was very reasonable. When we introduce a state space with contextual bandits, we now start to get a “combinatorial explosion” of possible state-action-reward tuples. For example, if we have a state space of 100 states, and each state is associated with the 10 actions, we now have 1000 different pieces of data we need to store and re-compute over. And in most of the problems we consider in this book, the state space is intractably large, thus a simple lookup table is just not feasible.

That’s where deep learning comes in. When properly trained, neural networks are great at learning abstractions that get rid of the details of little value. They can learn composable patterns and regularities in data such that they can effectively compress a large amount of data while retaining the important information. Hence, neural networks can be used to learn

complex relationships between state-action pairs and rewards without us having to store all such experiences as raw memories. We often call the part of an RL algorithm that makes the decisions based on some information the **agent**. In order to solve the contextual bandit we've been discussing, we'll employ a neural network as our agent. First though we will take a moment to introduce PyTorch, the deep learning framework we will be using to implement these networks.

2.4 Building Networks with PyTorch

There are many Deep Learning frameworks available today, with TensorFlow, MXNet and PyTorch probably being the most popular. We chose to use PyTorch for this book because of its simplicity, it allows you to write native-looking Python code and still get all the goodies of a good framework like automatic differentiation and built in optimization. We'll just give a quick up-front introduction to PyTorch here, but we'll explain more as we go along. If you need to brush up on basic Deep Learning, see the Appendix, we have a fairly detailed Deep Learning review section and more thorough coverage of PyTorch.

If you're comfortable with the NumPy multi-dimensional array, then you can almost just replace everything you do with numpy with PyTorch. For example, here we instantiate a 2x3 matrix in numpy:

```
>>> import numpy

>>> numpy.array([[1, 2, 3], [4, 5, 6]])
array([[1, 2, 3],
       [4, 5, 6]])
```

And here is how you instantiate the same matrix with PyTorch:

```
>>> import torch

>>> torch.Tensor([[1, 2, 3], [4, 5, 6]])
1 2 3
4 5 6
[torch.FloatTensor of size 2x3]
```

TENSORS. It's basically the same except in PyTorch we call multi-dimensional arrays **tensors**. Unsurprisingly, this is also the case for TensorFlow and other frameworks, so get used to seeing multi-dimensional arrays referred to as tensors. We can and do refer to the **tensor order**, which is basically how many indexed dimensions it has. This gets a little confusing because sometimes we speak of the dimension of a vector, in which case we just mean the length of the vector. But when we speak of the order of a tensor, we mean how many indices it has. A vector has one index, meaning every element can be "addressed" by a single index value, and hence is an order 1 tensor or 1-tensor for short. A matrix has two indices, one for each dimension, and is a 2-tensor. Higher order tensors may just be referred to as a k -tensor where k is the order, a non-negative integer. On the other end, a single number is actually a 0-tensor, or also called a **scalar**, since it has no indices.

AUTOMATIC DIFFERENTIATION. The most important features of PyTorch that we need and that NumPy doesn't offer is automatic differentiation and optimization. Let's say we want to setup a simple linear model to predict some data of interest, we can easily define the model using ordinary numpy-like syntax:

```
>>> x = torch.Tensor([2,4]) #input data
>>> m = torch.randn(2, requires_grad=True) #parameter 1
>>> b = torch.randn(1, requires_grad=True) #parameter 2
>>> y = m*x+b #linear model
>>> loss = (torch.sum(y_known - y))**2 #loss function
>>> loss.backward() #calculate gradients
>>> m.grad
tensor([ 0.7734, -90.4993])
```

You simply supply the `requires_grad=True` argument to PyTorch Tensors that you want to compute gradients for, and then call the `backward()` method on the last node in your computational graph, which will backpropagate gradients through all the nodes with `requires_grad=True`. You can then do gradient descent with the automatically computed gradients.

BUILDING MODELS. For most of this book, we'll be too lazy to even deal directly with automatically computed gradients. Instead we'll use PyTorch's `nn` module to easily setup a feedforward neural network model and then use the built in optimization algorithms to automatically train the neural network without every having to manually specify the mechanics of backpropagation and gradient descent. Here's a simple two layer neural network with an optimizer setup:

```
model = torch.nn.Sequential(
    torch.nn.Linear(10, 150),
    torch.nn.ReLU(),
    torch.nn.Linear(150, 4),
    torch.nn.ReLU(),
)
loss_fn = torch.nn.MSELoss()
optimizer = torch.optim.Adam(model.parameters(), lr=0.01)
```

We've setup a two-layer model with ReLU activation functions, defined a mean-squared error loss function, and setup an optimizer. All we have to do to train this model, given that we have some labeled training data, is start a training loop:

```
for step in range(100):
    y_pred = model(x)
    loss = loss_fn(y_pred, y_correct)
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()
```

The `x` variable is the input data to the model. The `y_correct` variable is a tensor representing the labeled, correct output. We make the prediction using the model, calculate the loss, and

then compute the gradients using the `backward()` method on the last node in the computational graph (which is almost always the loss function). Then we just run the `step()` method on the optimizer and it will run a single step of gradient descent. If we need to build more complex neural network architectures than the Sequential model, we can write our own Python class and inherit from PyTorch's module class, and then use that instead.

```
class MyNet(Module):
    def __init__(self):
        super(MyNet, self).__init__()
        self.fc1 = Linear(784, 50)
        self.fc2 = Linear(50, 10)

    def forward(self, x):
        x = F.relu(self.fc1(x))
        x = F.relu(self.fc2(x))
        return x

model = MyNet()
```

That's all you need to know about PyTorch for now to be productive with it.

2.5 Solving Contextual Bandits

We've built a simulated environment for a contextual bandit as we've described. The simulator includes the state (a number 0-9 representing 1 of the 10 websites in the network), reward generation (ad clicks), and a method to choose an action (which of 10 ads to serve). Below we demonstrate how to use the environment. The only part we need to build is the agent, which is generally the crux of any RL problem, since building an environment is usually just setting up input/output with some data source or plugging into an existing API.

```
from bandit_sim import *

env = ContextBandit(arms=10)
state = env.get_state()
reward = env.choose_arm(1)
print(state)
>>> 2
print(reward)
>>> 8
```

The simulator consists of a simple Python class called `ContextBandit` that can be initialized to a specific number of arms. For simplicity, the number of states equals the number of arms, but in general the state-space is often much larger than the action-space. The class has two methods, one is `get_state()` which is called with no arguments and will return a state sampled randomly from a uniform distribution. In most problems your state will come from a much more complex distribution. Calling `choose_arm(...)` will simulate placing an advertisement and returns a reward (e.g. proportional to the number of ad clicks). We need to always call `get_state` then `choose_arm`, in that order, to continually get new data to learn from. The `bandit_sim` module also includes a few helper functions such as the softmax

function and a one-hot encoder. Recall that a one-hot encoded vector is a vector where all but 1 element is set to 0. The only non-zero element is set to 1 and indicates a particular state in the state-space.

Rather than a single static reward probability distribution over N actions like our original bandit problem, the contextual bandit simulator sets up a different reward distribution over the actions for each state. That is, we will have N different softmax reward distributions over actions for each of N states. Hence we need to learn the relationship between the states and their respective reward distributions, then learn which action has the highest probability mass for a given state.

As with all of our projects in this book, we'll be using PyTorch to build the neural network. In this case, we're going to build a 2 layer feedforward neural network that uses rectified linear units (ReLU) as the activation function. The first layer accepts a 10-element one-hot (1-of-K) encoded vector of the state and the final layer returns a 10-element vector representing the predicted reward for each action given the state.

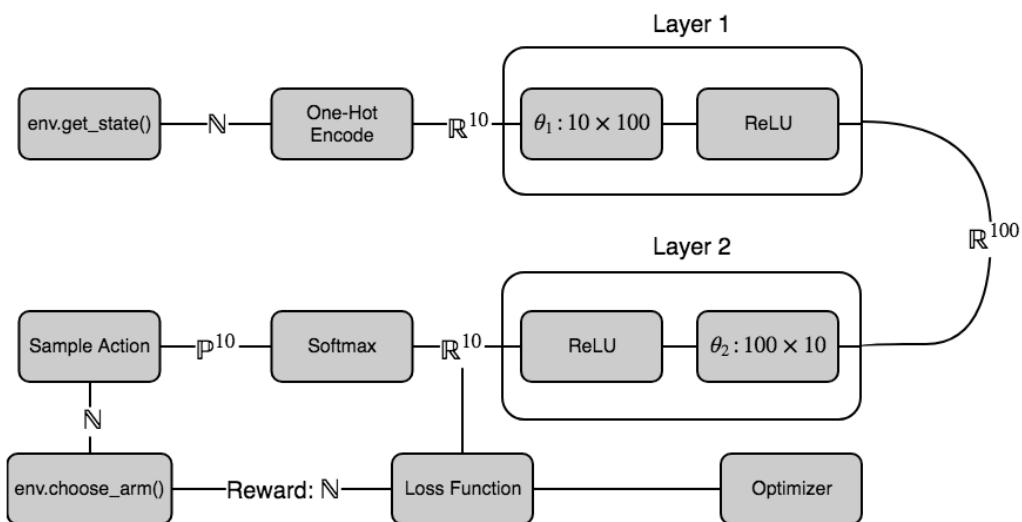


Figure 2.2: A computational graph for a simple 10-armed contextual bandit. The `get_state()` function returns a state value, which is transformed into a one-hot vector that becomes the input data for a 2 layer neural network. The output of the neural network is the predicted reward for each possible action, which is a dense vector that is run through a softmax to sample an action from the resulting probability distribution over the actions. The chosen action will return a reward and updates the state of the environment. θ_1 , θ_2 represent the weight parameters for each layer. The operation `mul` refers to matrix multiplication, which then gets passed to the activation function σ . Symbol reference: \mathbb{N} , \mathbb{R} , \mathbb{P} denote the natural numbers (i.e. 0, 1, 2, 3, ...), the real numbers (a floating point number, for our purposes), and a probability, respectively. The superscript indicates the length of the vector, so for example, P^{10} represents a 10-element vector where each element is a probability, such that all the elements sum to 1.

Figure 2.3 shows the forward pass of the algorithm as we've described. Unlike the lookup table approach, our neural network agent is going to learn to predict the rewards that each action will result in for a given state. Then we use the softmax function to give us a probability distribution over the actions and sample from this distribution to choose an arm. Choosing an arm will give us a reward, which we use to train our neural network.

For example, initially our neural network will produce a random vector such as [1.4, 50, 4.3, 0.31, 0.43, 11, 121, 90, 8.9, 1.1] when in state 0. We will run softmax over this vector and sample an action, most likely action 6 (from actions 0 - 9) since that is the biggest number in the vector. Choosing action 6 will generate a reward of say 8. So then we train our neural network to produce the vector [1.4, 50, 4.3, 0.31, 0.43, 11, 8, 90, 8.9, 1.1] since that is the true reward we received for action 6, leaving the rest of the values unchanged. So next time when the neural network sees state 0, it will produce a reward prediction for action 6 closer to 8. As we continually do this over many states and actions, the neural network will eventually learn to predict accurate rewards for each action given a state. Thus our algorithm will be able to choose the best action each time, maximizing our rewards.

```
import numpy as np
import torch as th
from torch.autograd import Variable
from bandit_sim import *

arms = 10
N, D_in, H, D_out = 1, arms, 100, arms
```

N is batch size, D_in is input dimension, H is hidden dimension and D_out is output dimension. Now we need to set up our neural network model. It is a simple sequential (feedforward) neural network with 2 layers as we described earlier.

```
model = th.nn.Sequential(
    th.nn.Linear(D_in, H),
    th.nn.ReLU(),
    th.nn.Linear(H, D_out),
    th.nn.ReLU(),
)
```

We'll use the mean squared error loss function here, but others will do.

```
loss_fn = th.nn.MSELoss(size_average=False)
```

Now we setup a new environment by instantiating the ContextBandit class, supplying the number of arms to its constructor. Remember, we've setup the environment such that the number of arms will be equal to the number of states.

```
env = ContextBandit(arms)
```

The main for-loop of the algorithm is very similar to our original N-armed bandit, however, we had the added step of needing to run a neural network and use the output to select an action. We'll define a function called train that accepts the environment instance we created above, the number of epochs we want to train for, and the learning rate. In the function we set a

PyTorch variable for the current state, which we need to one-hot encode using the `one_hot(...)` encoding function that we have omitted.

Once we enter the main training for-loop, we run our neural network model with the randomly initialized current state vector. It will return a vector that represents its guess for the values of each of the possible actions. At first, the model will output a bunch of random values since it is not trained. In any case, we run the softmax function over the model's output to generate a probability distribution over the actions and select an action using it. We select an action using the environment's `choose_arm(...)` function, which will return the reward generated for taking that action; it will also update the environment's current state. We turn the reward (which is a non-negative integer) into a one-hot vector that we use as our training data. So we run one step of backpropagation with this reward vector given the state we gave the model. Since we're using a neural network model as our action-value function, we no longer have any sort of action-value array storing "memories," everything is being encoded in the neural network's weight parameters.

Listing 2.1 The Main Training Loop

```
def train(env, epochs=5000, learning_rate=1e-2):
    cur_state = Variable(th.Tensor(one_hot(arms, env.get_state()))) #A
    optimizer = th.optim.Adam(model.parameters(), lr=learning_rate)
    for i in range(epochs):
        y_pred = model(cur_state) #B
        av_softmax = softmax(y_pred.data.numpy(), tau=2.0) #C
        av_softmax /= av_softmax.sum() #D
        choice = np.random.choice(arms, p=av_softmax) #E
        cur_reward = env.choose_arm(choice) #F
        one_hot_reward = y_pred.data.numpy().copy() #G
        one_hot_reward[choice] = cur_reward #H
        reward = Variable(th.Tensor(one_hot_reward))
        loss = loss_fn(y_pred, reward)

        optimizer.zero_grad()

        loss.backward()

        optimizer.step()
        cur_state = Variable(th.Tensor(one_hot(arms, env.get_state()))) #I
```

#A Get current state of the environment; convert to PyTorch Variable
#B Run neural net forward to get reward predictions
#C Convert reward predictions to probability distribution with softmax
#D Normalize distribution to make sure it sums to 1
#E Choose new action probabilistically
#F Take action, receive reward
#G Convert PyTorch tensor data to numpy array
#H Update one_hot_reward array to use as labeled training data
#I Update current environment state

When we train this network for 5000 epochs, we can plot the moving average of rewards earned over the training time (we omitted the code to produce such a graph). Our neural

network indeed learns a fairly good understanding of the relationship between states, actions and rewards for this contextual bandit. The maximum reward payout for any play is 10, and our average is topping off around 8.5, which is close to the mathematical optimum for this particular bandit. Our first deep reinforcement learning algorithm works! Okay... it's not a very deep network, but still!

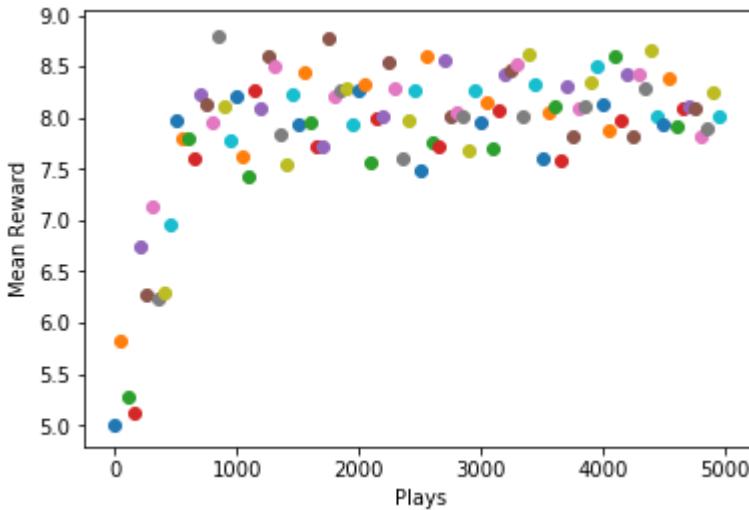


Figure 2.3: Training graph showing the average rewards for playing the contextual bandit simulator using a 2-layer neural network as the action-value function. We can see the average reward rapidly increases during training time, demonstrating our neural network is successfully learning.

2.6 The Markov Property

In our contextual bandit problem, our neural network led us to choose the best action given a state without reference to any other prior states. We just gave it the current state we're in and it produced the expected rewards for each possible action. This is an important property in reinforcement learning called the **Markov property**. A game (or any other control task) that exhibits the Markov property is said to be a **Markov Decision Process (MDP)**. With an MDP, the current state alone contains enough information to choose optimal actions to maximize future rewards. Modeling a control task as an MDP is a key concept in reinforcement learning.

The MDP model simplifies an RL problem dramatically as we do not need to take into account all previous states or actions, i.e. we don't need to have memory, we just need to analyze the present situation. Hence, we always attempt to model a problem as a (at least approximately) Markov decision processes. The card game Blackjack (also known as 21) is an MDP because we can play the game successfully by just knowing our current state (i.e. what cards we have and the dealer's one face-up card).

To test your understanding of the Markov property, consider each control problem/decision task in the list below and see if it has the Markov property or not:

- Driving a car
- Deciding whether to invest in a stock or not
- Choosing a medical treatment for a patient
- Diagnosing a patient's illness
- Predicting which team will win in a football game
- Choosing the shortest route (by distance) to some destination
- Aiming a gun to shoot a distant target

Okay, so let's see how you did, here are our answers and brief explanations:

- Driving a car can generally be considered to have the Markov property because you don't need to know what happened 10 minutes ago to be able to optimally drive your car. You just need to know where everything is right now and where you want to go.
- Deciding whether to invest in a stock or not does not meet the criteria of the Markov property since you would want to know the past performance of the stock in order to make a decision.
- Choosing a medical treatment seems to have the Markov property because you don't need to know the biography of a person to choose a good treatment for what ails them right now.
- In contrast, *diagnosing* (rather than treating) would definitely require knowledge of past states. It is often very important to know the historical course of a patient's symptoms in order to make a diagnosis.
- Predicting which football team will win does not have the Markov property since, like the stock example, you need to know the past performance of the football teams to make a good prediction.
- Choosing the shortest route to a destination has the Markov property because you just need to know the distance to the destination for various routes, which doesn't depend on what happened yesterday.
- Aiming a gun to shoot a distant target also has the Markov property since all you need to know is where the target is and perhaps current conditions like wind velocity and the particulars of your gun. You don't need to know the wind velocity of yesterday.

I hope you can appreciate that for some of those examples you could make arguments for or against it having the Markov property. For example, in diagnosing a patient, you may need to know the recent history of their symptoms but if that is documented in their medical record and we consider the full medical record as our current state, then we've effectively induced the Markov property. This is an important thing to keep in mind: many problems may not *naturally* have the Markov property, but often times we can induce it by jamming more information into the state.

DeepMind's deep Q-learning algorithm learned to play Atari games from just raw pixel data and the current score. Do Atari games have Markov property? Not exactly. Say the game is

Pacman, if our state is the raw pixel data from our current frame, we have no idea if that enemy a few tiles away is approaching us or moving away from us, and that would strongly influence our choice of actions to take. This is why DeepMind's implementation actually feeds in the last 4 frames of gameplay, effectively changing a non-Markov decision process into an MDP. With the last 4 frames, the agent has access to the direction and speed of all players.

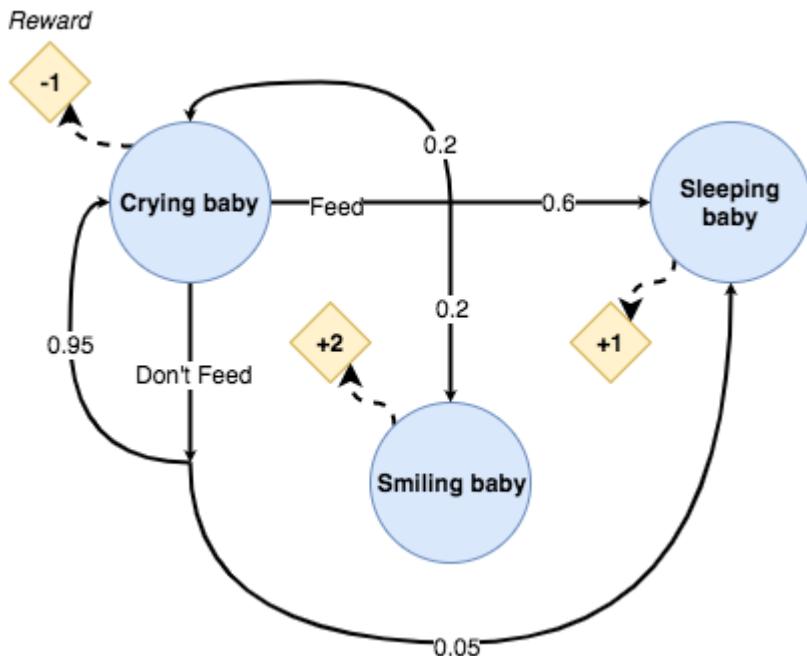


Figure 2.4: A simplified MDP diagram with 3 states and 2 actions. Here we model the parenting decision process for taking care of an infant. If the baby is crying, we can either administer food or not, and with some probability the baby will transition into a new state and receive a reward of -1, +1, or +2 (e.g. the baby's satisfaction).

Figure 2.2 gives a lighthearted example of a Markov decision process using all the concepts we've discussed so far. You can see there is a 3-element state space $S = \{\text{crying baby}, \text{sleeping baby}, \text{smiling baby}\}$, and a 2-element action space $A = \{\text{feed}, \text{don't feed}\}$. In addition, we have the transition probabilities noted, which are the maps from an action to the probability of an outcome state (we'll go over this again in the next section). Of course in real life, you as the “agent” have no idea what the transition probabilities are. If you did, then you would have a *model* of the environment. As we'll learn later, sometimes an agent does have access to a model of the environment, and sometimes not. In the cases where our agent does not have access to the model, we may want our agent to learn a model of the environment (which may just approximate the true, underlying model).

2.7 Predicting Future Rewards: Value and Policy Functions

Believe it or not, we actually smuggled in a lot of knowledge in the previous sections. The way we setup our solutions to the N-armed bandit and the contextual bandit are standard reinforcement learning methods, and as such, there is a whole bunch of established terminology and mathematics behind what we did. We introduced a few terms already such as state and action spaces, but we mostly just described things in natural language. In order to give you the ability to understand the latest RL research papers and make future chapters less verbose, it's important to become acquainted with the jargon and the mathematics.

So let's review and formalize what we've learned so far. A reinforcement learning algorithm essentially constructs an agent which acts in some environment. The environment is often a game, but is more generally whatever process produces states, actions and rewards. The agent has access to the current state of the environment, which is all the data about the environment at a particular time point, $s_t \in \mathcal{S}$. Using this state information, the agent takes an action $a_t \in \mathcal{A}$ which may deterministically or probabilistically change the environment to be in a new state s_{t+1} .

The probability associated with mapping a state to a new state by taking an action is called the **transition probability**. At the same time, the agent receives a reward r_t for having taken action a_t in state s_t leading to a new state s_{t+1} . And we know the ultimate goal of the agent (our reinforcement learning algorithm) is to maximize its rewards. It's really the state transition $s_t \rightarrow s_{t+1}$ that produces the reward, not the action per se, since the action may probabilistically lead to a bad state. If you're in an action movie (no pun intended) and you jump off a roof onto another roof, whether you land gracefully onto the other roof or miss it completely and fall to your peril is what's important (the two possible resulting states), not the fact that you jumped (the action).

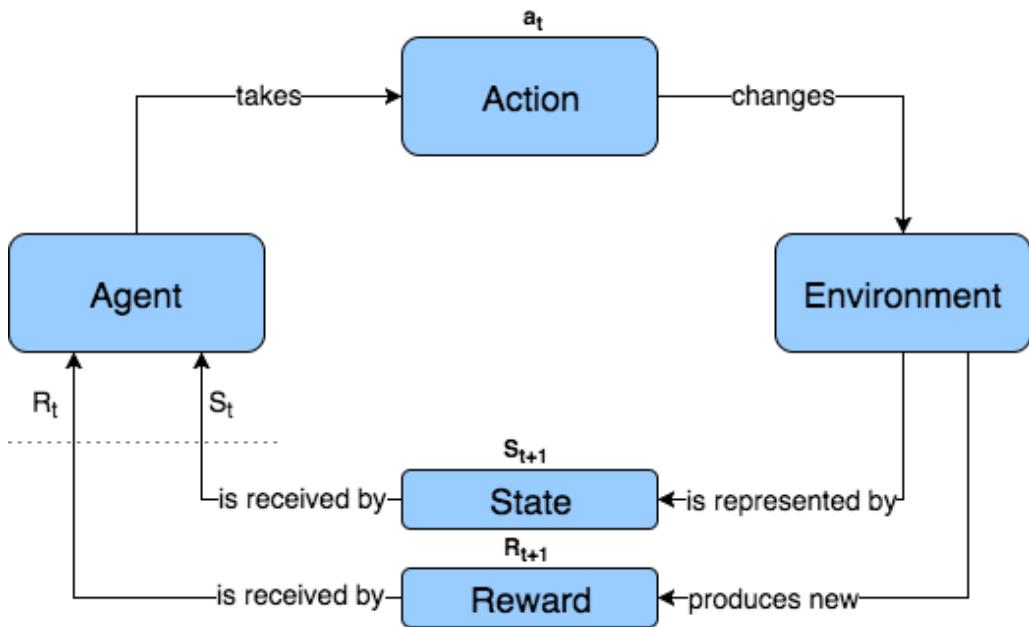


Figure 2.5: The general process of a reinforcement learning algorithm. The environment produces states and rewards. The agent takes an action a_t given a state s_t at time t and then receives a reward r_t . The agent's goal is to maximize rewards by learning to take the best actions in a given state.

POLICY FUNCTIONS. How exactly do we use our current state information to decide what action to take? This is where the key concepts of value functions and **policy functions** come into play, which we already have a bit of experience with. Let's first tackle policies. In words, a policy π is the “strategy” of an agent in some environment. For example, the strategy of the dealer in Blackjack is to always hit until she reaches a card value of 17 or greater.

Math

$$\pi: S \rightarrow \Pr(A / s), \text{ where } s \in S$$

English

A policy π is a mapping from states to the (probabilistically) best actions for those states.

Where s is a state and $\Pr(A | s)$ is a probability distribution over the set of actions A , given state s . The probability of each action in the distribution is the probability that that action will produce the greatest reward.

OPTIMAL POLICY The policy is the part of our reinforcement learning algorithm that chooses actions given its current state. We can then formulate the *optimal policy*. The optimal policy is the strategy that maximizes rewards.

Math	English
$\pi^* = \operatorname{argmax} E[R \pi]$	If we know the expected rewards for following any possible policy π , then optimal policy π^* is a policy that, when followed, produces the maximum possible rewards.

Remember, a particular policy is a map/function, so we have some sort of set of possible policies and the optimal policy is just an *argmax* (select the maximum) over this set of possible policies as a function of their expected rewards.

Again, the whole goal of a reinforcement learning algorithm (our agent) is to choose the actions that lead to the maximal expected rewards. But there are two ways we can train our agent to do this, directly or indirectly. That is, we can teach our agent to learn what actions are best directly given what state it is in, or we can teach it to learn which states are most valuable and then to take actions that lead to the most valuable states. This indirect method leads us to the idea of value functions.

VALUE FUNCTIONS are functions that map a state or a state-action pair to the **expected value** (i.e. expected reward) of being in some state or taking some action in some state. You may recall from statistics that the expected reward is just the long-term average of rewards received after being in some state or taking some action. When we speak of *the* value function, we usually mean a state-value function:

Math	English
$V_\pi: s \rightarrow E[R s, \pi]$	A value function V_π is a function that maps a state s to the expected rewards given that we start in state s and follow some policy π .

This is a function that accepts a state s and returns the expected reward of starting in that state and taking actions according to our policy π . It may not be immediately obvious why the value function depends on the policy. Consider that in our contextual bandit problem, if our policy was just to choose totally random actions (i.e. sample actions from a uniform distribution), then the value (expected reward) of a state would probably be pretty low since we're definitely not choosing the best possible actions. We want to use a policy that is not a uniform distribution over the actions, but is the probability distribution that would produce the maximum rewards when sampled.

With our first N-armed bandit problem we were already introduced to state-action value functions. These functions often go by the name **Q-function** or **Q-value**, which is where Deep Q-learning comes from since, as we'll see in the next chapter, deep learning algorithms can be used as Q-functions.

Math	English
$Q_{\pi} : (s, a) \rightarrow E[R a, s, \pi]$	Q_{π} is a function that maps a pair (s, a) of a state s and an action a to the expected reward of taking action a in state s given that we're using the policy (i.e. 'strategy') π

In fact, we sort of implemented a deep Q-network to solve our contextual bandit problem (except it was a pretty shallow neural network) since it was essentially acting as a Q-function. We trained it to produce accurate estimates of the expected reward of taking an action given a state. Our policy function was the softmax function over the output of the neural network.

2.8 Chapter Summary

We will be using the tools and terminology we developed in this chapter throughout the rest of the book so make sure you're comfortable with them before moving on.

- **State-spaces and Action-spaces:** State-spaces are the set of all possible states a system can be in. In Chess, this would be the set of all possible valid board configurations. An action is a function that maps a state s to a new state s' . An action may be stochastic such that it maps a state stochastically to a new state s' . There may be some probability distribution over the set of possible new states from which one is selected. The action-space is the set of all possible actions for a particular state.
- **Environment and Model:** The source of states, actions, and rewards. If we're building an RL algorithm to play a game, then the game is the environment. A model of an environment is an approximation of the state-space, action-space, and transition probabilities.
- **Reward and Expected Reward:** Rewards are signals produced by the environment that indicate the relative success of taking an action in a given state. Expected reward is a statistical concept that informally refers to the long-term average value of some random variable X (in our case, the reward), denoted $E[X]$. For example, in the N -armed bandit case, $E[R | a]$ ('the expected reward given action a ') is the long-term average reward of taking each of the N -actions. If we knew the probability distribution over the actions a then we could calculate the precise value the expected reward for a game of N plays as $E[R | a] = \sum_{i=1}^N a_i p_i r$ where N is the number of plays of the game, p_i refers to the probability of action a_i , and r refers to the maximum possible reward.
- **Agent:** An RL algorithm that learns to behave optimally in a given environment. Often implemented as a deep neural network. The goal of the agent is to maximize expected rewards, or equivalently, navigate to the highest value state.
- **Policy / Policy Function:** Informally, a particular strategy. Formally, a function that accepts a state and produces an action to take or produces a probability distribution over the action-space given the state. A common policy is the epsilon-greedy strategy

where with probability ϵ we take a random action in the action-space, and with probability $\epsilon-1$ we choose the best action we know of so far.

- **Value functions:** In general, any function that returns expected rewards given some relevant data. Without additional context, it typically refers to a state-value function, which is a function that accepts a state and returns the expected reward of starting in that state and acting according to some policy. The Q-value is the expected reward given a state-action pair, and the Q-function is a function that produces Q-values when given a state-action pair.
- **Markov Decision Process:** A decision-making process where it is possible to make the best decisions without reference to a history of prior states.

2.9 What's next?

We covered many of the foundational concepts in reinforcement learning just by using N-armed and contextual bandits as examples. We also got our feet wet with deep reinforcement learning in this chapter, but in the next chapter we will implement a full-blown Deep Q-network similar to the algorithm DeepMind used to play Atari games at superhuman levels. It will be a natural extension of what we've covered here.

3

Predicting the Best States and Actions: Deep Q-Networks

This chapter covers:

- Implementing the Q-function as a neural network
- Building a Deep Q-network using PyTorch to play Gridworld
- Counteracting “catastrophic forgetting” with experience replay
- Improving learning stability with target networks

3.1 The Q-function

In this chapter we start off where the deep reinforcement learning revolution began: DeepMind’s Deep Q-networks that learned to play Atari games. Although we won’t be using Atari games as our testbed quite yet, we will be building virtually the same system DeepMind did. We’ll be using a simple console-based game called Gridworld as our game environment. Gridworld is actually a family of similar games, but they all generally involve a grid board with a player (or agent), an objective tile (the “goal”), and possibly one or more special tiles that may be barriers or may grant negative or positive rewards. The player can move up, down, left or right and the point of the game is to get the player to the goal tile where the player will receive a positive reward. The player must not only reach the goal tile but must do so following the shortest path and may need to navigate through various obstacles.

We will be using a very simple Gridworld engine included in the GitHub repository for this book, which you can download at <<http://github.com/DeepReinforcementLearning/>> in the Chapter 3 folder.

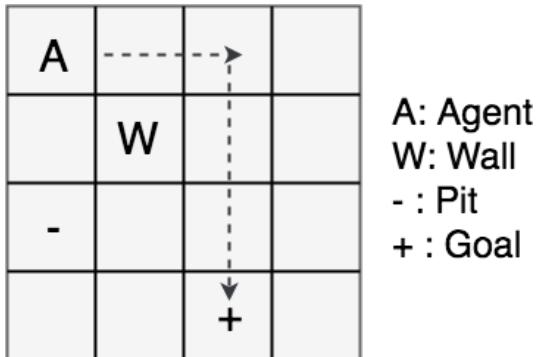


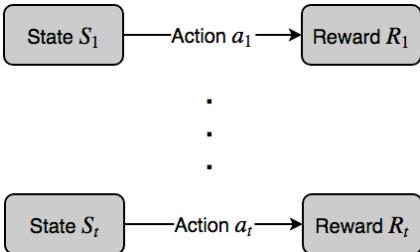
Figure 3.1: This is a simple Gridworld game setup. The agent (A) must navigate along the shortest path to the Goal (+) tile and avoid falling into the Pit (-).

The Gridworld game depicted in Figure 3.1 shows the simplest version of Gridworld we'll start with, and we'll progressively tackle more difficult variants of the game. Our goal is to train a deep RL agent to navigate the Gridworld board to the goal following the most efficient route every time. But before we get too far into that, let's review the key terms and concepts from the previous chapter that we will continue to use here.

The **state** is the information that our agent receives to make a decision on what action to take. It could be the raw pixels of a video game, sensor data from your autonomous vehicle, or, in the case of Gridworld, a tensor representing the position of all the objects on the grid.

The **policy**, denoted π , is the strategy our agent follows when provided a state. For example, a policy in blackjack might be to look at our hand (the state) and hit or stay randomly. Although this would be a terrible policy, the important point to stress is that the policy confers which actions we take. A better policy would be to always hit until we have 19.

The **reward** is the feedback our agent gets after taking an action, leading us to a new state. For a game of chess, we could reward our agent +1 when it performs the action that leads to a checkmate of the other player and -1 for an action that leads our agent to be checkmated. Every other state could be rewarded 0 since we do not know if the agent is winning or not.



Our agent makes a series of actions based upon its policy π and repeats this process until the episode ends. We call the weighted sum of the rewards while following a policy from the starting state S_1 the **value** of that state, or a state-value. We can denote this by the **value function** $V_\pi(s)$ that accepts an initial state and returns the expect total reward.

$$V_\pi(s) = \sum_{i=1}^t w_i R_i = w_1 R_1 + w_2 R_2 + \dots + w_t R_t$$

The coefficients w_1, w_2 , etc. are the weights we apply to the rewards before summing them. For example, we often want to weight more recent rewards greater than distant future rewards. This weighted sum is an expected value, a common statistic in many quantitative fields, and is often concisely denoted $E[R|\pi,s]$, read as “the expected rewards given a policy π and a starting state s ”. Similarly, there is an **action-value function** $Q_\pi(s, a)$ that accepts a state S and an action A and returns the value of taking that action given that state, or in other words $E[R + | \pi, s, a]$. Some RL algorithms or implementations will use one or the other. Importantly, if we base our algorithm on learning state-values (as opposed to action-values), we must keep in mind that the value of a state depends completely on our policy π . Using blackjack as an example, if we’re in the state of having a card total of 20, and have two possible actions, hit or stay, the value of this state is only high if our policy says to stay when we have 20. If our policy said to hit when we have 20, we would probably bust and lose the game, thus the value of that state would be low. In other words, the value of a state is equivalent to the value of the highest action taken in that state.

3.2 Navigating with Q-learning

In 2013, DeepMind published a paper entitled “Playing Atari with Deep Reinforcement Learning” that outlined their new approach to an old algorithm, which gave them enough performance to play 6 of 7 Atari 2600 games at record levels. Crucially, the algorithm they used only relied on analyzing the raw pixel data from the games just like a human. This paper really set off the field of deep reinforcement learning.

The old algorithm they modified is called Q-learning and it has been around for decades. Why did it take so long to make such significant progress? Well of course a large part is due to

the general boost that artificial neural networks (deep learning) got a few years prior with the use of GPUs that allowed training much larger networks. But a significant amount is due to the specific novel features DeepMind implemented to address some of the other issues that reinforcement learning algorithms struggled with. We'll be covering it all in this chapter.

WHAT IS Q-LEARNING. Okay so what is Q-learning, you ask? If you guessed it has something to do with the action-value function $Q_\pi(s, a)$ we previously described, you are right, but it's only a small part of the story. Many RL algorithms involve updating a value function (whether it's a state value or action-value) to achieve the objective, but not all such algorithms are Q-learning algorithms. Q-learning is a particular method to learn optimal action-values, but there are others. That is to say, value-functions and action-value functions are general concepts in RL that appear in many places, but Q-learning is a particular algorithm. Just like the goal of any investor is to make money, but there are many different kinds of investment strategies even though there are concepts common to all of them.

Believe it or not, we sort of implemented a Q-learning algorithm in the last chapter when we built a neural network to optimize the ad placement problem. The main idea of Q-learning is that your algorithm predicts the value of a state-action pair, and then you compare this prediction to the observed accumulated rewards at some later time point and then update the parameters of your algorithm so that next time it will make better predictions. That's essentially what we did last chapter when our neural network predicted the expected reward (value) of each action given a state, and then we would observe the actual reward we get and update our network accordingly. But that was a particular and simple implementation of a broader class of Q-learning algorithms that is described by the following update rule:

Math

$$Q(S_t, A_t) = Q(S_t, A_t) + \alpha [R_{t+1} + \gamma \max_a Q(S_{t+1}, a) - Q(S_t, A_t)]$$

Pseudocode

```
def get_updated_q_value(old_q_value, reward, state, step_size, discount):
    term2 = (reward + discount * max([Q(state, action) for action in actions]))
    term2 = term2 - old_q_value
    term2 = step_size * term2
    return (old_q_value + term2)
```

English

The Q-value at time t is updated to be the current predicted Q-value plus the amount of value we expect in the future given that we play optimally from our current state.

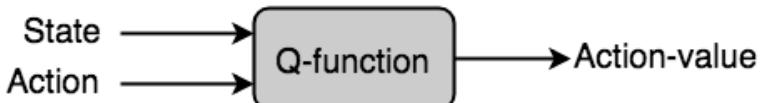
TACKLING GRIDWORLD.

Okay, so we've seen the formula for Q-learning. Let's take a step back and apply this formula to our Gridworld problem. Our goal in this chapter is to train a neural network to play a simple game, Gridworld, from scratch. All the agent will have access to is what the board looks like, the same as a human player would; the algorithm has no informational advantage. Moreover, we're starting with an un-trained algorithm, so it literally knows nothing at all about the world. It has no prior information about how games work or anything. The only thing we provided is the reward for reaching the goal. The fact that we will (trust us) be able to teach the algorithm to learn to play from nothing is actually quite impressive.

Unlike us humans who live in what appears to be a continuous flow of time, the algorithm lives in a discrete world, so something needs to happen at each discrete time step. First, at time step 1, the algorithm will "look" at the game board and make a decision about what action to take, then the game board will be updated, and so on.

Let's sketch out the details of this process now. Here's the sequence of events for a game of Gridworld.

1. We start the game in some state, we'll call it S_t . The state includes all the information about the game that we have. For our Gridworld example, the game state is represented as a 4x4x4 tensor. We will go into more detail about the specifics of the board when we implement the algorithm in a later section.
2. We feed the S_t data and a candidate action into a deep neural network (or some other fancy machine learning algorithm) and it produces a prediction of how valuable taking that action in that state is.



Remember, the algorithm is not predicting the reward we will get after taking a particular action, it's predicting the expected value or expected rewards, which is the long-term average reward we will get from taking an action in a state and then continuing to behave according to our policy π . We do this for a bunch (perhaps all) possible actions we could take in this state.

3. We decide to take an action, which we'll label A_t , e.g. because our neural network predicted it is the highest value action. After we take the action, we are now in a new state of the game, which we'll call S_{t+1} , and we receive or observe a reward, labelled R_{t+1} . Now we want to update our learning algorithm to reflect the actual reward we

received after taking the action it predicted was the best. Perhaps we got a negative reward or a really big reward, so we want to improve the accuracy of its predictions.

4. Next we run the algorithm using S_{t+1} as input and figure out which action our algorithm predicts has the highest value, we'll call this $\max_a Q(S_{t+1}, a)$. To be clear, this is a single value that reflects the highest predicted q-value given our new state and all possible actions.
5. Now we have all the pieces of our update term. We'll perform one iteration of training using some loss function, such as mean-squared error, to minimize the prediction error of our algorithm and the target prediction of $Q(S_t, A_t) + \alpha * [R_{t+1} + \gamma * \max_a Q(S_{t+1}, a) - Q(S_t, A_t)]$.

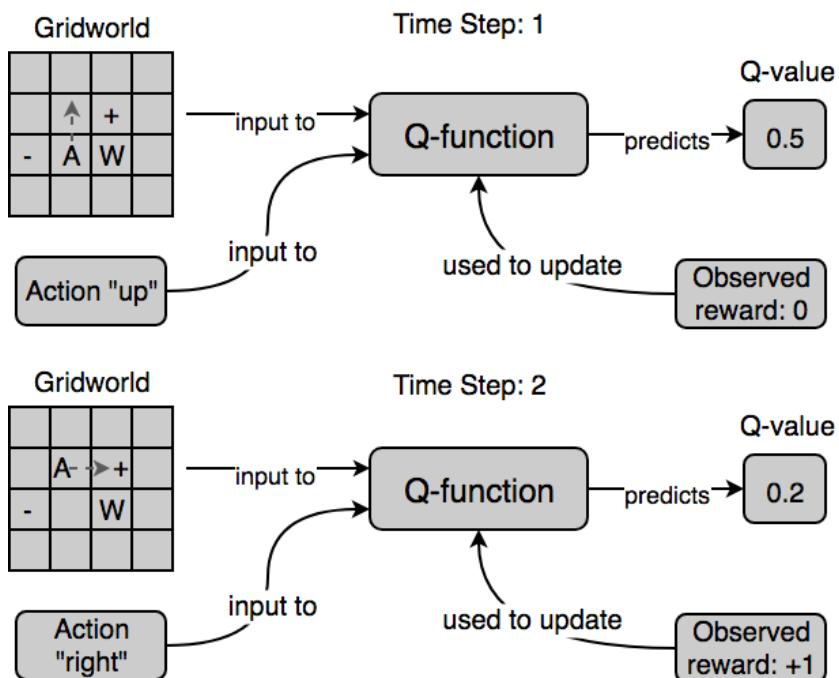


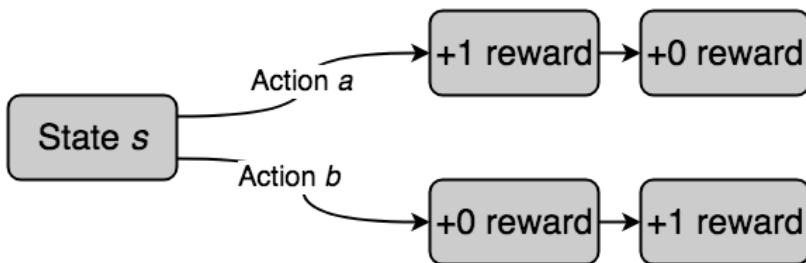
Figure 3.2: Schematic of Q-learning with Gridworld. The Q-function accepts a state and an action, and returns the predicted expected reward (i.e. value) of that state-action pair. After taking the action, we observe a reward, and using the update formula shown earlier, we use this observation to update the Q-function to make better predictions.

HYPERPARAMETERS.

The parameters α and γ are called hyperparameters since they're parameters that influence how the algorithm learns but are not involved in the actual learning. The parameter α is the **learning-rate** and is the same hyperparameter used to train many machine learning

algorithms. It controls how quickly we want the algorithm to learn from each move; a small value means it will only make small updates at each step whereas a large value means the algorithm will potentially make large updates.

DISCOUNT FACTOR. The parameter γ , the **discount factor**, is a variable between 0 and 1 and controls how much our agent discounts future rewards when making a decision. Let's take a simple example. Our agent has a decision between picking an action that leads to 0 reward then +1 reward or an action that leads to +1 and then 0 rewards.



Previously, we defined the value of a trajectory as the expected reward. Both trajectories provide +1 overall reward though, which sequence of actions should the algorithm prefer, or in other words, how can we break the tie? Well if the discount factor γ is less than 1, we will discount future rewards relative to recent rewards. In this simple case, even though both paths lead to a total of +1 rewards, action b gets the +1 reward later than action a , and since we will discount the future action, we prefer action a . In other words, we multiply the +1 reward observed with action b by a weighting factor less than 1, so we lower the reward from +1 to say only 0.8, hence now the decision is clear which action to take.

The discount factor comes up in real life as well as RL. Let's say that someone offers you \$100 now or \$110 one month from now. Most people would prefer to receive the money now because we discount the future to some degree, which makes sense since the future is someone uncertain (e.g. what if the person offering you the money dies in 2 weeks?).

In Q-learning, we face the same decision; how much do we consider future observed rewards when learning to predict Q-values? Unfortunately, there's no definitive answer to this, or to setting pretty much any of the hyperparameters we have control over. We just have to play around with these knobs and see what works best empirically.

It's worth pointing out that most games are *episodic*, meaning that there's multiple chances to take actions before the game is over, and many games like Chess don't naturally assign points to anything other than winning or losing the game. Hence the reward signal in these games is sparse, making it difficult for trial-and-error based learning to reliably learn anything, which would require seeing a reward fairly frequently. In Gridworld, we've designed the game so that any move that doesn't win the game receives a reward of 0, the winning move gets a reward of +1, and the losing move rewards -1. So it's really only the final move of the game where the algorithm can say "aha! Now I get it!" Since each episode of a

Gridworld game can be won in a fairly small number of moves, the sparse reward problem isn't too bad, but in other games it is such a significant problem that even the most advanced reinforcement learning algorithms have yet to reach human level performance. While beyond the scope of this book, one proposed method of dealing with this is to stop merely relying on the objective of maximizing expected rewards and instead instruct the algorithm to seek novelty and by doing so it will learn about its environment.

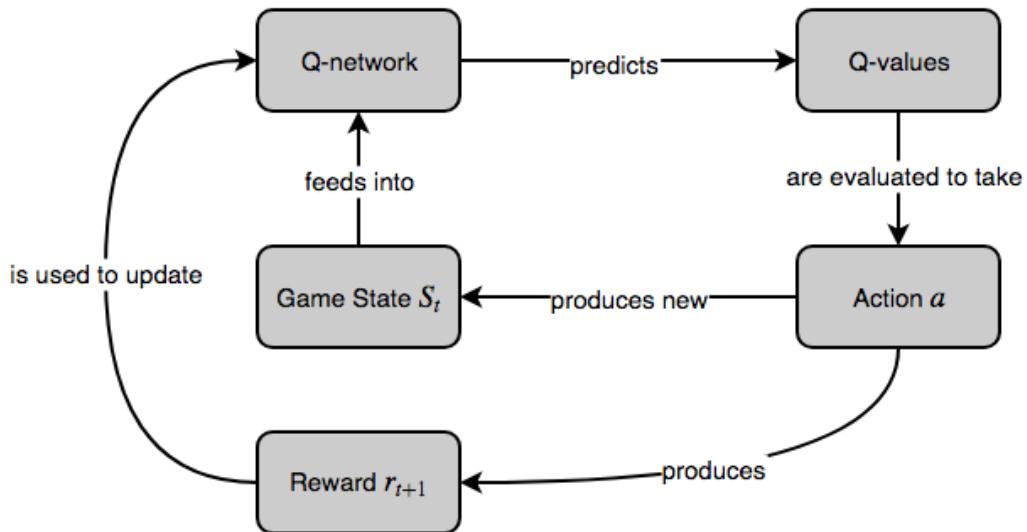


Figure 3.3: The general overview of Q-learning. We start in a game state S_t , which the Q-network (i.e. a neural network acting as a Q-function) uses to predict Q-values for the 4 available actions in Gridworld. The Q-values are used to select an action (e.g. we might just select the action associated with the highest predicted Q-value), which then results in a new game state S_{t+1} and a reward signal r_{t+1} . The reward is used to update the Q-network but minimizing the loss between the predicted Q-values and the observed reward.

BUILDING THE NETWORK Let's dig into how we will build our deep learning algorithm for this game. Recall that a neural network has a particular kind of architecture or network topology. When you build a neural network, you have to decide how many layers it should have, how many parameters each layer (i.e. the "width" of the layer) has, and how the layers are connected. Gridworld is simple enough that we don't need to build anything fancy. We can get away with a fairly straightforward feedforward neural network with only a few layers, using the typical rectified linear activation unit (ReLU).

The only parts that require some more careful thought are how we will represent our input data and how we will represent the output layer. We'll cover the output layer first. In our discussion of Q-learning, we said that the Q-function is a function that takes some state and some action and computes the value of that state-action pair, i.e. $Q(s, a)$. This is how the Q-function was originally defined. As we noted in the previous chapter, there is also just a state-

value function usually denoted $V_\pi(s)$ that computes the value of some state given you're following a particular policy π .

Generally, we want to use the Q-function because it can tell us the value of taking an action in some state, and therefore we can take the action that has the highest predicted value. But it would be rather wasteful if we separately computed the Q-values for every possible action given the state, even though the Q-function was originally defined that way. A much more efficient procedure, and the one that DeepMind employed in its implementation of Deep Q-Learning, is to instead recast the Q-function as a vector-valued function, meaning that instead of computing and returning a single Q-value for a single state-action pair, it will compute the Q-values for all actions given some state and return the vector of all those Q-values. So now we might represent this new version of the Q-function, $Q_A(s)$, where the subscript A denotes the set of all possible actions.

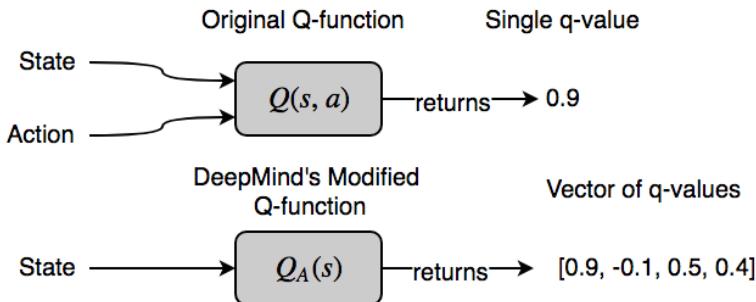


Figure 3.4: The original Q-function accepts a state-action pair and returns the value of that state-action pair, i.e. a single number. DeepMind used a modified vector-valued Q-function that accepts a state and returns a vector of state-action values, one for each possible action given the input state. The vector-valued Q-function is more efficient since you only need to compute the function once for all the actions.

Now it's quite easy to employ a neural network as our version of the Q-function; the last layer will simply produce an output vector of Q-values, one for each possible action. In the case of Gridworld there are only 4 possible actions ("up", "down", "left", "right") so the output layer will produce 4-dimensional vectors. We can then directly use the output of the neural network to decide what action to take using a simple -greedy approach or softmax. Just like DeepMind, we'll use the -greedy approach, and instead of using a static value like we did in the last chapter, we will initialize it to a large value (i.e. 1, so completely random selection of actions to start) and slowly decrement it so that after a certain number of iterations, the value will rest at some small value. In this way, we will allow the algorithm to explore and learn a lot in the beginning but then it will settle into maximizing rewards by exploiting what it has learned. Hopefully we set the decrementing process so that it will not under-explore or over-explore, but that will have to be tested empirically.

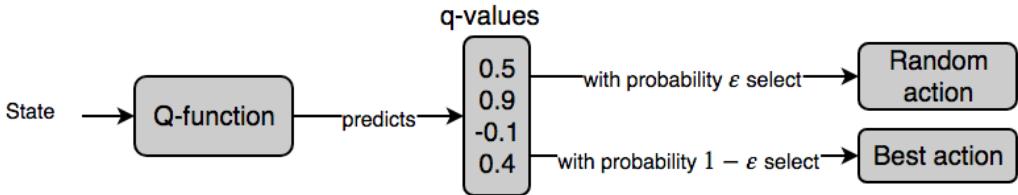


Figure 3.5: In an epsilon-greedy action selection method, we set a parameter ϵ to some value, e.g. 0.1, and with probability $\epsilon = 0.1$ we will randomly select an action (completely ignoring the predicted q-values) or with probability $1 - \epsilon = 0.9$, we select the action associated with the highest predicted q-value (the best known action). An additional helpful technique is to start with a high ϵ value, e.g. 1 and then slowly decrement it over the training iterations.

Okay, we have the output layer figured out, now to tackle the rest. In this book, we construct a network of just three layers with widths of 164 (input layer), 150 (hidden layer), 4 (output layer). You are welcome and encouraged to add more hidden layers and/or play with the size of the hidden layer as you will likely be able to achieve better results with a deeper network. We chose to implement a fairly shallow network here so that you can train the model with just your CPU (it takes our MacBook Air 1.7 GHz Intel Core i7 8GB RAM only a few minutes to train). We already discussed why the output layer is of width 4, but we haven't talked about the input layer yet. We need to first introduce the Gridworld game engine we will be using. We specifically developed a Gridworld game for this book and it is included in the GitHub repository for this chapter < <http://github.com/DeepReinforcementLearning/> >.

INTRODUCING THE GRIDWORLD GAME ENGINE. In the GitHub repository, you'll find a single file, `Gridworld.py`. Just copy and paste this file into whatever folder you'll be working out of. You can include it in your Python session by just running `from Gridworld import *`. The `Gridworld` module contains some classes and helper functions to run a Gridworld game instance. To create a Gridworld game instance, run:

Listing 3.1 Creating a Gridworld Game

```
from Gridworld import *
game = Gridworld(size=4, mode='static')
```

The Gridworld board is always square, so the size refers to one side dimension, i.e. in this case a 4x4 grid will be created. There are three ways to initialize the board. The first is to initialize it statically, so that the objects on the board are initialized at the same pre-determined locations. Second, you can set `mode='player'` so that just the player is initialized at a random position on the board. Lastly, you can also initialize so that all the objects are placed randomly (which is harder to learn for the algorithm) using `mode='random'`. We'll use all 3 eventually.

Now that we've created the game, let's play it. You call the `display` method to display the board, and the `makeMove` method to make a move. Moves are encoded with a single letter 'u'

for 'up', 'l' for 'left' and so on. After each move, you should display the board to see the effect. Additionally, after each move, you'll want to observe the reward/outcome of the move by calling the `reward` method. In Gridworld, every non-winning move receives a 0 reward. The winning move (reaching the goal) receives a +1 reward, or a -1 reward for the losing move (landing on the pit).

```
>>> game.display()
array([[ '+', '-', ' ', 'P'],
       [' ', 'W', ' ', ' '],
       [' ', ' ', ' ', ' '],
       [' ', ' ', ' ', ' ']], dtype='<U2')

>>> game.makeMove('d')
>>> game.makeMove('d')
>>> game.makeMove('l')
>>> game.display()
array([[ '+', '-', ' ', ' '],
       [' ', 'W', ' ', ' '],
       [' ', ' ', 'P', ' '],
       [' ', ' ', ' ', ' ']], dtype='<U2')
>>> game.reward()
0
```

Now let's take a look at how the game state is actually represented since we will need to feed this into our neural network. Run:

```
>>> game.board.render_np()
array([[[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 1, 0],
       [0, 0, 0, 0]],

      [[1, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]],

      [[0, 1, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]],

      [[0, 0, 0, 0],
       [0, 1, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0]]], dtype=uint8)>>> game.board.render_np().shape
(4, 4, 4)
```

Each matrix is a 4x4 grid of zeros and a single 1 indicates the position of a particular object. Each matrix encodes the position of one of the 4 objects: the player, the goal, the pit and the wall. If you compare the result from `display` with the game state, you can see that the first matrix encodes the position of the player, the second matrix encodes position

of the goal, the third matrix encodes the position of the pit, and the last matrix encodes the position of the wall.

In other words, the 1st dimension of this 3-tensor is divided into 4 separate grid planes, where each plane represents the position of each element. So below is an example where the player is at grid position (2,2), the goal is at (0,0), the pit is at (0,1) and the wall is at (1,1) where (row, column). All other elements are 0s.

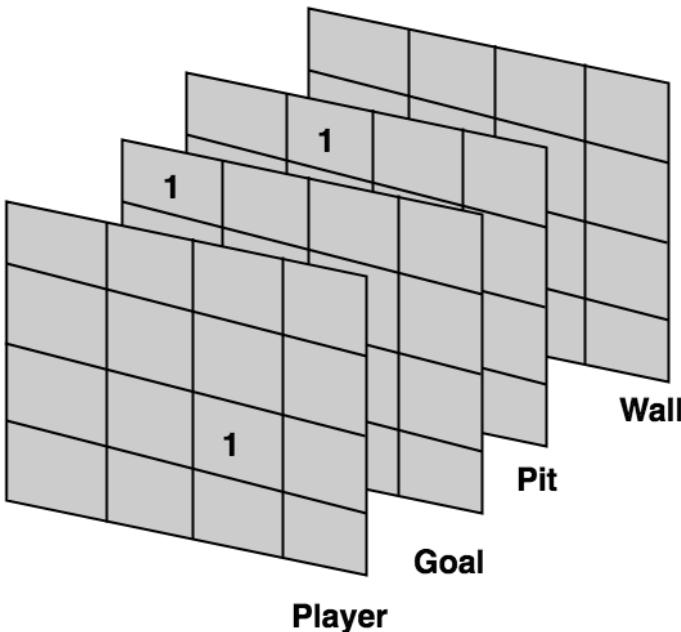


Figure 3.6: This is how the Gridworld board is represented as a numpy array. It is a $4 \times 4 \times 4$ tensor, composed of 4 “slices” of a 4×4 grid. Each grid slice represents the position of an individual object on the board and contains a single 1 whereas all other elements are 0s. The position of the 1 indicates the position of that slice’s object.

While we could in principle build a neural network that can operate on a $4 \times 4 \times 4$ tensor, it is easier to just flatten it into a 1-tensor (vector). A $4 \times 4 \times 4$ tensor has $4^3 = 64$ total elements, so the input layer of our neural network must be accordingly shaped. The neural network will have to learn what this data means and how it relates to maximizing rewards. Remember, the algorithm will know absolutely nothing to begin with.

NEURAL NETWORK AS THE Q-FUNCTION. Now for the fun part. Let’s build our neural network that will serve as our Q function. As you know, in this book we’ll be using PyTorch for all our deep learning models, but if you’re more comfortable with another framework such as TensorFlow or MXnet, then it should be fairly straightforward to port the models. Here’s the general architecture for the model we will build:

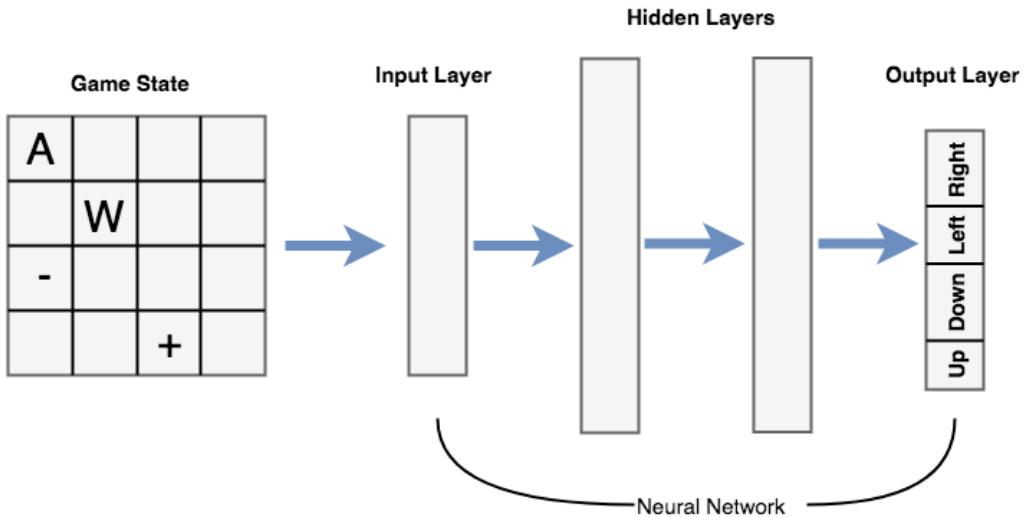


Figure 3.7: The neural network model we will use to play Gridworld. The model has an input layer that can accept a 64-length game state vector, some hidden layers, and an output layer that produces a 4-length vector of Q-values for each action, given the state.

To implement this with PyTorch, we'll use the `nn` module, which is the higher-level interface for PyTorch, similar to Keras for TensorFlow.

Listing 3.2 Neural Network Q-function

```
import numpy as np
import torch
from torch.autograd import Variable
from Gridworld import *
from IPython.display import clear_output
import random
from matplotlib import pylab as plt

l1 = 64
l2 = 150
l3 = 100
l4 = 4

model = torch.nn.Sequential(
    torch.nn.Linear(l1, l2),
    torch.nn.ReLU(),
    torch.nn.Linear(l2, l3),
    torch.nn.ReLU(),
    torch.nn.Linear(l3,l4)
)
loss_fn = torch.nn.MSELoss(size_average=True)
learning_rate = 1e-3
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)
```

```
gamma = 0.9
epsilon = 1.0
```

So far all we've done is setup the neural network model, define a loss function, the learning rate, setup an optimizer, and define a couple parameters. If this were a simple classification neural network, then we'd almost be done. We'd just setup a for-loop to iteratively run the optimizer to minimize the model error with respect to the data. It's more complicated with reinforcement learning, which is probably why you're reading this book. We covered the main steps we'd need to run through earlier, but let's zoom in a little.

Below is the implementation for the main loop of the algorithm. In broad strokes:

1. Setup a for-loop to number of epochs
2. In the loop, setup while loop (while game is in progress)
3. Run Q network forward.
4. We're using an epsilon greedy implementation, so at time t with probability ϵ we will choose a random action. With probability $1-\epsilon$ we will choose the action associated with the highest Q value from our neural network.
5. Take action a as determined in (4), observe new state s' and reward r_{t+1}
6. Run the network forward using s' . Store the highest Q value, max Q.
7. Our target value to train the network is $R_{t+1} + \gamma * \max Q_A(S_{t+1})$ where γ (gamma) is a parameter between 0 and 1.
8. Given that we have 4 outputs and we only want to update/train the output associated with the action we just took, our target output vector is the same as the output vector from the first run, except we change the one output associated with our action to the result we compute using the Q-learning formula.
9. Train the model on this 1 sample. Repeat process 2-9

[insert blog diagram of steps 1-9]

Just to be clear, when we first run our neural network and get an output of action-values like this

```
array([[-0.02812552, -0.04649779, -0.08819015, -0.00723661]])
```

our target vector for one iteration may look like this:

```
array([[-0.02812552, -0.04649779, 1, -0.00723661]])
```

where we just changed a single entry to the value we want to update. One detail to

One detail to include in the code before we move on. The Gridworld game engine's makeMove method expects a character such as 'u' to make a move, however, our Q-learning algorithm only knows how to generate numbers, so we need a simple map from numeric keys to our action characters:

```
action_set = {
    0: 'u',
    1: 'd',
    2: 'l',
```

```
    3: 'r',
}
```

Okay, let's actually get to coding the main training loop.

Listing 3.3 Q-learning: Main Training Loop

```
epochs = 1000
losses = [] #A
for i in range(epochs): #B
    game = Gridworld(size=4, mode='static') #C
    state_ = game.board.render_np().reshape(1,64) + np.random.rand(1,64)/10.0 #D
    state = Variable(torch.from_numpy(state_).float()) #E
    status = 1 #F
    while(status == 1): #G
        qval = model(state) #H
        qval_ = qval.data.numpy()
        if (random.random() < epsilon): #I
            action_ = np.random.randint(0,4)
        else:
            action_ = (np.argmax(qval_))

        action = action_set[action_] #J
        game.makeMove(action) #K
        new_state_ = game.board.render_np().reshape(1,64) + np.random.rand(1,64)/10.0
        new_state = Variable(th.from_numpy(new_state_).float()) #L
        reward = game.reward()
        newQ = model(new_state.reshape(1,64)).data.numpy()
        maxQ = np.max(newQ) #M
        y = np.zeros((1,4))
        y[:] = qval_[:]
        if reward == -1: #N
            update = (reward + (gamma * maxQ))
        else:
            update = reward
        y[0][action_] = update #O
        y = Variable(torch.from_numpy(y).float())
        loss = loss_fn(qval, y) #P
        print(i, loss.item())
        optimizer.zero_grad()
        loss.backward()
        losses.append(loss.data[0])
        optimizer.step()
        state = new_state
        if reward != -1: #Q
            status = 0
            clear_output(wait=True)
    if epsilon > 0.1: #R
        epsilon -= (1/epochs)
```

#A Create a list to store loss values so we can plot the trend later

#B The main training loop

#C For each epoch, we start a new game

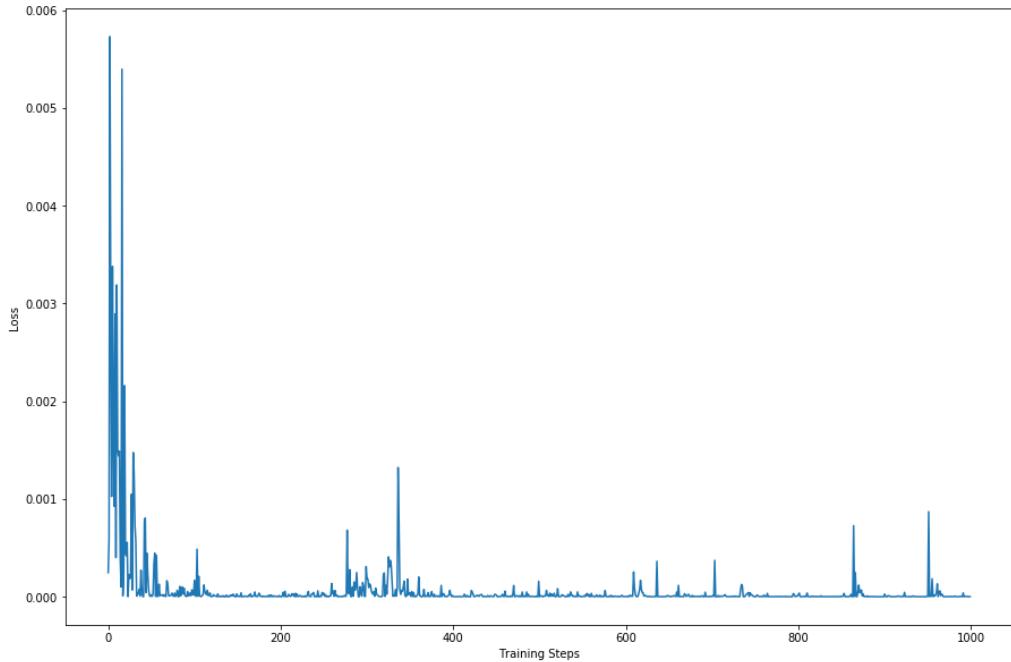
#D After we create the game, we extract the state information and add a small amount of noise

#E We need to convert the numpy array into a PyTorch Tensor and then into a PyTorch Variable

```
#F Use the status variable to keep track of whether or not the game is still in progress
#g While this game is still in progress, we'll play to completion then start a new epoch
#H Run the Q-network forward to get its predicted q-values for all the actions
#I Select an action using the epsilon-greedy method
#J We have to translate the numerical action into one of the action characters that our Gridworld game expects
#K After selecting an action using the epsilon greedy method, we take the action
#L After making a move, we get the new state of the game
#M Find the maximum q-value predicted from the new state
#N Calculate the target q-value
#O Create a copy of the qval array and then update the one element corresponding to the action we took
#Q If reward is -1 then we know the game hasn't been won or lost and is still in progress
#R Decrement the epsilon value each epoch
```

NOTE: Why did we add noise to the game state? Because it helps prevent “dead neurons” that can happen with the use of rectified linear units (ReLU) as our activation function. Basically, since most of the elements in our game state array are 0s they won’t play nice with ReLU, which is technically non-differentiable at 0. Hence, we add just a tiny bit of noise so that none of the values in the state array are exactly 0. It also might help with overfitting.

Go ahead and run the training loop, 1000 epochs will be enough. Once it’s done, you can plot the losses to see if the training looks successful (i.e. the loss more or less decreases over training time). Here’s the plot we get:



The loss plot is pretty noisy but clearly a moving average of the plot is significantly trending toward zero. This gives us some confidence the training worked, but we'll never know until we test it. We've written up a simple function that allows us to test the model on a single game.

Listing 3.4 Testing the Q-network

```
def test_model(model, mode='static'):
    i = 0
    test_game = Gridworld(mode=mode)
    state_ = test_game.board.render_np().reshape(1,64) + np.random.rand(1,64)/10.0
    state = Variable(torch.from_numpy(state_).float())
    print("Initial State:")
    print(test_game.display())
    status = 1
    #while game still in progress
    while(status == 1):
        qval = model(state)
        qval_ = qval.data.numpy()
        action_ = np.argmax(qval_) #take action with highest Q-value
        action = action_set[action_]
        print('Move #: %s; Taking action: %s' % (i, action))
        test_game.makeMove(action)
        state_ = test_game.board.render_np().reshape(1,64) +
        np.random.rand(1,64)/10.0
        state = Variable(torch.from_numpy(state_).float())
        print(test_game.display())
        reward = test_game.reward()
        if reward != 0:
```

```

    status = 0
    print("Reward: %s" % (reward,))
    i += 1
    if (i > 15):
        print("Game lost; too many moves.")
        break

```

The test function is essentially just the same as the code in our training loop except we don't do any loss calculation or backpropagation, we're just running the network forward to get the predictions. Let's see if it learned how to play Gridworld!

```

>>> test_model(model, 'static')

Initial State:
[[ '+ - - ' 'P' ]
 [ ' - W - ' ]
 [ ' - - - ' ]
 [ ' - - - ' ]]

Move #: 0; Taking action: d
[[ '+ - - ' 'P' ]
 [ ' - W - ' ]
 [ ' - - - ' ]
 [ ' - - - ' ]]

Move #: 1; Taking action: d
[[ '+ - - ' 'P' ]
 [ ' - W - ' ]
 [ ' - - - ' ]
 [ ' - - - ' ]]

Move #: 2; Taking action: l
[[ '+ - - ' 'P' ]
 [ ' - W - ' ]
 [ ' - - P ' ]
 [ ' - - - ' ]]

Move #: 3; Taking action: l
[[ '+ - - ' 'P' ]
 [ ' - W - ' ]
 [ ' - P - ' ]
 [ ' - - - ' ]]

Move #: 4; Taking action: l
[[ '+ - - ' 'P' ]
 [ ' - W - ' ]
 [ ' P - - ' ]
 [ ' - - - ' ]]

Move #: 5; Taking action: u
[[ '+ - - ' 'P' ]
 [ ' P - W ' ]
 [ ' - - - ' ]
 [ ' - - - ' ]]

Move #: 6; Taking action: u
[[ '+ - - ' 'P' ]
 [ ' - W - ' ]
 [ ' - - - ' ]
 [ ' - - - ' ]]

Reward: 10

```

Can we get a round of applause for our Gridworld player here? Clearly it knows what it's doing; it went straight for the goal! But let's not get too excited; this was the static version of the game, which is really easy. If you use our test function with the `mode='random'`, we'll find some disappointment:

```
>>> testModel(model, 'random')

Initial State:
[[ '+', ' ', 'P'],
 [ 'W', ' ', ' '],
 [ ' ', ' ', ' '],
 [ ' ', ' ', ' ']]

Move #: 0; Taking action: d
[[ '+', ' ', ' '],
 [ 'W', ' ', 'P'],
 [ ' ', ' ', ' '],
 [ ' ', ' ', ' ']]

Move #: 1; Taking action: d
[[ '+', ' ', ' '],
 [ 'W', ' ', ' '],
 [ ' ', ' ', 'P'],
 [ ' ', ' ', ' ']]

Move #: 2; Taking action: l
[[ '+', ' ', ' '],
 [ 'W', ' ', ' '],
 [ ' ', 'P', ' '],
 [ ' ', ' ', ' ']]

Move #: 3; Taking action: l
[[ '+', ' ', ' '],
 [ 'W', ' ', ' '],
 [ 'P', ' ', ' '],
 [ ' ', ' ', ' ']]

Move #: 4; Taking action: l
[[ '+', ' ', ' '],
 [ 'W', ' ', ' '],
 [ 'P', ' ', ' '],
 [ ' ', ' ', ' ']]

Move #: 5; Taking action: u
[[ '+', ' ', ' '],
 [ 'P', 'W', ' '],
 [ ' ', ' ', ' '],
 [ ' ', ' ', ' ']]

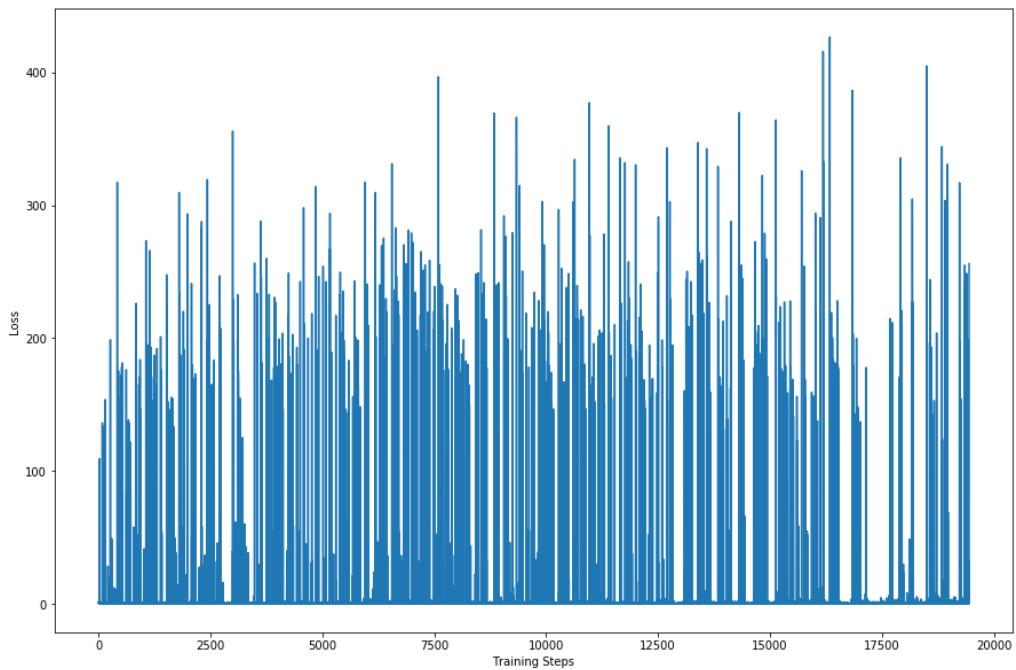
Move #: 6; Taking action: u
[[ 'P', '+', ' '],
 [ 'W', ' ', ' '],
 [ ' ', ' ', ' '],
 [ ' ', ' ', ' ']]

Move #: 7; Taking action: d
[[ '+', ' ', ' '],
 [ 'P', 'W', ' '],
 [ ' ', ' ', ' '],
 [ ' ', ' ', ' ']]

# we omitted the last several moves to save space

Game lost; too many moves.
```

This is actually really interesting, look carefully at the moves that the network is making. The player starts off the game only 2 tiles to the right of the goal, if it *really* knew how to play the game, it would just take the shortest path to the goal. Instead it starts moving down and to the left, just like it would in the static game mode. It seems like the model just memorized the particular board it was trained on and didn't generalize at all. Ah, but maybe we just need to train it with the game mode set to random, and then it will really learn right? Try it, go ahead. Re-train it with random mode. Maybe you'll be luckier than us, but this is what our loss plot looks like with random mode and 1000 epochs:



Well, that doesn't look pretty. There's no sign that any significant learning is happening at all with random mode. We didn't show these results, but for us, the model *did* seem to learn how to play with "player" mode where only the player is randomly placed on the grid. In any case, this is a big problem, reinforcement learning wouldn't be worth anything if all it could do is learn how to memorize or weakly learn. But indeed, this is a problem that the DeepMind team faced and one they solved.

3.3 Preventing Catastrophic Forgetting: Experience Replay

We're slowly building up our skills and we want our algorithm to train on the harder variant of the game where every new game the all the board pieces are randomly placed on the grid. It can't just memorize a sequence of steps to take as before, it needs to be able to take the

shortest path to the goal (without stepping into the pit) from what the initial board configuration is. It needs to develop a more sophisticated representation of its environment.

CATASTROPHIC FORGETTING The main problem we encountered in the previous section when we tried to train our model on random mode has a name, it's called **catastrophic forgetting**. It's actually a very important issue that is associated with gradient descent-based training methods in *online* training. Online training is what we've been doing: we backpropagate after each move as we play the game.

Imagine that in game #1 that our algorithm is training on (learning Q-values for) the player is placed in between the pit and the goal such that the goal is on the right and the pit is on the left.

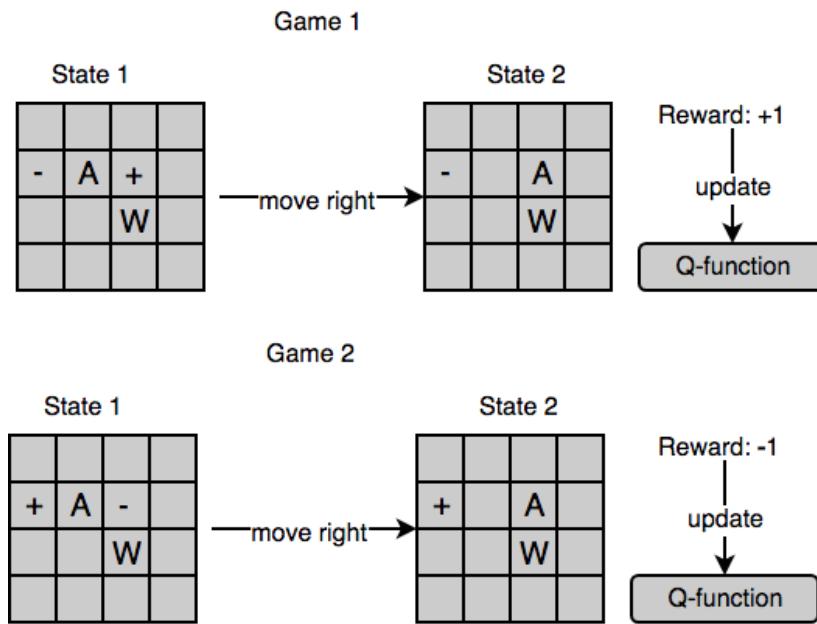


Figure 3.8: Catastrophic forgetting. The idea is that when two game states are very similar and yet lead to very different outcomes, the q-function will get “confused” and won’t be able to learn what to do. In this example, the catastrophic forgetting happens because the q-function learns from game state 1 that taking action “right” leads to a +1 reward, but then game state 2, which looks very similar, gets a reward of -1 after moving right, so the algorithm then forgets what it previously learned about game state 1, overall resulting in essentially no significant learning at all.

Using an epsilon-greedy strategy, the player takes a random move and by chance takes a step to the right and hits the goal. Great, the algorithm will try to learn that this state-action pair is associated with a high value by updating its weights in such a way that the output will more closely match the target value (i.e. via backpropagation). Now, the second game gets

initialized and the player is again in between the goal and pit but this time the goal is on the *left* and the pit is on the right. Perhaps to our naive algorithm, the state *seems* very similar to the last game. Since last time moving right gave a nice positive reward, the player chooses to make one step to the right again, but this time it ends up in the pit and gets -1 reward. The player is thinking "what is going on, I thought going to the right was the best decision based on my previous experience." So now it may do backpropagation again to update its state-action value but because this state-action is very similar to the last learned state-action it may override its previously learned weights.

This is the essence of catastrophic forgetting. There's a push-pull between very similar state-actions (but with divergent targets) that results in this inability to properly learn anything. We generally don't have this problem in the supervised learning realm because we do randomized batch learning, where we don't update our weights until we've iterated through some random subset of our training data and compute the sum or average gradient for the batch, and this sort of averages over the targets and stabilizes the learning.

EXPERIENCE REPLAY. Catastrophic forgetting is probably not something we have to worry about with the first variant of our game because the targets are always stationary, and indeed the model successfully learned how to play it. But with the random mode, it's something we need to consider, and that is why we need to implement something called **experience replay**. Experience replay basically gives us batch updating in an online learning scheme. It's actually not a big deal to implement; here's how it works.

Experience replay:

1. In state s , take action a , observe new state s_{t+1} and reward r_{t+1}
2. Store this as a tuple (s, a, s_{t+1}, r_{t+1}) in a list.
3. Continue to store each experience in this list until we have filled the list to a specific length (up to you to define)
4. Once the experience replay memory is filled, randomly select a subset (again...you need to define the subset size)
5. Iterate through this subset and calculate value updates for each; store these in a target array (e.g. y_{train}) and store the state s of each memory in X_{train}
6. Use X_{train} and y_{train} as a minibatch for batch training. For subsequent epochs where the array is full, just overwrite old values in our experience replay memory array.

Experience Replay

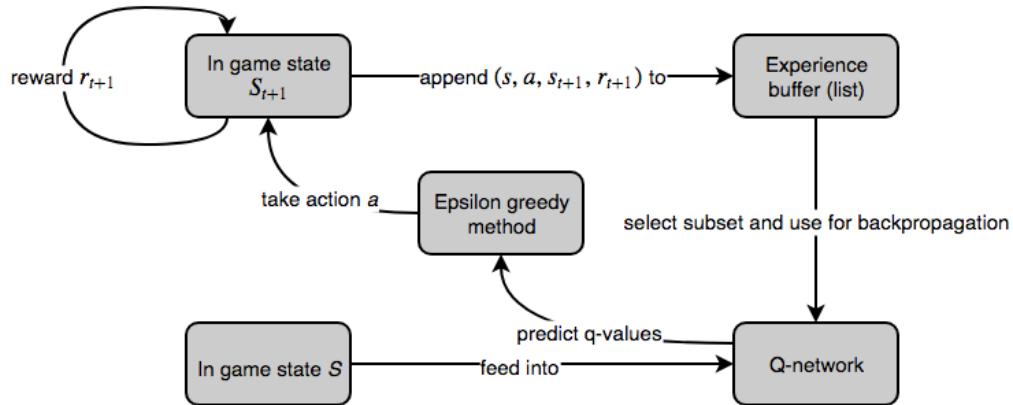


Figure 3.9: This is the general overview of experience replay, a method to mitigate a major problem with online training algorithms: catastrophic forgetting. The idea is to employ minibatching by storing past experiences and then using a random subset of these experiences to update the Q-network, rather than just the single most recent experience.

Thus, in addition to learning the action-value for the action we just took, we're also going to use a random sample of our past experiences to train on to prevent catastrophic forgetting.

So here's the same training algorithm from above except with experience replay added. Remember, this time we're training it on the harder variant of the game where all the board pieces are randomly placed on the grid.

Listing 3.5 Experience Replay

```
epochs = 3000
losses = []
batchSize = 100 #A
buffer = 500 #B
replay = [] #C
max_moves = 50 #D
h = 0
for i in range(epochs):
    game = Gridworld(size=4, mode='random')
    state_ = game.board.render_np().reshape(1,64) + np.random.rand(1,64)/100.0
    state = Variable(torch.from_numpy(state_).float())
    status = 1
    mov = 0
    while(status == 1):
        mov += 1
        qval = model(state)
        qval_ = qval.data.numpy()
        if (random.random() < epsilon):
            action = np.random.randint(0,4)
```

```

else:
    action_ = (np.argmax(qval_))

action = action_set[action_]
game.makeMove(action)
new_state_ = game.board.render_np().reshape(1,64) +
np.random.rand(1,64)/100.0
new_state = Variable(torch.from_numpy(new_state_).float())
reward = game.reward()

if (len(replay) < buffer): #E
    replay.append((state, action_, reward, new_state))
else: #F
    replay.pop(0)
replay.append((state, action_, reward, new_state))
minibatch = random.sample(replay, batchSize) #G
X_train = Variable(torch.empty(batchSize, 4, dtype=torch.float))
y_train = Variable(torch.empty(batchSize, 4, dtype=torch.float))
h = 0
for memory in minibatch: #H
    old_state, action_m, reward_m, new_state_m = memory
    old_qval = model(old_state)
    newQ = model(new_state_m).data.numpy()
    maxQ = np.max(newQ)
    y = torch.zeros((1,4))
    y[:] = old_qval[:]
    if reward == 0:
        update = (reward_m + (gamma * maxQ))
    else:
        update = reward_m
    y[0][action_m] = update
    X_train[h] = old_qval
    y_train[h] = Variable(y)
    h+=1

loss = loss_fn(X_train, y_train)
print(i, loss.item())
optimizer.zero_grad()
loss.backward()
losses.append(loss.data[0])
optimizer.step()

state = new_state
if reward != 0 or mov > max_moves:
    status = 0
    mov = 0
if epsilon > 0.1:
    epsilon -= (1/epochs)

```

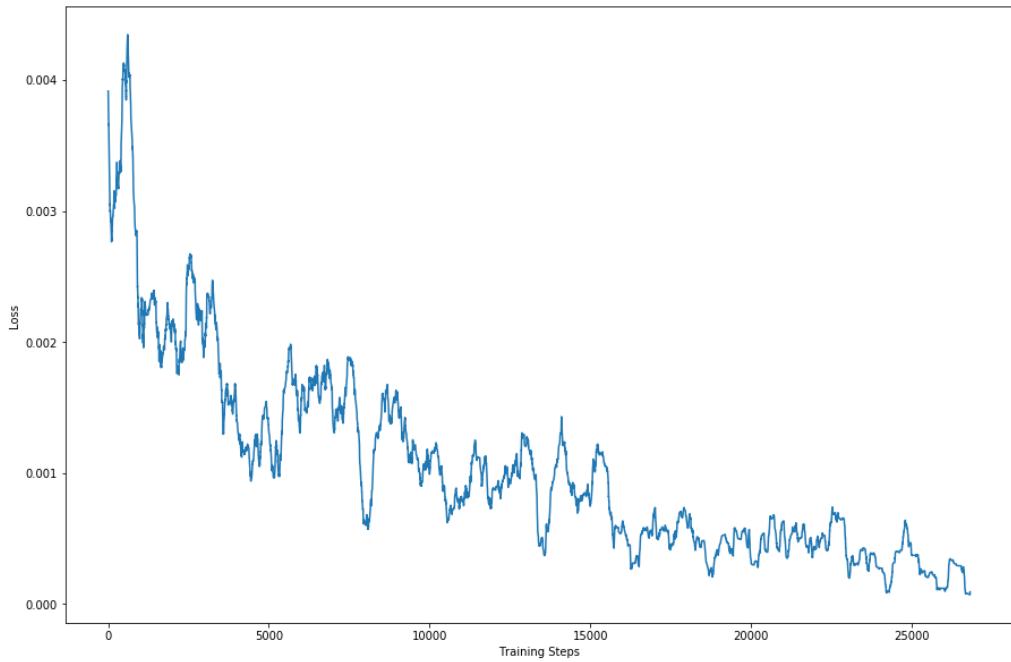
#A The number of samples from the experience replay buffer used as minibatches
#B The size of the experience replay buffer
#C The experience replay buffer, a list that will store tuples of state and reward data
#D The maximum number of moves allowed before we decide to start a new game
#E If the buffer has not been filled up, just add to it
#F If the buffer is full, remove first item and add new item
#G Sample a minibatch from the replay buffer
#H Iterate through each experience in the minibatch

We ran for 3000 epochs this time since it's a more difficult game, but otherwise the Q-network model is the same as before. When we test the algorithm, it seems to play most of the games correctly. We wrote an additional testing script to see the percentage of games it wins out of 1000 plays.

Listing 3.6 Testing the performance

```
max_games = 1000
wins = 0
for i in range(max_games):
    win = test_model(model, mode='random', display=False)
    if win:
        wins += 1
win_perc = float(wins) / float(max_games)
print("Games played: {0}, # of wins: {1}".format(max_games,wins))
print("Win percentage: {}".format(win_perc))
```

When we run Listing 3.6 on our trained model, we got 86.5% wins out of 1000 games, which is certainly a lot better than random but is not nearly what we would expect if the algorithm really knew what it was doing (although you could probably improve the accuracy with a much longer training time). Once you actually know how to play, you should be able to win every single game. There's a small caveat that some of the initialized games may actually be impossible to win and thus the win percentage may not ever reach 100%. The Gridworld game engine does eliminate most of the impossible board configurations but there's a small number that can still get through. What's holding us back from getting into the 95%+ accuracy territory? Well let's have a look at our loss plot. Here we plotted the running average loss plot (yours may vary significantly):



You can see it's definitely trending downward but looks pretty unstable. This is the type of plot you'd be a bit surprised to see in a supervised learning problem, but is quite common in bare deep reinforcement learning. While the experience replay mechanism helps with training stabilization by reducing catastrophic forgetting, there are still other related sources of instability.

3.4 Improving Stability with a Target Network

So far we've been able to successfully train a deep reinforcement learning algorithm to learn and play Gridworld with a deterministic static initialization and a slightly harder version where the player is placed randomly on the board each game. Unfortunately, even though the algorithm appears to learn how to play, it is quite possible it is just memorizing all the possible board configurations since on a 4x4 board it's not that many. The hardest variant of the game is where the player, goal, pit and wall are all initialized randomly each game, making it much more difficult for the algorithm to memorize. This ought to enforce some amount of actual learning, but as we saw, we're still experiencing difficulty with learning this variant. To help address this, we're going to add another dimension to the updating rule that will smooth out the value updates.

LEARNING INSTABILITY. One potential problem that DeepMind identified when they published their deep Q-network paper was that if you just keep updating the Q-network's (i.e. the neural

network serving the role as Q-function) parameters after each move, you might cause instabilities to arise. The idea is that, since the actual rewards may be sparse (you only get a significant positive reward when you win the game or significant penalty upon losing), if you update on every single step where most steps you're not seeing any significant reward, you may cause the algorithm to start behaving erratically. For example, the Q-network might predict a high value for the "up" action in some state, then it moves up, and by chance it lands on the goal and wins, so we update the Q-network to reflect the fact that it was rewarded +1. The next game, however, it thinks "up" is a really fantastic move and predicts a high q-value, but then it moves up and gets a -1 reward, so we update and now it thinks "up" is not so great after all, but then a few games later moving up leads to winning again. You can see how this might lead to a kind of oscillatory behavior where the predicted q-value never settles to a reasonable value but just keeps getting jerked around. Of course this is very similar to the catastrophic forgetting problem.

This is not just a theoretical issue, it's something that DeepMind observed in their own training and had to come up with a solution. The solution they devised is to split the Q-network into two copies each with their own model parameters: the "regular" Q-network and a copy called the target network (symbolically denoted θ -network, read "Q hat"). The target network is identical to the Q-network in the beginning before we've done any training, but its own parameters lag behind the regular Q-network in terms of how they're updated. Let's run through the sequence of events again with the target network in play (we'll leave out the details of experience replay).

Target Network:

1. Initialize Q-network with parameters (weights) θ_Q (read "theta Q")
2. Initialize target network as copy of Q-network, but with separate parameters θ_T (read "theta T"), and we set $\theta_T = \theta_Q$.
3. Use epsilon greedy strategy with Q-network q-values to select action a
4. Observe reward and new state r_{t+1}, s_{t+1}
5. Target network q-value will be set to r_{t+1} if the episode has just been terminated (i.e. the game is won or lost) or to $r_{t+1} + \gamma \max_{a'} Q_{\theta_T}(s_{t+1})$ otherwise (notice use of target network here)
6. Backpropagate the target q-value through the Q-network (not the target network)
7. Every Cnumber of iterations, set $\theta_T = \theta_Q$ (i.e. set the target network parameters equal to the Q-network's parameters)

Q-Learning with a Target Network

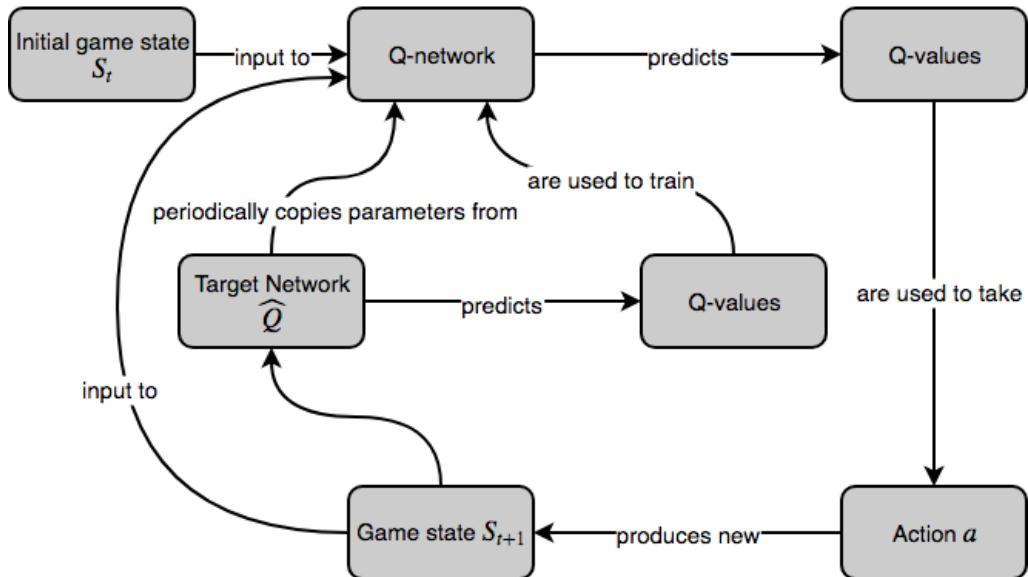


Figure 3.10: This is the general overview for q-learning with a target network. It's a fairly straightforward extension of the normal q-learning algorithm, except that you have a second q-network called the target network whose predicted q-values are used to backpropagate through and train the main Q-network. The target network's parameters are not trained, but are periodically synchronized with the Q-network's parameters. The idea is that using the target network's q-values to train the Q-network will improve the stability of training.

Notice that that only time we use the target network \hat{Q} is to calculate the target q-value for backpropagation through the Q-network. The idea is that we update the Q-network's parameters on each training iteration, but we decrease the effect that recent updates have on the action selection, hopefully improving stability. The code is getting a bit long now with both experience replay and a target network, so we're just going to show a portion of the full code and leave it to you to checkout the book's GitHub <<http://github.com/DeepReinforcementLearning/>> where you'll find all the code for this chapter. The following code is identical to Listing 3.5 except for a few lines that add in the target network capability.

Listing 3.7 Target Network

```
model3 = torch.nn.Sequential(
    torch.nn.Linear(11, 12),
    torch.nn.ReLU(),
    torch.nn.Linear(12, 13),
    torch.nn.ReLU(),
    torch.nn.Linear(13,14),
```

```

)
model3_ = copy.deepcopy(model3) #A

#B

epochs = 5000
losses = []
batchSize = 250
buffer = 2000
replay = []
max_moves = 100
c = 500 #C
c_step = 0
h = 0
for i in range(epochs):
    game = Gridworld(size=4, mode='random')
    state_ = game.board.render_np().reshape(1,64) + np.random.rand(1,64)/100.0
    state = Variable(torch.from_numpy(state_).float())
    status = 1
    mov = 0
    #while game still in progress
    while(status == 1):
        c_step += 1
        if c_step > c:
            model3_.load_state_dict(model3.state_dict()) #D
            c_step = 0
        mov += 1
        qval = model3(state)

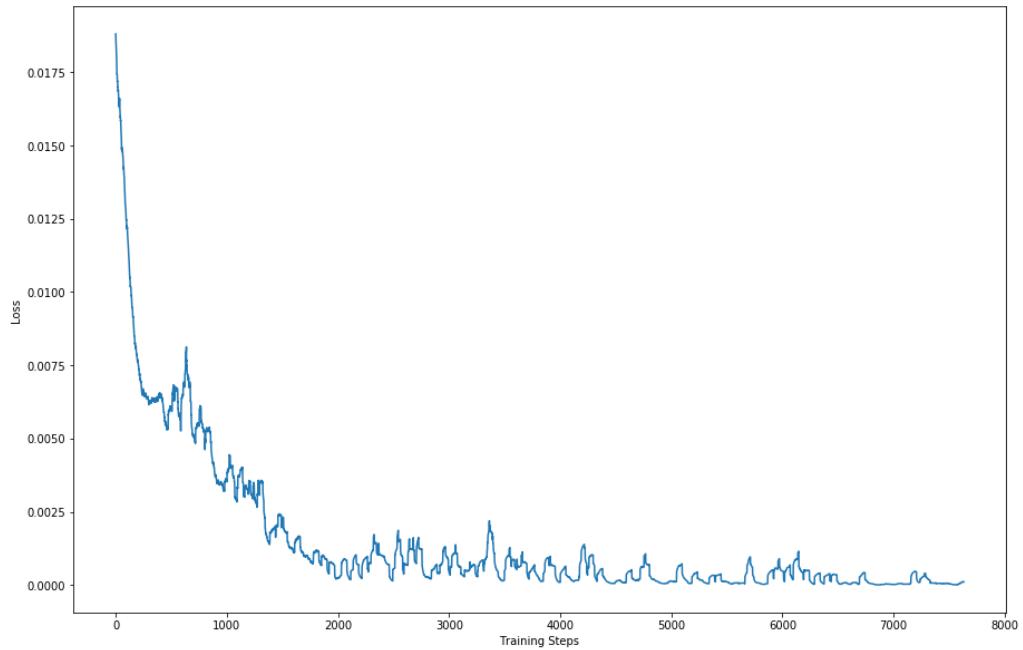
#E

        for memory in minibatch:
            old_state, action_m, reward_m, new_state_m = memory
            old_qval = model3(old_state)
            newQ = model3_(new_state_m).data.numpy() #F
            maxQ = np.max(newQ) #G

#A We create a second model by making an identical copy of the original Q-network model.
#B Code omitted
#C This is the parameter that controls how often we will synchronize model3_ (target network) with model3 (Q-network)
#D Every 50 training steps we synchronize the target network's parameters with the q-network
#E Code omitted
#F We use the target network's predicted q-values to calculate the target q-value for training the Q-network
#G Rest of code omitted

```

When we plot the loss for a target network approach plus experience replay, we get a nicely decreasing trend. In any case, you'll want to experiment with the hyperparameters such as the experience replay buffer size, the batch size, the target network update frequency, and the learning rate. Unfortunately, the performance can be quite sensitive to these.



And if you run the test script, you should be getting over 90% accuracy. We're only training up to 5000 epochs, where each epoch is a single game. The number of possible game configurations (i.e. the size of the state-space) is approximately 43,680 ($16 \times 15 \times 14 \times 13$), so we're only sampling about $5000/43680 = 0.11$ or 11% of the total number of possible starting game states. If the model can successfully play games it has never seen before, then we have some confidence it has generalized. If you're getting good results with the 4x4 board, you should try training an agent to play a 5x5 board or larger by changing the size parameter when creating a Gridworld game instance, e.g.

```
>>> game = Gridworld(size=6, mode='random')
>>> game.display()

array([[' ', '+', ' ', ' ', ' ', ' '],
       [' ', ' ', ' ', ' ', ' ', ' '],
       [' ', ' ', 'W', ' ', ' ', ' '],
       [' ', ' ', ' ', ' ', ' ', ' '],
       [' ', ' ', ' ', ' ', 'P', ' '],
       [' ', ' ', ' ', ' ', ' ', ' ']], dtype='<U2')
```

DeepMind's Deep Q-Network

Believe it or not, but in this chapter we basically built the Deep Q-Network (DQN) that DeepMind originally introduced in 2015 that learned to play old Atari games at superhuman performance levels. DeepMind's DQN used an epsilon-greedy

action-selection strategy, experience replay, and a target network. Of course the details of our implementation are different since we are playing a custom Gridworld game and DeepMind was training on raw pixels from real video games. For example, one difference worth noting is that they actual input the last 4 frames of a game into their Q-network. The reason is that a single frame in a video game is not enough information to determine the speed and direction of the objects in the game, which is important to know when deciding what action to take.

You can read more about the specifics of DeepMind's DQN by searching for their paper "Human-level control through deep reinforcement learning." One thing to note is that they used a neural network architecture consisting of two convolutional layers followed by two fully connected layers. In our case we used 3 fully connected layers. It would be a worthwhile experiment to build a model with a convolutional layer at first and try training with Gridworld. One huge advantage of convolutional layers is that they are independent of the size of the input tensor. When we use a fully connected layer, for example, we had to make the first dimension 64, in our case we used a parameter matrix for the first layer. With a convolutional layer, however, it can be applied to input data of any length. This would allow you to train a model on a 4x4 grid and see if it generalizes enough to be able to play on a 5x5 or bigger grid. Go ahead, try it!

3.5 Summary

We've covered a lot in this chapter. And once again we've smuggled in a lot of fundamental reinforcement learning concepts. We could have pushed a bunch of academic definitions in your face to start, but we resisted the temptation, and decided to get to coding as quickly as possible and then tell you the definitions afterward. Let's review what we've accomplished and fill in a few terminological gaps.

In this chapter we covered a particular RL algorithm called Q-learning. Q-learning has nothing to do with deep learning or neural networks on its own, it is only an abstract mathematical construct. Q-learning refers to solving a control task by learning a function called a Q-function. You give the Q-function a state (e.g. a game state) and it predicts how valuable all the possible actions are that you could take given the input state, which we call q-values. You decide what to do with these q-values. You might decide to just take the action that corresponds to the highest q-value (a greedy approach), or you might opt for a more sophisticated selection process. As we learned in chapter 2, you have to balance exploration (trying new things) versus exploitation (taking the best action you know of). In this chapter, we used the standard epsilon-greedy approach to select actions, where we initially take random actions to explore, and then progressively switch our strategy to taking the highest value actions.

Back to the Q-function. The Q-function must be learned from the data we give it. It has to learn how to make accurate q-value predictions of states. The Q-function could be anything really, anything from an unintelligent database to a complex deep learning algorithm. Since deep learning is the best class of learning algorithms we have at the moment, we choose to employ neural networks as our Q-functions. This means that "learning the Q-function" is the same as training a neural network with backpropagation.

One important concept about Q-learning that we held until now is that it is an **off-policy** algorithm, in contrast to **on-policy** algorithms. You already know what a policy is from last chapter: it's the strategy our algorithm uses to maximize rewards over time. If a human is

learning to play Gridworld, they might employ a policy that first scouts all possible paths toward the goal and selects the one that is shortest. Another policy might be to just randomly take actions until you land on the goal. An off-policy reinforcement learning algorithm like Q-learning means that the choice of policy does not affect the ability to learn accurate q-values. Indeed, our Q-network could learn accurate q-values if we selected actions at random since eventually it would experience a number of winning and losing games and infer the values of states and actions. Of course, this is terribly inefficient, the policy matters only insofar as it helps us learn with the least amount of data. In contrast, an on-policy algorithm will explicitly depend on the choice of policy or will directly aim at learning a policy from the data.

Another key concept we've saved until now is the notion of **model-based** versus **model-free** algorithms. To make sense of this, we first need to understand what a model is. We sort of use this term informally to refer to a neural network, for example, or it's often used to mean any kind of statistical model, others being a linear model or a Bayesian graphical model. In another context, we might say a model is a mental or mathematical representation of how something in "the real world" works. If we understand exactly how something works (i.e. what it's composed of and how those components interact) then we can not only explain data we've already seen, but we can predict data we haven't yet seen.

For example, weather forecasters build very sophisticated models of the climate that take into account many relevant variables and are constantly measuring real-world data. Then they can use their models to predict the weather to some degree of accuracy. There's an almost cliché statistics mantra that "all models are wrong, but some are useful," meaning that it is impossible to build a model that 100% corresponds to reality (if that were the case, you'd basically have built a reality simulator), there will always be data or relationships that we're missing, but nonetheless, many models capture enough truth about some system we're interested in that they're useful for explanation and prediction.

If we could build an algorithm that could figure out how Gridworld works, then it would have inferred a model of Gridworld, and it would be able to perfectly play it. In Q-learning, all we gave the Q-network was a numpy tensor. It had no *a priori* model of Gridworld, but it still learned to play by trial and error. We did not task the Q-network with figuring out how Gridworld works, its only job was to predict expected rewards. Hence, Q-learning is a model-free algorithm.

As the human architects of algorithms, we may be able to engineer in some of our own domain knowledge about a problem as a model. We could then supply this model to a learning algorithm and then let it figure out the details to optimize our problem. This would be a model-based algorithm. For example, most Chess playing algorithms are model-based, that is, they know how Chess works, they know the rules of the games and what the result of taking certain moves will be. The only part that isn't known (and we would want the algorithm to figure out) is what sequence of moves will win the game. With a model in hand, the algorithm can actually make long-term plans in order to achieve its aim.

In many cases, we want to employ algorithms that can progress from being model-free to planning with a model. For example, a robot learning how to walk may start to learn by trial

and error (model-free), but once it's figured out the basics of walking, it can start to infer a model of its environment and then plan a sequence of steps to get from point A to B (model-based). We'll continue to explore on and off-policy and model-based and free algorithms in the rest of the book.

3.6 What's next?

Q-learning is about training an agent to learn the most accurate Q-function for an environment. We can then use this learned Q-function to figure out what action to take. In the next chapter we'll learn about an algorithm that will help us build a network that can approximate the policy function.

4

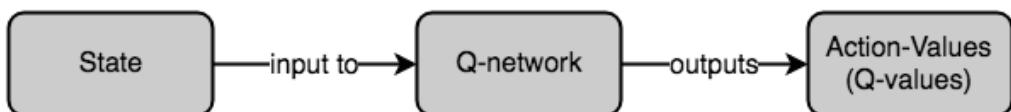
Learning to Pick the Best Policy: Policy Gradient Methods

This chapter covers:

- Implementing the policy function as a neural network
- Introduction to OpenAI Gym API
- Applying the REINFORCE algorithm on the OpenAI Cartpole problem

4.1 Policy Function using Neural Networks

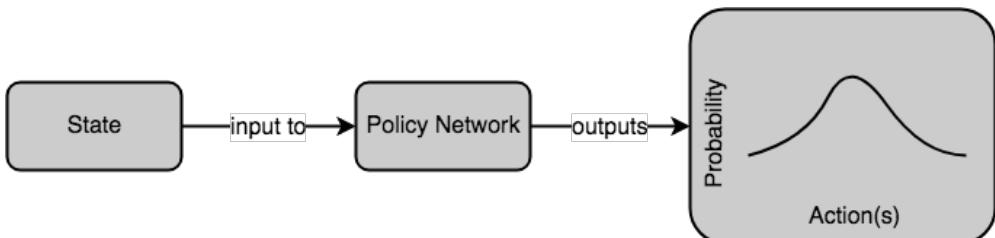
In the previous chapter we discussed Deep Q-networks, an off-policy algorithm where we approximated the Q-function with a neural network. The output of the Q-network were q-values corresponding to each action for a given state, and recall that value means the expected (i.e. weighted average or sum) of rewards.



Using these predicted Q-values from the Q-network, we could select actions to perform using some strategy. The strategy we employed in the last chapter was the epsilon-greedy approach where we select an action at random with probability ϵ and with probability $1-\epsilon$ we select the action associated with the highest q-value (the action the Q-network predicts is the best given its experience so far). There are other policies that we could have followed, such as using a softmax layer on the q-values, or any number of other ways of selecting actions. What if we

skip selecting a policy and instead train a neural network to output an action directly? If we do that, then our neural network ends up being a policy function, or a policy network. Remember from chapter 3, a policy function $\pi: \text{State} \rightarrow P(\text{Action} | \text{State})$ accepts a state and returns the best action, or more precisely, it will return a probability distribution over the actions and we can sample from this distribution to select actions. If a probability distribution is an unfamiliar concept to you, don't worry, we'll discuss it more throughout the chapter and the book.

Neural Network as the policy function. In this chapter we introduce a class of algorithms where we approximate the policy function $\pi(s)$ instead of the value function V_π or Q . That is, instead of training a network that outputs action-values, we are training a network to output (the probability of) actions.

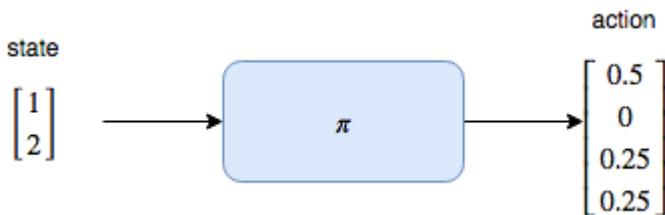


So in contrast to the Q-network, the policy-network tells us exactly what to do given the state we're in. No further decisions necessary. All we need to do is randomly sample from the probability distribution $P(A | s)$, and we get an action to take. The actions that are most likely to be beneficial will have the highest chance of being selected from random sampling. Imagine the probability distribution $P(A | s)$ as a jar filled with little notes with an action written on them. In a game with 4 possible actions, there will be notes with labels 1-4. If our policy network predicts that action 2 is the most likely to result in the highest reward, then it will fill this jar with a lot of little notes labeled 2, and less notes labeled 1, 3 and 4. In order to select an action then, all we do is close our eyes and grab a random note from the jar. We're most likely to choose action 2, but sometimes we'll grab another action and that gives us the opportunity to explore. So using this analogy, every time the state of the environment changes, we give the state to our policy network and it uses that to fill the jar with a new set of labeled notes representing the actions in different proportions and then we randomly pick from the jar.

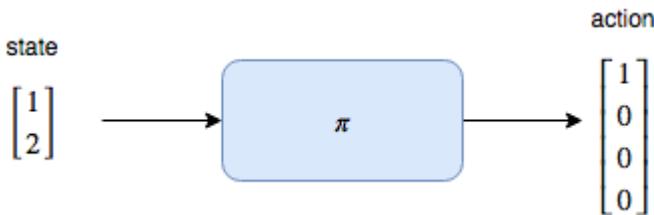
This class of algorithms is called policy gradient methods and has a few important differences from the DQN algorithm which we will explore in this chapter. There are a few advantages of this approach over value prediction methods. One is that, as we already discussed, we no longer have to worry about devising an action-selection strategy like epsilon-greedy, we just sample from the actions. Remember we spent a lot of time cooking up methods to improve the stability of training our DQN, we had to use experience replay and target networks and there are a number of other methods in the academic literature that we

could have used. A policy network tends to simplify some of the complexity we dealt with when using a Q-network.

Stochastic Policy Gradient. There are many different flavors of policy gradient methods. We will be starting with the stochastic policy gradient method, which is what we just described. Stochastic policy gradient means that the output of our neural network is an action vector that represents a probability distribution.



The policy we follow is to select an action from this probability distribution. This also means that if our agent ends up in the same state twice, we may not end up taking the same action every time. In the above example, we feed our function the state, which is $(1,2)$, and the output is an action vector. Our agent will have a 0.50 probability of going left, no chance of going up, 0.25 probability of going right, and 0.25 probability of going down.



If the environment is static and there is a deterministic strategy, we expect the probability distribution to converge to a more deterministic action vector as shown above.

I forget...What's a probability distribution?

Let's be concrete. In Gridworld, we had 4 possible actions: up, down, left, right. We call this our action-set or actions-space, since we can describe it mathematically as a set, e.g. $A = \{\text{up}, \text{down}, \text{left}, \text{right}\}$ where the curly braces indicate a set (a set in mathematics is just an abstract un-ordered collection of things with certain operations defined). So what does it mean to apply a probability distribution over this set of actions?

Probability is actually a very rich and even controversial topic in its own right. There are varying philosophical opinions on what exactly probability means. To some people, the probability means that, if you were to flip a coin a very large number of times (ideally an infinite number of times, mathematically speaking) then the probability of a fair coin turning up heads is equal to the proportion of heads in that infinitely long sequence of flips. That is, if we flip a fair coin 1,000,000 times, we expect about half of the flips to be heads and the other half tails, and hence the probability is

equal to that proportion. This is a frequentist interpretation of probability since probability is interpreted as the long-term frequency of some event repeated many times.

In contrast, another school of thought interprets probability only as a degree of belief, a subjective assessment of how much I can predict an event given the knowledge I currently possess. This degree of belief is often called a credence. The probability of a fair coin turning up heads is 0.5 or 50% because, given what I know about the coin, I don't have any reasons to predict heads more than tails or tails more than heads, and hence I split my belief evenly across the two possible outcomes. Hence, anything that we can't predict deterministically (i.e. with probability 0 or 1, nothing in between) results from a lack of knowledge.

You're free to interpret probabilities however you want since it doesn't affect our calculations, but in this book we tend to implicitly use the credence interpretation of probability. So for our purposes, applying a probability distribution over the set of actions in Gridworld, $A=\{up,down,left,right\}$ means to assign a degree of belief (a real number between 0 and 1) to each action in the set such that all the probabilities sum to 1. We interpret these probabilities as the probability that an action is the best action to maximize the expected rewards, given that we're in a certain state.

Concretely, a probability distribution over our action set A is denoted $P(A):A \rightarrow [0, 1]$, meaning that $P(A)$ is a map from a set A to a set of real numbers between 0 and 1. In particular, each element $a_i \in A$ is mapped to a single number between 0 and 1 such that the sum of all these numbers for each action is equal to 1. We might represent this map for our Gridworld action set as just a vector, where we identify each position in the vector with an element in the action-set, e.g. $[up, down, left, right] \rightarrow [0.25, 0.25, 0.10, 0.4]$. This map is called a probability mass function (PMF).

What we just described is actually a discrete probability distribution, since our action-set was discrete (a finite number of elements). If our action-set was infinite, i.e. a continuous variable like velocity, then we would call this a continuous probability distribution and instead we would need to define a probability density function (PDF).

The most common example of a PDF is the normal (also known as Gaussian, or just bell-curve) distribution. If we have a probability with a continuous action, say a car game where we need to control the velocity of the car from 0 to some maximum value, which is a continuous variable, how might we do this with a policy network? Well, we could drop the idea of probability distribution and just train the network to produce the single value of velocity that it predicts is best, but then we risk not exploring enough (and it is difficult to train such a network). A lot of power comes from a little bit of randomness. The kind of neural networks we employ in this book only produce vectors (or tensors more generally) as output, so they can't produce a continuous probability distribution—we have to be more clever. A PDF like a normal distribution is defined by two parameters, the mean and variance. Once we have those, we have a normal distribution that we can sample from. So we can just train a neural network to produce mean and standard deviation values that we then plug into the normal distribution equation and sample from that.

Don't worry, if this isn't all making sense now, we will continue to go over it again and again as these concepts are ubiquitous in reinforcement learning and machine learning more broadly.

But in many problems the environment is not static. Think of playing rock, paper, scissors. When playing against a player for the first time, there is no best action the optimal strategy and we would select each action with a 1/3 chance. If we were to this with a DQN algorithm and the values for each action were the same, we need to think carefully about what to do with the Q-values to split the tie. This is to say that there are often cases where there may be two or more actions with approximately equivalent value predictions, so we need a policy to determine how to break the tie, for example by flipping a coin and selecting one of the equivalently valued actions randomly. This tie-breaking mechanism adds complexity to the

algorithm. However, with a stochastic policy network, the need to take actions probabilistically in a stochastic environment is baked in to how the network works.

Exploration. Recall from the previous chapter that we needed our policy to include some randomness that would allow us to visit non-optimal states during training. For DQNs we followed the epsilon-greedy policy where there was a chance we would not follow the action that led to the greatest reward. If we always selected the action that led to the maximum predicted reward, then we'd never discover the even better actions and states available to us. For the stochastic policy gradient method, because our output is a probability distribution there should be a small chance that we explore all spaces, and only after sufficient exploration will the action distribution converge to producing the single best action. Or if the environment has an element of randomness, then the probability distribution will retain some probability mass to each action. When we initialize our model in the beginning, the probability of our agent picking each action should be approximately equal or uniform since the model has zero information about which action is better.

There is a variant of policy gradient called deterministic policy gradient (DPG) where there is a single output that the agent will always follow. In the case of Gridworld for example, it would produce a 4-dimensional binary vector with a 1 for the action to be taken and 0s for the other actions. This causes the agent to not explore properly if it always follows the output since there's no randomness in the action selection. Since the output of a deterministic policy function for a discrete action set would be discrete values, it is also difficult to get this working in the fully differentiable manner that we are accustomed to with deep learning, so we'll focus on stochastic policy gradients. Building a notion of uncertainty (e.g. using probability distributions) into the models is generally a good thing.

4.2 Reinforcing Good Actions: The Policy Gradient Algorithm

From the previous sections, we understand that there is a class of algorithms which attempts to create a function that outputs a probability distribution over actions and that this policy function $\pi(s)$ can be implemented with a neural network.

Defining An Objective. Recall that neural networks need an objective function that is differentiable with respect to the network weights (parameters). In the last chapter we trained the Deep Q-network by a minimizing mean square error (MSE) loss function with respect to its predicted q-values and the target q -value. We had a nice formula for calculating the target q-value based on the observed reward since q-values are just averaged rewards (i.e. expectations), so this was not much different from a how we would normally train a supervised deep learning algorithm.

With a policy network that gives us a probability distribution over actions given a state, $P(A | s)$, how do we train this? There's no obvious way to map our observed rewards after taking an action to updating $P(A | s)$. Training the DQN was not much different than a supervised learning problem, because our Q-network generated a vector of predicted Q-values, and using some formula we were able to generate the target q-value vector, and then

we just minimized the error between the Q-network predictions and our target. With a policy network, we're predicting actions directly, and there is no way to come up with a target vector of what actions we should have taken instead, given the rewards. All we know is whether the action lead to positive or negative rewards. In fact, what the best action is secretly depends on a value function, but with a policy network we're specifically trying to avoid computing these action-values directly.

Let's go through an example to see how we might optimize our policy network. Let's start with some notation. Our policy network is denoted π and is parameterized by a vector θ , this represents all of the weights of the neural network. As you know, neural networks have parameters in the form of multiple weight matrices, however, for the purposes of easy notation and discussion, it is standard to consider all the network parameters together as a single long vector, that we denote θ (*theta*).

Whenever we run the policy network forward the parameter vector θ is fixed, the variable is the data that gets fed into the policy network (i.e. the state). Hence, we denote the parameterized policy as π_θ . Whenever we want to indicate that some input to a function is fixed, we will include it as a subscript rather than as an explicit input like $\pi(x, \theta)$ where x is some input data (i.e. the state of the game). Notation like $\pi(x, \theta)$ suggests θ is a variable that changes along with x , whereas π_θ indicates that θ is a fixed parameter of the function.

Let's say we give our initially untrained policy network π_θ some initial game state of Gridworld denoted s , and run it forward by computing $\pi_\theta(s)$. It returns a probability distribution over the 4 possible actions, for example [0.25, 0.25, 0.25, 0.25]. (It is a bit unrealistic that it would return a perfectly uniform distribution like that, but that won't affect our example). We sample from this distribution and since it's a uniform distribution, we essentially take a random action. We continue to take actions by sampling from the produced action distribution until we reach the end of the episode.

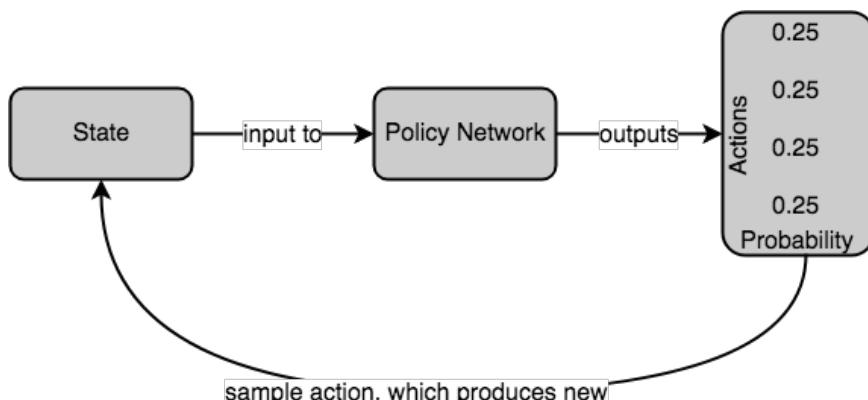


Figure 4.1: The general overview of policy gradients for an environment with 4 possible discrete actions. First we input the state to the policy network, which produces a probability distribution over the actions, then we sample from this distribution to take an action, which produces a new state.

Remember, some games like Gridworld are episodic, meaning that there is a well-defined start and end point to a round of the game. In Gridworld, we start the game in some initial state, and play until we either hit the pit, land on the goal, or we take too many moves. So an episode is a sequence of states, actions, and rewards from an initial state to the terminal state where we win or lose the game. We denote this:

Notation (episode):

$$\varepsilon = (S_0, A_0, R_1), (S_1, A_1, R_2), \dots, (S_{t-1}, A_{t-1}, R_t)$$

Each tuple is one time-step of the Gridworld game (or a Markov decision process more generally). After we've reached the end of the episode at time t , we've collected a bunch of historical data on what just happened. Let's say that by chance we hit the goal after just 3 moves determined by our policy network. Here's what our episode looks like:

$$\varepsilon = (S_0, 3, 0), (S_1, 1, 0), (S_2, 3, +1)$$

We've encoded the actions as integers from 0 to 3 (referring to array indices of the action vector) and left the states denoted symbolically since they're actually 64-length vectors. What is there to learn from in this episode? Well we won the game, indicated by the +1 reward in the last tuple, so our actions must have been "good" to some degree, so given the states we were in, we should encourage our policy network to make those actions more likely next time. We want to *reinforce* those actions that led to a nice positive reward. We will address what happens when our agent loses (receives a terminal reward of -1) later in this section, but in the meantime, we will focus on positive reinforcement.

Positive Reinforcement. We want to make small, smooth updates to our gradients to encourage the network to take assign more probability to these winning actions in the future. Let's focus on the last experience in the episode with state S_2 . Remember, we're assuming our policy network produced the action probability distribution [0.25, 0.25, 0.25, 0.25] since it is untrained, and in the last time step we took action 3 (corresponding to element 4 in the action probability array) and it resulted in us winning the game with a +1 reward. We want to positively reinforce this action given state S_2 , such that whenever the policy network encounters S_2 or a very similar state, it will be more confident in predicting action 3 as the highest probability action to take.

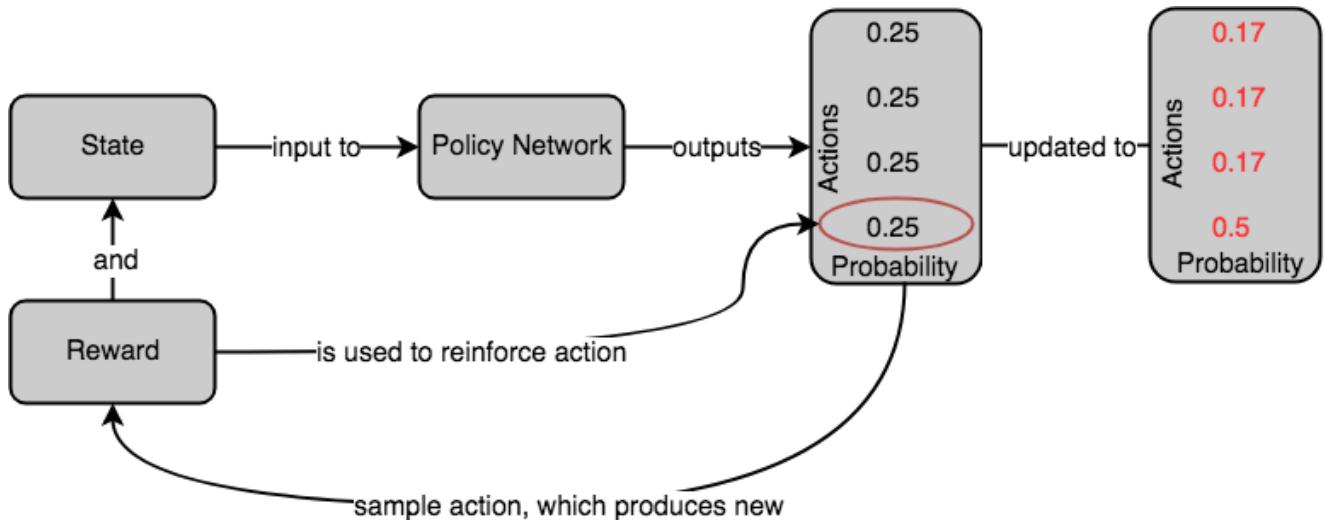


Figure 4.2: One action is sampled from the policy network's probability distribution, it produces a new state and reward. The reward signal is used to reinforce the action that was taken, that is, increase the probability of that action given the state (if the reward is positive) or decrease if the reward was negative. Notice that we only received information about action 3 (element 4) but since probabilities must sum to 1, we have to lower the probabilities of the other actions.

A naïve approach might be to make a target action distribution $[0, 0, 0, 1]$ so that our gradient descent will move the probabilities from $[0.25, 0.25, 0.25, 0.25]$ close to $[0, 0, 0, 1]$, maybe ending up as $[0.167, 0.167, 0.167, 0.5]$. This is something we often do in the supervised learning realm when we are training a softmax-based image classifier. But in that case, there is a single correct classification to an image and there is no temporal association between each prediction. In our RL case, we want more control over how we make these updates. First, we want to make small, smooth updates because we want to maintain some stochasticity in our action sampling to adequately explore the environment. Secondly, we want to be able to weight how much we assign credit to each action for earlier actions. Let's review some more notation first before diving into these two problems.

Recall, our policy network is typically denoted π_θ when we are running it forward (i.e. using it for to produce action probabilities), because we think of the network parameters θ as being fixed and the input state is what varies. Hence calling $\pi_\theta(s)$ for some state s will return a probability distribution over the possible actions given a fixed set of parameters. When we are training the policy network, we need to vary the parameters with respect to a fixed input to find a set of parameters that optimizes our objective (i.e. minimize a loss or maximizes a utility function), i.e. $\pi_s(\theta)$.

NOTATION (CONDITIONAL PROBABILITY): The probability of an action given the parameters of the policy network is denoted $\pi_s(a | \theta)$. This makes it clear that the probability of an action a explicitly depends on the parameterization of the policy network. In general, we denote a conditional probability as $P(x | y)$ read “the probability distribution over x given y .” This means, we have some function that takes a parameter y and returns a probability distribution over some other parameter x .

In order to reinforce action 3, we want to modify our policy network parameters θ such that we increase $\pi_s(a_3 | \theta)$. So our objective function merely needs to maximize $\pi_s(a_3 | \theta)$ where a_3 is action 3 in our example. Before training $\pi_s(a_3 | \theta) = 0.25$ but we want to modify θ such that $\pi_s(a_3 | \theta) > 0.25$. Because all of our probabilities must sum to 1, this means maximizing $\pi_s(a_3 | \theta)$ will minimize the other action probabilities. And remember, we prefer to set things up so that we’re minimizing an objective function instead of maximizing, since it plays nice with PyTorch’s built-in optimizers, so we should instead tell PyTorch to minimize $1 - \pi_s(a | \theta)$. This loss function approaches 0 as $\pi_s(a | \theta)$ nears 1 and so we are encouraging the gradients to maximize $\pi_s(a | \theta)$ for the action we took. We will subsequently drop the subscript a_3 as it should be clear from the context which action we’re referring to.

Log Probability. Mathematically this should make sense. But alas, due to computation imprecisions we need to make adjustment to this formula to stabilize the training. One problem is that probabilities are bounded between 0 and 1 by definition, so the range of values that the optimizer can operate over is limited and small. Sometimes probabilities may be extremely tiny or very close to one, and this runs into numerical issues when optimizing on a computer with limited numerical precision. If we instead use a surrogate objective, namely $-\log \pi_s(a | \theta)$ (where \log is the natural logarithm), then we have an objective that has a larger “dynamic range” than raw probability space and this makes it easier to compute. There are a few other reasons for using log-probabilities rather than raw probabilities but suffice it to say that log-probabilities are in general just easier to work with. If we set our objective as $-\log \pi_s(a | \theta)$ instead of $1 - \pi_s(a | \theta)$ our loss still abides by the intuition that the loss function approaches 0 as $\pi_s(a | \theta)$ approaches 1, while decreasing $\pi_s(a | \theta)$ will increase objective. Our gradients will be tuned to try to increase $\pi_s(a | \theta)$ to 1, where $a =$ action 3, for our running example.

Credit Assignment. Okay, our objective function is $-\log \pi_s(a | \theta)$, but this assigns equal weight to every action in our episode. The weights in the network that produced the last action will be updated to the same degree as the first action. Why shouldn’t that be the case? Well it makes sense that the last action right before the reward “deserves more credit” for winning the game than does the first action in the episode. For all we know, the first action was actually sub-optimal, but then we later made a comeback and hit the goal. Or in other words, our confidence in how “good” each action diminishes the further we are from the point of reward. In a game of chess, we attribute more credit to last move made than the first one. We’re very confident that the move that directly led to us winning was a good move, but we become less confident the further back we go. How much did the move from 5 time steps ago contribute to winning? We’re not so sure.

We express this by multiplying the magnitude of the update by the discount factor, which we learned from previous Chapter 3 ranges from 0 to 1. The action right before the episode ends will have a discount factor of 1, meaning it will receive the full gradient update, while earlier moves will be discounted by a fraction such as 0.5 and therefore the gradient steps will be smaller.

Let's add those into our objective (loss) function. Our final objective function that we will tell PyTorch to minimize is $-\gamma_t * G_t * \log \pi_s(a | \theta)$. Remember γ_t is the discount factor and the subscript t tells us its value will depend on the time step t , since we want to discount more distant actions more than more recent ones. The parameter G_t is called the total return, or future return, at time step t . It is the return we expect to collect from time step t until the end of the episode and can be approximated by simply adding the rewards from some state in the episode until the end of the episode.

$$G_t = r_t + r_{(t+1)} + \dots + r_{(T-1)} + r_T$$

In Gridworld, all rewards are 0 except for the winning or losing reward, so the return is equal to the terminal reward. In other environments, however, positive or negative rewards may be given at each time step. So in our earlier example with three time steps that we ended up winning, we could calculate G_t as followed:

$$G_0 = 0 + 0 + 1 = 1$$

$$G_1 = 0 + 1 = 1$$

$$G_2 = 1$$

This is before we apply any discount though. Actions temporally more distant from the received reward should be weighted less than actions closer. From the start to terminal state, the sequence of discounted rewards in Gridworld if we win a game might look something like [0.970, 0.980, 0.99, 1.0]. The last action led to the winning state of +1, and is not discounted at all. The previous action is assigned a scaled reward by multiplying the terminal reward with the γ_{t-1} discount factor, which we've set to 0.99.

The discount is exponentially decayed from 1, i.e. $\gamma_t = \gamma_0^{T-t}$ meaning that the discount at time t is calculated as the starting discount (here 0.99) exponentiated to the integer time distance from the reward. The length of the episode (total number of time steps) is denoted T and the local time step for a particular action is t . For $T-t=0$, $\gamma_{T-0} = 0.99^0 = 1$. For $T-t=2$, the $\gamma_{T-2} = 0.99^2 = 0.9801$ and so on. Each time step back, the discount factor is exponentiated to the distance from the terminal step, which results in an exponential decay of the discount factor the more distant (and irrelevant) the action was to the reward outcome.

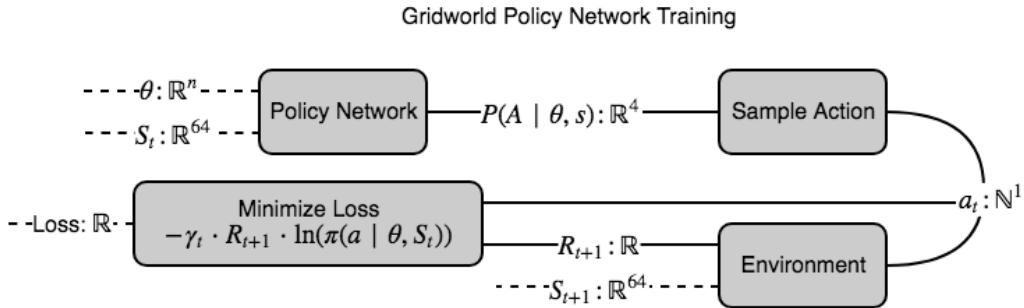


Figure 4.3: A string diagram for training a policy network for Gridworld. The policy network is a neural network parametrized by θ (the weights) and accepts an input state that is a 64-dimensional vector. It produces a discrete 4-dimensional probability distribution over the actions. The sample action box samples an action from the distribution and produces an integer as the action, which is given to the environment (to produce a new state and reward) and to the loss function so we can reinforce that action. The reward signal is also fed into the loss function, which we attempt to minimize with respect to the policy network parameters.

Negative Reinforcement. And there we have it! We defined an objective function that will guide the weights in network to positively reinforce actions that led to rewards and the degree of reinforcement needs to be scaled in proportion to the amount of rewards and a discount factor (denoted y). But what about episodes where we lose the game? This same objective function works even if we lose game (received a negative reward at the end) because our objective function will include a **negative** total return value instead of a positive one. Before including the total return value in our objective function, our objective function was just $-\log \pi_s(a | \theta)$ which encourages the action taken to be taken again. But when include the return value back into the equation, we are multiplying the function by a negative number, which effectively discourages the action that was taken to be taken again in a similar state. Hopefully the mathematics of this all is starting to make sense, but the actual implementation in code may not be obvious yet. We're getting there.

4.3 Working with OpenAI Gym

To illustrate how policy gradients work we've been using Gridworld as an example since it is already familiar to you from last chapter. However, we thought we should use a different problem to actually implement the policy gradient algorithm for variety and also as a chance to introduce the OpenAI Gym. The OpenAI Gym is an open source suite of environments with a common API that is perfect for testing reinforcement learning algorithms. If you come up with some new Deep RL algorithm, testing it on a few of the environments in the Gym is a great place to get some idea of how well it is performing. The Gym contains very easy environments that can be "solved" by simple linear regression all the way to ones that all but require a sophisticated deep RL approach. There are games, robotic control and other types of environments. There's probably something in there you'll be interested in.

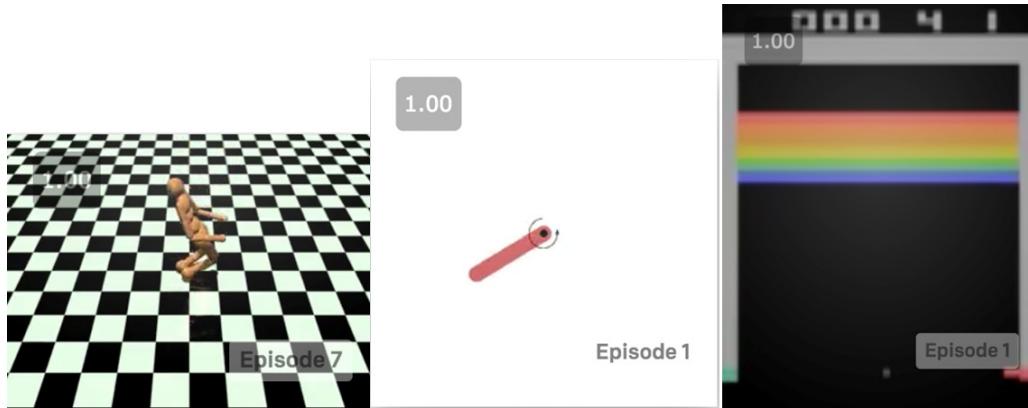


Figure 4.4: Three example environments provided by OpenAI's gym environment. The OpenAI gym provides hundreds of environments to test your reinforcement learning algorithms on.

OpenAI lists all of their currently supported environments on their website (<https://gym.openai.com/envs/>) and at the time of this writing they are broken down into 7 categories.

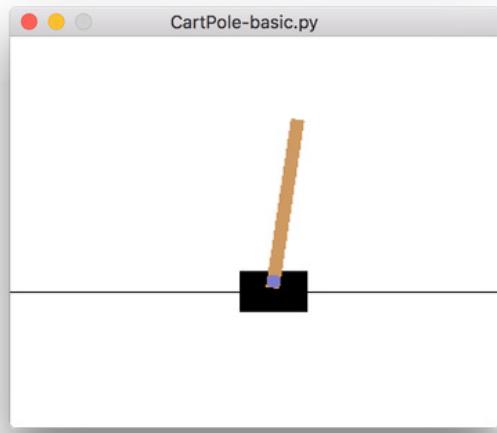
1. Algorithms
2. Atari
3. Box2D
4. Classic Control
5. MuJoCo
6. Robotics
7. Toy Text

They used to have board games, which included games like Go as a section, but removed it in a previous version (removed in v0.9.6). But don't worry, we have forked this library and provided a means for you to access the Go Game in a later chapter. In the meantime, you can just work with the latest version (v0.9.6). You can also view the entire list of environments from the OpenAI registry in your python shell with the following code snippet.

Listing 4.1 OpenAI Gym

```
from gym import envs
envs.registry.all()
```

There are hundreds of environments to choose from (797 in v0.9.6). Unfortunately, some of these environments require licenses (MuJoCo) or external dependencies (Box2D, Atari) and will therefore require a bit of setup time. As of now, we will be starting with a simple example, CartPole, to avoid any unnecessary complications and to get us coding right away.



CartPole. The CartPole falls under the Classic Control section above and has a very simple objective – don’t let the pole fall over. It’s the game equivalent of trying to balance a pencil on the tip of your finger. In order to balance the pole successfully, you have to apply just the right amount of small left and right movements to the cart. In this environment, there are only two actions that correspond to making a small push left or right. In the OpenAI Gym API, all actions are simply represented as integers from 0 to whatever the total number of actions are for the particular environment, so in Cartpole the possible actions are 0 and 1. The state is represented as an array of size four that indicates the cart position, cart velocity, pole angle and pole velocity. We receive a reward of +1 for every step the pole has not fallen over, which is when the pole angle is more than 12° from the center or the cart position is outside the window. Hence, the goal of Cartpole is to maximize the length of the episode since each time returns a positive +1 reward. More information can be found on the OpenAI gym github page (<https://github.com/openai/gym/wiki/CartPole-v0>). Note, not every problem has a nice specification page as CartPole but we will define the scope of the problem beforehand in all subsequent chapters.

The OpenAI Gym API. The OpenAI Gym has been built to be incredibly easy to use and there is less than half a dozen methods that you’ll routinely use. We have already seen one earlier in Listing 4.1 where we listed out all available environments. Another important method is creating our environment as shown below.

Listing 4.2 OpenAI Gym

```
import gym
env = gym.make('CartPole-v0')
```

From now on we will be interacting solely with this `env` variable. We need a way to observe the current state of the environment and then to interact with it. Thankfully, there are only two methods you need to do this.

Listing 4.3 OpenAI Gym

```
first_state = env.reset()
action = env.action_space.sample()
state, reward, done, info = env.step(action)
```

The `reset` method initializes our environment and returns the first state. For this example, we used the `sample` method of the `env.action_space` object to sample a random action. Soon enough, we'll sample actions from a trained policy network that will act as our reinforcement learning agent. Once we initialized our environment we are free to interact with it via the `step` method. The `step` method returns four important variables that our training loop needs access to in order to run. The first parameter `state` represents the next state after we take the action. The second parameter `reward` is the reward at that time step, which for our CartPole problem is 1 unless the pole has fallen down. The third parameter `done` is a Boolean that indicates whether or not a terminal state has been reached. For our CartPole problem this would initially always return false until the pole has fallen or the cart has moved outside the window. The last parameter `info` is a dictionary with diagnostic information that may be useful for debugging, however, we will not use it.

That's basically all you need to get most environments up and running in OpenAI Gym.

4.4 The REINFORCE Algorithm

So now that we how to create an OpenAI gym environment and have hopefully developed an intuition for the policy gradient algorithm, let's dive in to getting a working implementation. Our discussion of policy gradients in the previous section was actually of a particular algorithm that has been around for decades (like most of deep learning and reinforcement learning) called REINFORCE (yes, it's always fully capitalized). We're going to consolidate what we learned previously, formalize it, and then turn it into glorious Python code.

Let's run through the steps of the algorithm with the Cartpole example.

1. Create our policy network. We build and initialize a neural network that serves as a policy network. The policy network will accept state vectors as inputs and produces a (discrete) probability distribution over the possible actions. You can think of "the agent" as a thin wrapper around the policy network that samples from the probability distribution to take an action. Remember, an agent in reinforcement learning is whatever function or algorithm takes a state and returns a concrete action that will be executed in the environment. Let's express this in code.

Listing 4.4 Cartpole Policy Gradients

```
import gym
import numpy as np
```

```

import torch

l1 = 4
l2 = 150
l3 = 2

model = torch.nn.Sequential(
    torch.nn.Linear(l1, l2),
    torch.nn.LeakyReLU(),
    torch.nn.Linear(l2, l3),
    torch.nn.Softmax()
)

learning_rate = 0.0009
optimizer = torch.optim.Adam(model.parameters(), lr=learning_rate)

```

That should all look fairly familiar to you at this point. The model is only two layers with a leaky ReLU activation function for the first layer and the Softmax function for the last layer. We chose the leaky ReLU because it performed better empirically. We saw the Softmax function back in Chapter 2, it just takes an array of numbers and squishes them into a range of 0 to 1 and makes sure they all sum to 1, basically creating a discrete probability distribution out of any list of numbers (that are not probabilities to start with). For example, $\text{softmax}([-1, 2, 3]) = [0.0132, 0.2654, 0.7214]$. Unsurprisingly, the softmax will turn the bigger numbers into larger probabilities.

2. Have the Agent Interact with the environment. The agent consumes the state and takes an action a probabilistically. More specifically, the state is input to the policy network, which then produces the probability distribution over the actions $P(A | \theta, s_i)$ given its current parameters and the state. Note, capital A refers to the set of all possible actions given the state whereas small a generally refers to a particular action. The policy network might return a discrete probability distribution in the form of a vector such as $[0.25, 0.75]$ for our two possible actions in Cartpole. This means the policy network predicts action 0 is the best with 25% probability and action 1 is the best with 75% probability (or confidence). We call this array `pred`.

Listing 4.5 Cartpole Policy Gradients

```

pred = model(torch.from_numpy(state1).float()) #G
action = np.random.choice(np.array([0,1]), p=pred.data.numpy()) #H
state2, reward, done, info = env.step(action) #I

#G Call policy network model to produce predicted action probabilities
#H Sample an action from the probability distribution produced by the policy network
#I Take the action, receive new state and reward. The info variable is produced by the environment but is irrelevant

```

The environment responds to the action by producing a new state s_2 , and a reward r_2 . We will store those into two arrays (a *states* array and an *actions* array) for when we need to update our model after the episode ends. We then plug the new state into our model, get a

new state and reward, store those, and repeat until the episode ends (the pole falls over and the game is over).

3. Training the model. We train the policy network by updating the parameters to minimize the objective/loss function. This involves three steps: calculate the probability of the action actually taken at each time step, multiply it by the discounted return, and then use that to backpropagate and minimize the loss. Calculating the probabilities of the action taken is easy enough, we can use the stored past transitions to re-compute the probability distributions using the policy network, except this time, we extract just the predicted probability for the action that was actually taken. We'll denote this quantity $P(a_t | \theta, s_t)$; this is a single probability value like 0.75.

To be concrete, let's say the current state is s_5 (state at time step 5) and we input that into the policy network and it returns $P_\theta(A | s_5) = [0.25, 0.75]$. We sample from this distribution and take action $a=1$ (the second element in the action array), and after this the pole falls over and the episode has ended. The total duration of the episode was $T=5$. For each of these 5 time steps, we took an action according to $P_\theta(A | s_t)$ and we store the specific probabilities of the actions that were actually taken, $P_\theta(a | s_t)$, in an array, so it might look like $[0.5, 0.3, 0.25, 0.5, 0.75]$. We simply multiply these probabilities by the discounted rewards (explained below), take the sum, multiply it by -1 and call that our overall loss for this episode. Unlike Gridworld, in Cartpole, the last action is the one that loses the episode, so we discount it the most since it probably had the least affect in losing (since it takes several bad moves in a row to drop the pole). In Gridworld we would do the opposite and discount the first action in the episode the most since it would be the least responsible for winning or losing.

Minimizing this objective will tend to increase those probabilities $P_\theta(a | s_t)$ weighted by the discounted rewards. So every episode we're tending to increase $P_\theta(a | s_t)$ but for a particularly long episode (i.e. we're doing well in the game and get a large end-of-episode return), we will increase the $P_\theta(a | s_t)$ to a greater degree, and hence, on average over many episodes we will reinforce the actions that are good while the bad actions will get left behind. Since probabilities must sum to 1, if we increase the probability of a good action, that automatically steals probability mass from the other presumably less good actions. Without the use of this redistributive nature of probabilities, this whole scheme wouldn't work (i.e., everything good and bad would just tend to increase).

Calculating future rewards. We will multiply $P_\theta(a_t | s_t)$ by the total reward (aka return) we received after this state. As mentioned earlier in the section, we can get the total reward by just summing the rewards (which is just equal to the number of time steps the episode lasted in Cartpole) and create a return array that starts with the episode duration and decrements by 1 until 1. If the episode lasted 5 time steps, then the return array would be $[5, 4, 3, 2, 1]$. This makes sense because our first action should be rewarded the most, since it is the least responsible for the pole falling and losing the episode. In contrast, the action right before the pole fell is the worst action and should have the smallest reward. But this is a linear decrement, we want to discount the rewards exponentially.

So we compute the discounted rewards. We make an array of γ_t by taking our γ parameter which may be set to 0.99, for example, and exponentiating it according to the distance from the end of the episode. For example, we start with `gamma_t = [0.99, 0.99, 0.99, 0.99, 0.99]`, then have arrange another array of exponents `exp = [1,2,3,4,5]` and compute `torch.power(gamma_t, exp)`, which will give us: `[1.0, 0.99, 0.98, 0.97, 0.96]`.

Loss Function. As we discussed previously, we make our loss function the negative log-probability of the action given the state, scaled by the reward returns. In PyTorch this defined as: `-1 * torch.sum(r * torch.log(preds))`. We compute the loss with the data we've collected for the episode, and run the torch optimizer to minimize the loss.

Let's run through some actual code.

Listing 4.5 Cartpole Policy Gradients

```
def discount_rewards(rewards, gamma=0.99):
    lenr = len(rewards)
    d_rewards = torch.pow(gamma, torch.arange(lenr)) * rewards #A
    d_rewards = (d_rewards - d_rewards.mean()) / (d_rewards.std() + 1e-07) #B
    return d_rewards

#A Compute exponentially decaying rewards
#B Normalize the rewards by subtracting the mean and dividing out the standard deviation
```

Here we define a special function to compute the discounted rewards given an array of rewards that looks like `[50,49,48,47,...]` if the episode lasted 50 time steps. It essentially turns this linear sequence of rewards into an exponentially decaying sequence of rewards, e.g. `[50.0000, 48.5100, 47.0448, 45.6041, ...]` and then it subtracts the mean to make the sequence to be zero-centered. Lastly it normalizes the sequence by dividing by the standard deviation, to end up with a sequence like: `[1.9257, 1.8240, 1.7240, 1.6256, ...]`. The first half of the sequence will be positive numbers while the second half will be negative numbers. The reason for this normalization step is just to improve the learning efficiency and stability since it keeps the return values within the same range no matter how big the raw return is. It will still work without normalization, just not as reliably.

Backpropagate. Now that we have all the variables in our objective function we can calculate the loss and then backpropagate to adjust the parameters. We define our loss function below.

Listing 4.5 Cartpole Policy Gradients

```
def loss_fn(preds, r): #A
    return -1 * torch.sum(r * torch.log(preds)) #B
```

#A The loss function expects an array of action probabilities for the actions that were taken and the discounted rewards.

#B It computes the log of the probabilities, multiplies by the discounted rewards, sums them all and flips the sign.

Full training loop. Initialize, collect experiences, calculate the loss from those experiences, backpropagate and repeat. Below defines the full training loop of our REINFORCE agent.

Listing 4.6 Cartpole Policy Gradients

```

env = gym.make('CartPole-v0')
MAX_DUR = 200
MAX_EPISODES = 500 #A
gamma_ = 0.99 #B
for episode in range(MAX_EPISODES):
    state1 = env.reset()
    done = False #C
    t = 0
    obs = [] #D
    actions = [] #E
    while not done: #F
        pred = model(torch.from_numpy(state1).float()) #G
        action = np.random.choice(np.array([0,1]), p=pred.data.numpy()) #H
        state2, reward, done, info = env.step(action) #I
        obs.append(state1) #J
        actions.append(action) #K
        state1 = state2
        t += 1
        if t > MAX_DUR: #L
            break;
    ep_len = len(obs) # M
    rewards = torch.arange(ep_len, 0, -1) #N
    preds = torch.zeros(ep_len) #O
    d_rewards = discount_rewards(rewards, gamma_) #P
    for j in range(ep_len): #Q
        state = obs[j]
        action = int(actions[j])
        pred = model(torch.from_numpy(state).float())
        preds[j] = pred[action] #R

    loss = loss_fn(preds, d_rewards)
    losses.append(loss)
    optimizer.zero_grad()
    loss.backward()
    optimizer.step()

#A The number of training episodes
#B The discount factor
#C The done variable is set by the environment and indicates if the game is still in play
#D An array to store the state observations during an episode
#E An array to store the actions taken during an episode
#F Continue taking actions until episode is done
#G Call policy network model to produce predicted action probabilities
#H Sample an action from the probability distribution produced by the policy network
#I Take the action, receive new state and reward. The info variable is produced by the environment but is irrelevant
#J Add the state to our storage array of states
#K Add the action taken to the storage array of actions taken
#L If the episode is exceeding some defined max number of time steps, quit the episode.
#M Now the episode has ended, entering training steps. ep_len is the duration of the episode
#N Create an array of rewards associated to each action taken
#O Setup an array to store the predicted probabilities of the actions actually taken

```

```
#P Compute the discounted rewards
#Q Revisit each state in the storage array of states
#R Fill in the array to store the probability of the actions actually taken, then run the optimizer
```

The code does exactly what we outlined earlier. We start an episode, use the policy network to take actions, record the states and actions we observe, and then once we break out of an episode, we have to re-compute the predicted probabilities to use in our loss function. If you run this code, you should be able to plot the episode duration against the episode number and will hopefully see a nicely increasing trend.

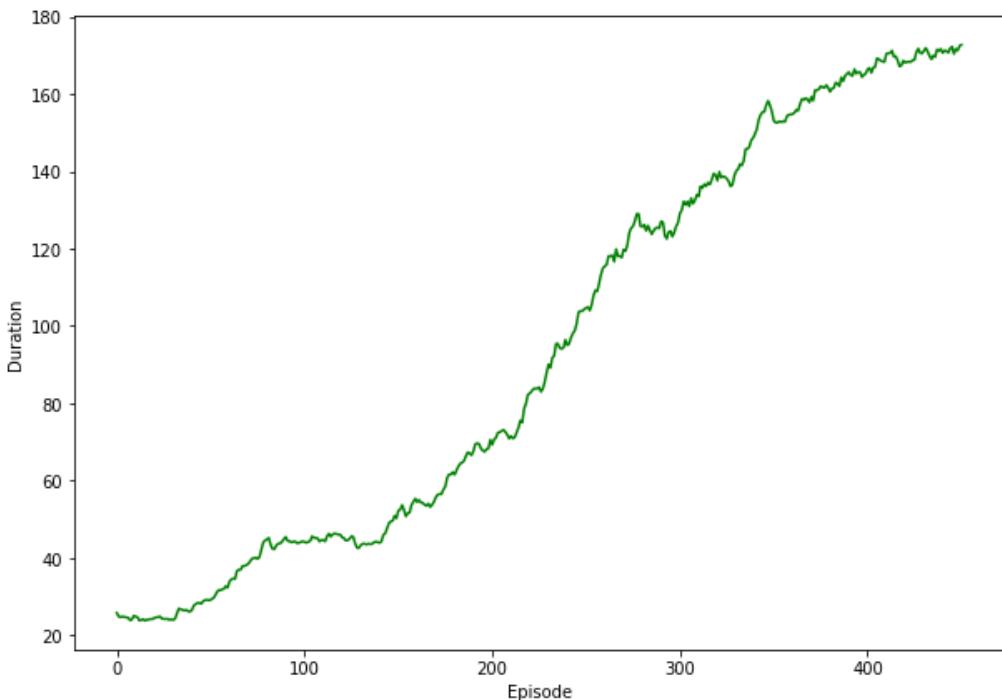


Figure 4.5: After training the policy network to 500 epochs, we get a plot that demonstrates the agent really is learning how to play cartpole. Note this is a moving average plot with a window of 50 to smooth the plot.

The agent learns how to play Cartpole! The nice thing about this example is that it should be able to train in under 1 minute on your laptop with just the CPU. The state of cartpole is just a 4-dimensional vector and our policy network is only 2 small layers, so it's much faster to train than the DQN we made to play Gridworld. OpenAI's documentation says that the game is considered "solved" if the agent can play an episode beyond 200 time-steps. Although the plot looks like it tops off at around 180, that's because it's a moving average plot, so there are

episodes that it reaches 200. Also, we capped the episode duration at 200, so if you increase the cap it will be able to play even longer.

4.5 Summary and what's next

In this chapter we covered the REINFORCE algorithm, one of the earliest versions of the policy gradient algorithms.

REINFORCE is an effective and very simple way of training a policy function. But it's a little too simple. For Cartpole, it works very well since the state space is simple and there are only two actions. If we're dealing with an environment with many more possible actions, then reinforcing all of them each episode and hoping that on average it will only reinforce the good actions becomes less and less reliable. In the next two chapters we explore more sophisticated ways of training the agent.

5

Tackling more complex problems with Actor-Critic methods

This chapter covers:

- The limitations of the REINFORCE algorithm described in the previous chapter
- Introducing a critic to improve sample efficiency and decrease variance
- Using the advantage function to speed up convergence
- Speeding up the model by parallelizing training

In the previous chapter we introduced a vanilla version of a policy gradient method called REINFORCE. The REINFORCE algorithm is generally implemented as an episodic algorithm, meaning that we only apply to update to our model parameters after the agent has completed an entire episode (and collecting rewards along the way). Recall the policy is a function $\pi:S \rightarrow P(a)$, that is, a function that takes a state and returns a probability distribution over actions. Then we sample from this distribution to get an action, such that the most probable action (the “best” action) is most likely to be sampled. At the end of the episode, we compute the *return* of the episode, which is essentially the sum of the discounted rewards in the episode. If action 1 was taken in state A and resulted in a return of +10, then the probability of action 1 given state A will be increased a little, whereas if action 2 was taken in state A and resulted in a return of -20 then the probability of action 2 given state A will decrease. Essentially, we minimized this loss function:

$$\text{loss} = -\log(P(a | S)) * R$$

This says “minimize the (logarithm) of the probability of the action a given state S times the return R.” So if the reward is a big positive number and $P(a_1 | S_A)=0.5$, for example, then

minimizing this loss will involve increasing this probability. So with REINFORCE we just keep sampling episodes (or trajectories more generally) from the agent and environment and periodically update the policy parameters by minimizing this loss.

WHY LOG-PROBABILITIES?

Remember, we only apply the logarithm to the probability because a probability is bounded between 0 and 1 whereas the log-probability is bounded from $-\infty$ (negative infinity) to 0, so given that numbers are represented by a finite number of bits, we can represent very small (close to 0) or very large (close to 1) probabilities without underflowing or overflowing the computer's numerical precision. Logarithms also have nicer mathematical properties that we don't need to cover, but that is why you'll almost always seen log-probabilities used in algorithms and machine learning papers even though we are conceptually interested in just the raw probabilities themselves.

By sampling a full episode, we get a pretty good idea of the "true value" of an action because we can see its downstream effects rather than just its immediate effect (which may be misleading due to randomness in the environment) and this full episode sampling is under the umbrella of Monte Carlo approaches. But not all environments are episodic, and sometimes we want to be able to make updates in an incremental or *online* fashion, i.e. making updates at regular intervals irrespective of what is going on in the environment. Our Deep Q-network did well in the non-episodic setting and could be considered an online-learning algorithm but it required an experience replay buffer in order to effectively learn.

The replay buffer was necessary because true online learning where parameter updates are made after each action is taken would be unstable due to the inherent variance (randomness) in the environment. An action taken once may by chance result in a big negative reward, but in expectation (average long-term rewards) it is a good action, so updating after a single action may result in erroneous parameter updates that will ultimately prevent adequate learning.

In this chapter, we introduce a new kind of policy gradient method called distributed advantage actor-critic (DA2C) that will have the online-learning advantages of DQN without a replay buffer and the advantages of policy methods where we can directly sample actions from the probability distribution over actions, thereby eliminating the need for choosing a policy (such as the epsilon-greedy policy) that we needed with DQN.

5.1 Combining the value and policy function

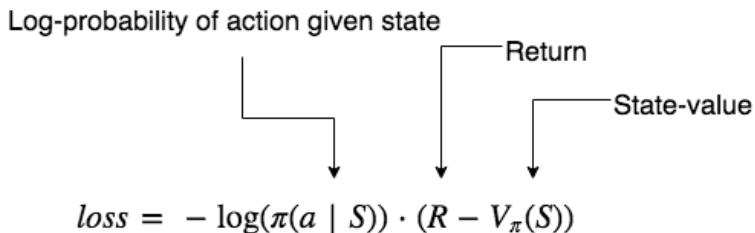
Q-learning (e.g. DQN) uses an action-value function to directly model the value (i.e. expected reward) of an action given a state. This is a very intuitive way of solving a Markov decision process (MDP) since we only observe states and rewards so it makes sense to predict the rewards and then just take actions that have high predicted rewards. On the other hand, we saw the advantage that direct policy learning (e.g. policy gradients) has, namely we get a true conditional probability distribution over actions, $P(a|S)$, that we can directly sample from to

take an action. Naturally someone decided it might be a good idea to combine these two approaches to get the advantages of both.

In building such a combined value-policy learning algorithm, we will start with the policy learner as the foundation. There are two challenges we want to overcome to increase the robustness of the policy learner:

1. We want to improve our sample efficiency by updating more frequently and
2. We want to decrease the variance of the reward we used to update our model.

These problems are related since the reward variance depends on how many samples we collect (i.e. more samples yields less variance). The idea behind a combined value-policy algorithm is to use the value learner to reduce the variance in the rewards used to train the policy. That is, instead of minimizing the REINFORCE loss that included direct reference to the observed return R from an episode, we instead add a baseline value such that the loss is now:



Where $V(S)$ is the value of state S , which is the state-value function (only a function of the state) rather than an action-value function (a function of both state and action), although an action-value function could be used as well. This quantity $V(S)-R$ is termed the **advantage**. Intuitively, the advantage quantity tells you how much better an action is relative to what you expected.

VALUES DEPEND ON THE POLICY

Remember that the value function (state or action-value) implicitly depends on the choice of policy, hence we ought to write $V_\pi(S)$. to make it explicit, however we drop the π subscript for notational simplicity. The policy's influence on the value is crucial, since a policy of taking random actions all of the time would result in all states being more or less equally low value.

Imagine that we're training a policy on a simple game with discrete actions and a small discrete state-space such that we can use a vector where each position in the vector represents a distinct state and the element is the average rewards observed after that state is visited. This look-up table would be the $V(S)$. So we might sample action 1 from the policy and observe reward +10, but then we use our value look-up table and see that on average we get +4 after visiting this state, so the advantage of action 1 given this state is $10 - 4 = +6$. This means that when we took action 1, we got a reward that was significantly better than what we expected based on past rewards from that state, which suggests that was a good action.

Compare this to the case where we take action 1 and receive reward +10 but our value look-up table says we expected to see +15, so the advantage is $10 - 15 = -5$, suggesting this was a relatively bad action despite the fact we still received a reasonably large positive reward.

Rather than using a look-up table of course, we will use some sort of parameterized model such as a neural network that can be trained to predict expected rewards for a given state. So we want to simultaneously train a policy neural network and a state or action-value neural network.

Algorithms of this sort are called **actor-critic** methods, where “actor” refers to the policy since that’s where the actions are generated from and “critic” refers to the value function, since that’s what (in part) tells the actor how good its actions are. Since we’re using $R-V(S)$ to train the policy rather than just $V(S)$, this is called **advantage actor-critic**.

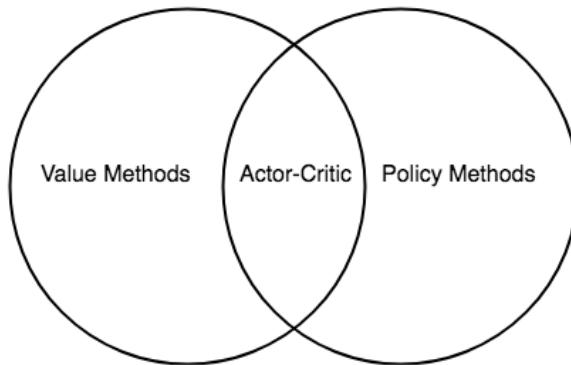


Figure 5.1

VALUE BASELINE VERSUS ACTOR-CRITIC

Technically what we have described so far would not considered a true actor-critic method by some since we’re only using the value function as a baseline and not using it to “bootstrap” by making a prediction about a future state based on the current state. We will see how bootstrapping comes into play soon.

The policy network has the issue of a sensitive loss function that depends on the rewards collected at the end of the episode. If we naively tried to make online updates then, depending on the type of environment, we may never learn anything because the rewards may be too sparse.

In Gridworld, for example, the reward is 0 on every move except for the end of the episode. So the vanilla policy gradient method wouldn’t know what action to reinforce, since the vast majority of the time all the actions end up resulting in the same reward of 0. In contrast, a Q-network can learn decent q -values even when the rewards are sparse because it **bootstraps**. When we say an algorithm bootstraps we mean it can make a prediction from a prediction.

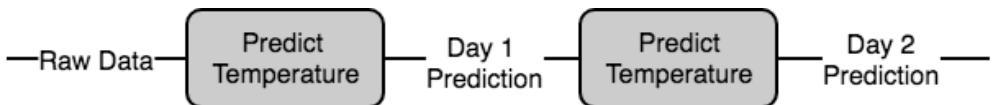


Figure 5.2

If I ask you what the weather is going to be like in 2 days from now, you might first predict what the weather will be tomorrow, and then base your 2-day prediction off that. You're bootstrapping. Of course, if your first prediction was bad, your second may be even worse, so bootstrapping introduces a source of **bias**. Bias is a systematic deviation from the true value of something, in this case, the true q-values. On the other hand, making predictions from predictions introduces a kind of "self-consistency" that results in lower **variance**. Variance is exactly what it sounds like, a lack of precision in the predictions, i.e. predictions that vary a lot. With the temperature example, if I make my day 2 temperature prediction based on my day 1 prediction, it will likely not be too far from my day 1 prediction.

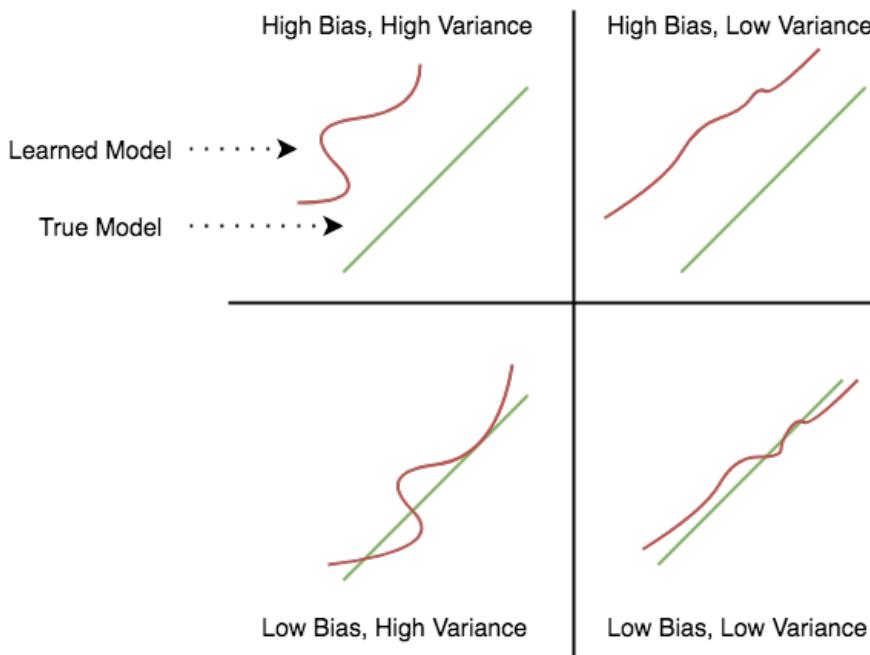


Figure 5.3: The bias-variance tradeoff is a fundamental machine learning concept that says any machine learning model will have some degree of systematic deviation from the true data distribution and some degree of variance. You can try to reduce the variance of your model but it will always come at the cost of increased bias.

Bias and variance are key concepts relevant to basically all of machine learning, not just deep learning or deep reinforcement learning. Generally, if you reduce bias you will increase variance and vice versa. For example, if I ask you to predict the temperature for tomorrow and the next day, you could tell me a specific temperature: "The 2-day temperature forecast is 20.1 C and 20.5 C." This is a high-precision prediction, you've given me a temperature prediction to a tenth of a degree! But you don't have a crystal ball, so your prediction is almost surely going to be systematically off, hence biased toward whatever your prediction procedure involved. Or you could have told me: "The 2-day temperature forecast is 15-25 C and 18-27 C." In this case, your prediction has a lot of spread or variance since we're giving fairly wide ranges, but low bias, i.e. you have a good chance of the real temperatures falling in your intervals. This spread might be because your prediction algorithm didn't give undue weight to any of the variables used for prediction, hence not particularly biased in any direction. Indeed, machine learning models are often **regularized** by imposing a penalty on the size of the parameters during training. Regularization essentially means to modify your machine learning procedure in a way to mitigate overfitting.

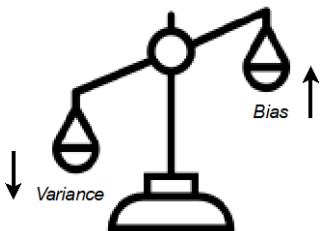


Figure 5.4: The bias-variance tradeoff. Increasing model complexity can reduce bias but will increase variance. Reducing variance will increase bias.

So we want to combine the potentially high-bias, low-variance value prediction with the potentially low-bias, high-variance policy prediction to get something with moderate bias and variance, and therefore something that will work well in the online setting. The role of the critic is hopefully starting to become clear. The actor (policy network) will take a move, but the critic (state-value network) will tell the actor how good or bad the action was, rather than only using the potentially sparse raw reward signals from the environment. Thus the critic will be a term in the actor's loss function. The critic, just like with Q-learning, will learn directly from the reward signals coming from the environment, however the sequence of rewards will depend on the actions taken by the actor, so the actor affects the critic too, albeit more indirectly.

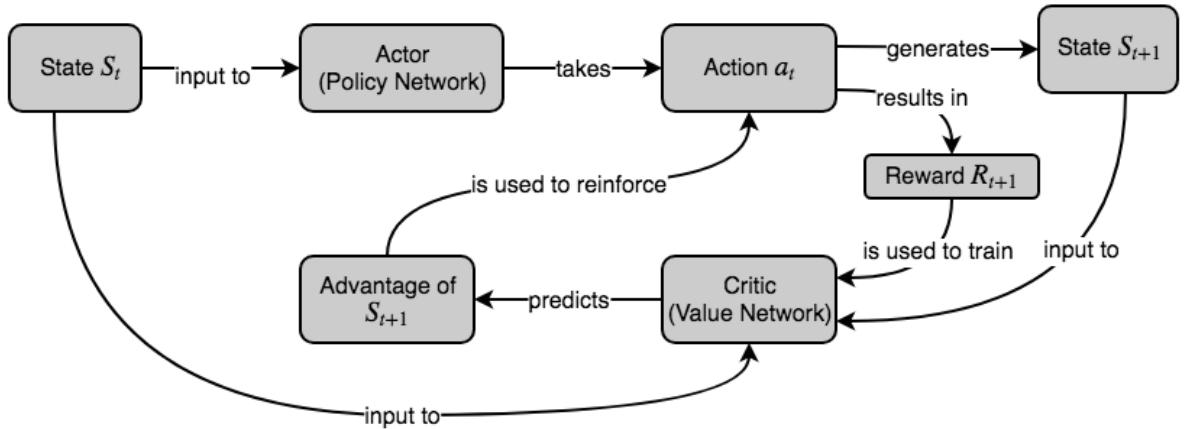


Figure 5.5: The general overview of actor-critic models. First, the actor predicts the best action and chooses the action to take, which generates a new state. The critic network computes the value of the old state and the new state. The relative value of S_{t+1} is called its advantage, and this is the signal used to reinforce the action that was taken by the actor.

The actor is trained in part by using signals coming from the critic, but how exactly do we train a state-value function as opposed to the action-value (Q)-functions we're more accustomed to? With action-values we computed the expected return (i.e. sum of future discounted rewards) for a given state-action pair. Hence we could predict whether a state-action pair would result in a nice positive reward, a bad negative reward, or something in between. But recall with our DQN, our Q -network returned separate action-values for each possible discrete action, so if we employ a reasonable policy like epsilon-greedy, then the state-value will essentially be the highest action-value. Thus the state-value function just computes this highest action-value rather than separately computing action-values for each action.

5.2 Distributed Training

We presented the advantage actor-critic part of the distributed advantage actor-critic (DA2C), now this section is about the distributed part. For virtually all deep learning models we do batch training where a random subset of our training data is batched together and we compute the loss for this entire batch before we backpropagate and do gradient descent. This is necessary because the gradients if we trained with a single datum at a time would have too much variance and the parameters would never converge on their optimal values. We need to average out the noise in a batch of data to get the real signal before updating the model parameters.

For example, if you're training an image classifier to recognize hand-drawn digits and you only train it one image at a time, the algorithm will think that the background pixels are just as important as the digits in the foreground because it can only see the signal when averaged

together with other images. The same concept applies in reinforcement learning, which is why we had to use an experience replay buffer with DQN.

Having a sufficiently large replay buffer is requires a lot of memory, and in some cases, a replay buffer is impractical. A replay buffer is possible when your reinforcement learning environment and agent algorithm follow the strict criteria of a Markov decision process, in particular, the Markov property. Recall the Markov property says that the optimal action for a state S_t can be computed without reference to any prior states S_{t+1} , i.e. there is no need to keep a history of previously visited states. For simple games this is the case, but for more complex environments, it may be necessary to remember the past in order to select the best option now.

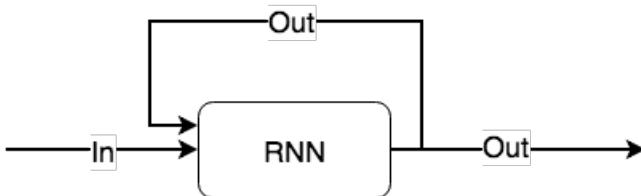


Figure 5.6: A generic recurrent neural network (RNN) layer processes a sequence of data by incorporating its previous output with the new input. Thus an RNN will not work properly with single experiences in an experience replay buffer.

Indeed, in many complex games it is common to use recurrent neural networks (RNNs) like a long short-term memory (LSTM) network or a Gated Recurrent Unit (GRU). These RNNs can keep an internal state that can store traces of the past. They are particularly useful for natural language processing (NLP) tasks where keeping track of preceding words or characters is critical to being able to encode or decode a sentence. Experience replay doesn't work with an RNN unless your replay buffer stores entire trajectories or full episodes since the RNN is designed to process sequential data.

One solution is to run multiple copies of the agent in parallel each with separate instantiations of the environment. By distributing multiple independent agents across different CPU processes, we can collect a varied set of experiences and therefore get a sample of gradients that we can average together to get a lower variance mean gradient. This eliminates the need for experience replay and allows us to train an algorithm in a completely online fashion, visiting each state only once as it appears in the environment.

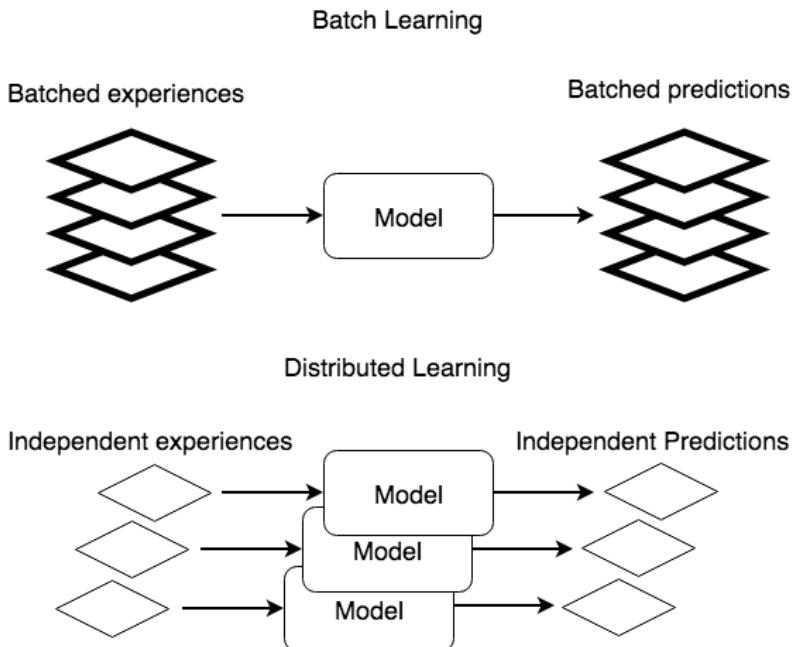


Figure 5.7: The most common form of training a deep learning model is to feed a batch of data together into the model to return a batch of predictions. Then we compute the loss for each prediction and average or sum all the losses before backpropagating and updating the model parameters. This averages out the noise present in each individual datum. Alternatively, we can run multiple models each taking a single piece of data and making a single prediction, backpropagate through each model to get the gradients and then sum or average the gradients before making any parameter updates.

MULTIPROCESSING VERSUS MULTITHREADING

Modern desktop and laptop computers have central process units (CPUs) with multiple cores, which are independent processing units capable of running computations simultaneously. Therefore, if you can split a computation into pieces that can be computed separately and combined later, you can get dramatic speedups. The operating system software abstracts the physical CPU processors into virtual processes and threads. A process contains its own memory space and threads run within a single process.

Multithreading is like when people multi-task, i.e. they can work on only one thing at a time but switch between different tasks while one task is idle; therefore tasks are not truly simultaneously performed with multithreading. Multithreading is really effective when your task requires a lot of input/output operations such as reading and writing data to the hard disk. When data is being read into RAM from the hard disk, computation on the CPU is idle waiting for the required data, so during that time the operating system can use the idle CPU time to work on a different task and then switch back when the I/O operation is done.

Running machine learning models generally does not require I/O operations; machine learning is limited by computation speed, therefore ML benefits from true simultaneous computation with multiprocessing.

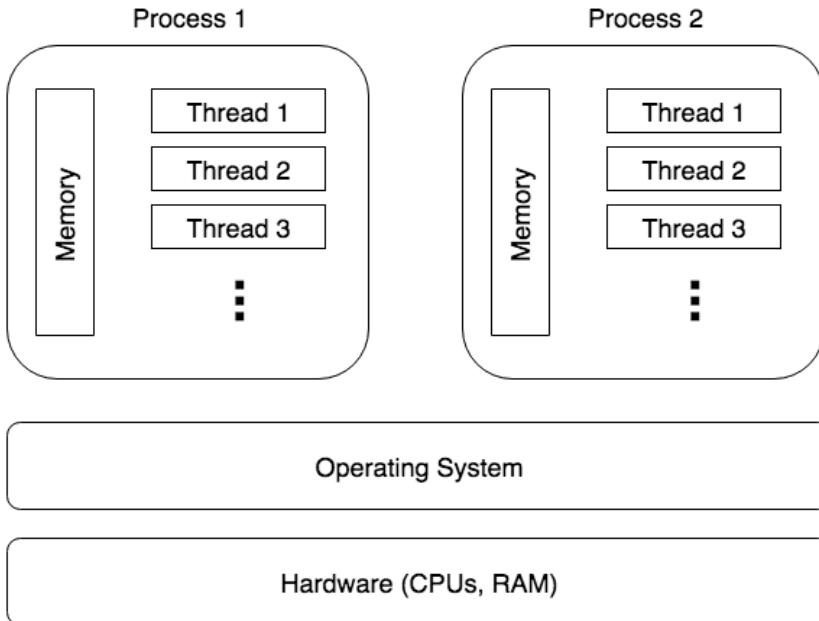


Figure 5.8: Processes are an abstraction of the underlying CPU hardware created by the operating system. If you have two CPUs, then you can run two simultaneous processes. However, the operating system will let you spawn more than 2 virtual processes and it will figure out how to multi-task between them. Each process has its own memory address space and can have multiple threads. A thread is a task that can be run and while one task is waiting for an external process to finish (such as an input/output operation), the OS can let another thread run. This maximizes the usage of whatever CPUs you have.

Large machine learning models all but require graphics processing units (GPUs) to perform efficiently, however, distributed models on multiple CPUs can be competitive in some cases. Python provides a library called `multiprocessing` that makes multiprocessing very easy. Additionally, PyTorch wraps this library and has a method for allowing a model's parameters to be shared across multiple processes. Let's see a simple example of multiprocessing.

A contrived simple example is that we have an array with the numbers 0, 1, 2, 3 ... 64 and we want to square each number. Since squaring a number does not depend on any other numbers in the array, we can easily parallelize this across multiple processors.

Listing 5.1: Introduction to multiprocessing

```
import multiprocessing as mp
import numpy as np
def square(x): #A
    return np.square(x)
x = np.arange(64) #B
>>> print(x)
array([ 0,  1,  2,  3,  4,  5,  6,  7,  8,  9, 10, 11, 12, 13, 14, 15, 16,
       17, 18, 19, 20, 21, 22, 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33,
```

```

34, 35, 36, 37, 38, 39, 40, 41, 42, 43, 44, 45, 46, 47, 48, 49, 50,
51, 52, 53, 54, 55, 56, 57, 58, 59, 60, 61, 62, 63])
>>> mp.cpu_count()
8
pool = mp.Pool(8) #C
squared = pool.map(square, [x[8*i:8*i+8] for i in range(8)]) #D
>>> squared
[array([ 0,  1,  4,  9, 16, 25, 36, 49]),
 array([ 64,  81, 100, 121, 144, 169, 196, 225]),
 array([256, 289, 324, 361, 400, 441, 484, 529]),
 array([576, 625, 676, 729, 784, 841, 900, 961]),
 array([1024, 1089, 1156, 1225, 1296, 1369, 1444, 1521]),
 array([1600, 1681, 1764, 1849, 1936, 2025, 2116, 2209]),
 array([2304, 2401, 2500, 2601, 2704, 2809, 2916, 3025]),
 array([3136, 3249, 3364, 3481, 3600, 3721, 3844, 3969])]
```

#A This function just takes an array and squares each element

#B Setup an array with a sequence of numbers

#C Setup a multiprocessing processor pool with 8 processes

#D Use the pool's map function to apply the square function to each array in the list and return the results in a list

Here we simply define a function square that takes an array and squares it. This is the function that will get distributed across multiple processes. We create some toy data that is simply the list of numbers 0 to 63 and rather than sequentially squaring them in a single process, we chop up the array into 8 pieces and compute the squares for each piece independently on a different processor.

You can see how many hardware processors your computer has using the `mp.cpu_count()` function, you can see we have 8. Many modern computers may have say 4 independent hardware processors but will have twice as many “virtual” processors via something called hyperthreading. Hyperthreading is a performance trick by some processors that can allow two processes to run essentially simultaneously on one physical processor. It is important not to create more processes than there are CPUs on your machine as the additional processes will essentially function as threads where the CPU will have to rapidly switch between processes.

We setup a processor pool of 8 processes with `mp.Pool(8)` and then use `pool.map` to distributed the square function across the 8 pieces of data. You can see we get a list of 8 arrays with all their elements squared just as we wanted. Processes will return as soon as their complete so the order of the elements in the returned list will be unpredictable and may not always been in the order they were mapped.

We’re going to need a bit more control over our processes than a processor Pool allows, so we will create and start a bunch of processes manually.

Listing 5.2: Manually starting individual processes

```

def square(i, x, queue):
    print("In process {}".format(i))
    queue.put(np.square(x))
processes = [] #A
queue = mp.Queue() #B
x = np.arange(64) #C
for i in range(8): #D
```

```

start_index = 8*i
proc = mp.Process(target=square,args=(i,x[start_index:start_index+8], queue))
proc.start()
processes.append(proc)

for proc in processes: #E
    proc.join()

for proc in processes: #F
    proc.terminate()
results = []
while not queue.empty(): #G
    results.append(queue.get())
>>> results
[array([ 0,  1,  4,  9, 16, 25, 36, 49]),
 array([256, 289, 324, 361, 400, 441, 484, 529]),
 array([ 64,   81, 100, 121, 144, 169, 196, 225]),
 array([1600, 1681, 1764, 1849, 1936, 2025, 2116, 2209]),
 array([576, 625, 676, 729, 784, 841, 900, 961]),
 array([1024, 1089, 1156, 1225, 1296, 1369, 1444, 1521]),
 array([2304, 2401, 2500, 2601, 2704, 2809, 2916, 3025]),
 array([3136, 3249, 3364, 3481, 3600, 3721, 3844, 3969])]

#A Setup a list to store a reference to each process
#B Setup a multiprocessing queue, a data structure than can be shared across processes
#C Setup some toy data, a sequence of numbers
#D Start 8 processes with the square function as the target and an individual piece of data to process
#E Wait for each process to finish before returning to the main thread
#F Terminate each process
#G Convert the multiprocessing queue into a list

```

This is more code but functionally the same as what we did before with the `Pool`, but now its easy to share data between processes using special shareable data structures in the multiprocessing library and to have more control over the processes. We modify our `square` function a little to accept an integer representing the process ID, the array to square, and a shared global data structure called a `queue` that we can put data into and extract from using the `.get()` method.

Next we setup a list to hold the instances of our processes, the shared queue object and create our toy data as before. We then enter a loop to create (in our case) 8 processes and start them using the `.start()` method, then we add them to our processes list so we can access them later. Next we run through the processes list and call each processes `.join()` method, this makes it so we wait to return anything until all the processes have finished. Then we call each processes `.terminate()` method to ensure it is killed. Lastly, we collect all the elements of the queue into a list and print it out. The results look the same as with the process Pool except their in a random order. That's really all there is to distributing a function across multiple CPU processors.

5.3 Advantage Actor-Critic

Now that we know how to distribute computation across processes, we can get back to the real reinforcement learning. In this section we put together the pieces of the full distributed advantage actor-critic model. To allow fast training and to compare to the previous chapter, we will also use the CartPole game as our test environment, however you can easily adapt the algorithm to a more difficult game such as Pong in OpenAI Gym and you can find such an implementation at this chapter's GitHub page:

< <https://github.com/DeepReinforcementLearning/DeepReinforcementLearningInAction> >

While we presented the actor and critics as two totally separate functions, we can actually combine them into a single neural network with two output "heads." That is, instead of a normal neural network that returns a single vector, ours will return two different vectors, one for the policy and one for the value. This allows for some parameter sharing between the policy and value that can make things more efficient since some of the information needed to compute values is also probably useful to predicting the best action for the policy. But if a two-headed neural network seems too exotic right now, go ahead and write two separate neural networks, it will work just fine.

Let's see some pseudocode for what the algorithm looks like and then we'll translate to Python.

Listing 5.3: Pseudocode for Online Advantage Actor-Critic

```
gamma = 0.9
for each epoch do {
    state = environment.get_state()
    value = critic(state)
    policy = actor(state)
    action = policy.sample()
    next_state, reward = environment.take_action(action)
    value_next = critic(next_state)
    advantage = reward + (gamma * value_next - value)
    loss = -1 * policy.logprob(action) * advantage
    minimize(loss)
```

This is very simplified pseudocode but it gets the main idea across. The important part to point out is the advantage calculation. Consider the case where we take action 1 receive reward +10, the value prediction is +5, and the value prediction for the next state is +7. We discount the value of the next state (since future predictions are always less valuable than currently observed reward) by the gamma discount factor, so our $advantage = 10 + 0.9*7 - 5 = 10 + (6.3 - 5) = 10 + 1.3 = +11.3$. Since the difference between the next state value and the current state value is positive, it increases the overall value of the action we just took so we will reinforce it more. Notice that the advantage function *bootsraps* because it computes a value for the current state and action based on predictions for a future state.

In this chapter we're going to use our DA2C model on Cartpole again, which is episodic, so if we do a full Monte Carlo update (i.e. update after the full episode is complete) then

`value_next` will always be 0 for the last move (since there is no next state if the episode is over), thus the advantage term actually reduces to `advantage = reward - value`, which is the value baseline we discussed at the beginning of the chapter. The full advantage expression $A = r_{t+1} + \gamma * v(s_{t+1}) - v(s_t)$ is used when we do online or **N-step learning**.

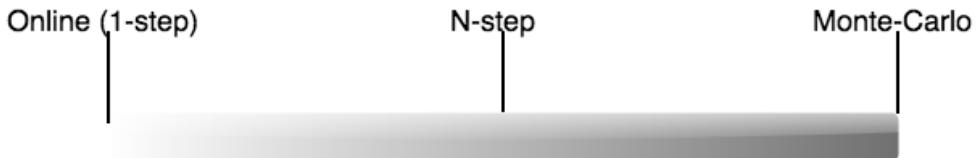


Figure 5.9

N-step learning is what's in between fully online learning and waiting for a full episode (i.e. Monte Carlo) before updating. As the name suggests, we accumulate rewards over N-steps and then compute our loss and backpropagate. The number of steps can be anywhere from 1 (which reduces to fully online learning) to the maximum number of steps in the episode (Monte Carlo), but usually we pick something in between to get the advantages of both. We will first show the episodic actor-critic algorithm and then we will adapt it to N-step with N set to 10.

Alright, we're ready to get to the coding of an actor-critic model to play Cartpole. As usual, let's sketch out the sequence of steps.

1. Setup our actor-critic model, a two-headed model (alternatively you can setup two independent actor and critic networks). The model accepts a Cartpole state as input, which is a vector of 4 real numbers. The actor head is just like the policy network (actor) from the previous chapter, so it outputs a 2-dimensional vector representing a discrete probability distribution over the 2 possible actions. The critic outputs a single number representing the state-value. The critic is denoted $v(s)$ and the actor is denoted $\pi(s)$. Remember that $\pi(s)$ returns the log-probabilities for each possible action, in our case 2 actions.
2. While in current episode
 - 2.1 Define hyper parameter: γ (gamma, discount factor)
 - 2.2 Start a new episode, in initial state s_t
 - 2.3 Compute value $v(s_t)$ and store in list.
 - 2.4 Compute $\pi(s_t)$, store in list, sample and take action a_t
 - Receive new state s_{t+1} and reward r_{t+1} . Store reward in list.
3. Training.
 - 3.1 Initialize $R=0$. Loop through rewards in reverse order to generate returns

$$R=r_t + \gamma * R$$

3.2 Minimize the actor loss:

$$-I * \gamma_t * (R - v(s_t)) * \pi(a | s)$$

3.3 Minimize critic loss:

$$(R - v)^2$$

4. Repeat for new episode.

Listing 5.4 Cartpole Actor-Critic Model

```
import torch
from torch import nn
from torch import optim
import numpy as np
from torch.nn import functional as F
import gym
import torch.multiprocessing as mp #A
class ActorCritic(nn.Module): #B
    def __init__(self):
        super(ActorCritic, self).__init__()
        self.l1 = nn.Linear(4,25)
        self.l2 = nn.Linear(25,50)
        self.actor_lin1 = nn.Linear(50,2)
        self.l3 = nn.Linear(50,25)
        self.critic_lin1 = nn.Linear(25,1)
    def forward(self,x):
        x = F.normalize(x,dim=0)
        y = F.relu(self.l1(x))
        y = F.relu(self.l2(y))
        actor = F.log_softmax(self.actor_lin1(y),dim=0) #C
        c = F.relu(self.l3(y.detach()))
        critic = torch.tanh(self.critic_lin1(c)) #D
        return actor, critic #E
```

#A PyTorch wraps Python's built-in multiprocessing library and the API is the same
#B Define a single combined model for the actor and critic
#C The actor head returns the log-probabilities over the 2 actions
#D The critic returns a single number bounded between -1 and +1
#E We simply return the actor and critic results as a tuple

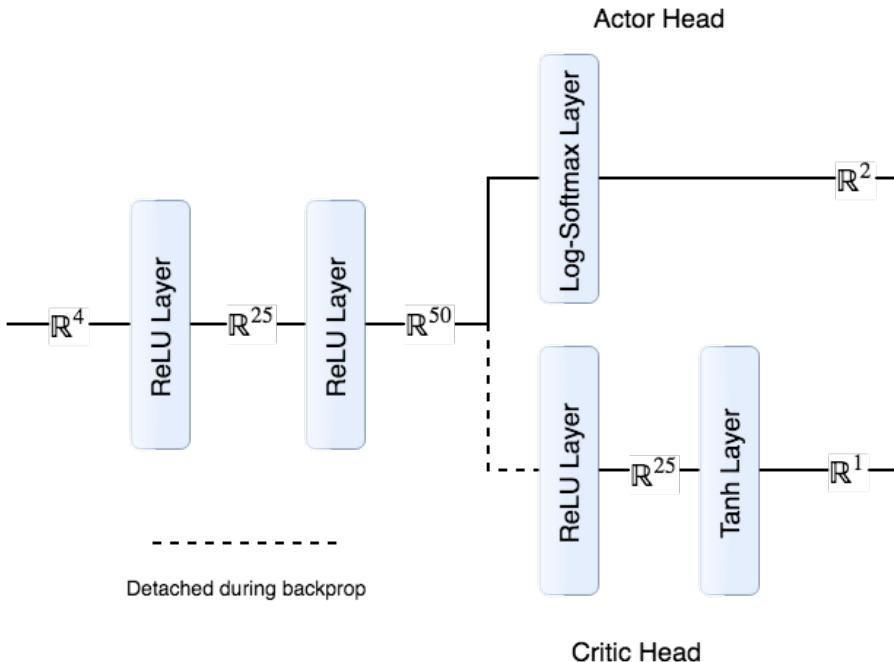


Figure 5.10: This is an overview of the architecture for our two-headed actor-critic model. It's overall very simple with two shared linear layers and then a branching point where the output of the first two layers is sent to a log-softmax layer of the actor head and also sent to another ReLU layer of the critic head before finally passing through a tanh layer. This model returns a 2-tuple of tensors rather than a single tensor.

For CartPole, we have a fairly simple neural network other than having two output heads. First we normalize the input so that the state values are all within the same range, then the first two layers are ordinary linear layers with the ReLU activation function. Then we fork the model into two paths. The first path is the actor head that takes the output of layer 2 and applies another linear layer and then the `log_softmax(...)` function. The `log_softmax` is logically equivalent to doing `log(softmax(...))` but the combined function is more numerically stable since if you compute the functions separately you might end up with overflowed or underflowed probabilities after the `softmax`.

The second path is the critic head, which applies a linear layer and ReLU to the output of layer 2, but notice we call `y.detach()`, which detaches the `y` node from the graph and thus the critic loss won't backpropagate and modify the weights in layer 1 and 2, only the actor will cause the weights to be modified. This is not a crucial feature but it improves the training time a bit by reducing the conflict between what the actor and critic want. With two-headed models, it often makes sense to make one head the dominant head and control most of the parameters by detaching the other head from the first several layers. Lastly, the critic applies

another linear layer with the tanh activation function that bounds the output to the interval $(-1,1)$, which is perfect for Cartpole since the rewards are $+1$ and -1 .

Listing 5.5: Distributing the training

```

MasterNode = ActorCritic() #A
MasterNode.share_memory() #B
processes = [] #C
params = {
    'epochs':1000,
    'n_workers':7,
}
counter = mp.Value('i',0) #D
for i in range(params['n_workers']):
    p = mp.Process(target=worker, args=(i,MasterNode,counter,params)) #E
    p.start()
    processes.append(p)
for p in processes: #F
    p.join()
for p in processes: #G
    p.terminate()

print(counter.value,processes[1].exitcode) #H

#A Create a global, shared actor-critic model
#B The share_memory() method will allow the parameters of the model to be shared across processes rather than
copied
#C Setup a list to store our instantiated processes
#D Shared global counter using multiprocessing's built-in shared object. The 'i' parameter indicates the type as integer.
#E Start a new process that runs the worker function
#F "Join" each process to wait for it to finish before returning to main process
#G Make sure each process is terminated
#H Print the global counter value and the first process' exit code (should be 0)

```

This is exactly the same setup we had when demonstrating how to split up an array across multiple processes, except this time we're going to be running a function called `worker` that will run our CartPole reinforcement learning algorithm.

Listing 5.6: The main training loop

```

def worker(t, worker_model, counter, params):
    worker_env = gym.make("CartPole-v1")
    worker_env.reset()
    worker_opt = optim.Adam(lr=1e-4, params=worker_model.parameters()) #A
    worker_opt.zero_grad()
    for i in range(params['epochs']):
        worker_opt.zero_grad()
        values, logprobs, rewards = run_episode(worker_env,worker_model) #B
        actor_loss,critic_loss,eplen =
        update_params(worker_opt,values,logprobs,rewards) #C
        counter.value = counter.value + 1 #D

```

```

#A Each process runs its own isolated environment and optimizer but share the model
#B The run_episode function plays an episode of the game, collecting data along the way
#C We use the collected data from run_episode to run one parameter update step

```

```
#D counter is a globally shared counter between all the running processes
```

The `worker` function is the function that each individual process will run separately. Each worker (i.e. process) will create its own CartPole environment and its own optimizer but will share the actor-critic model, which is passed in as an argument to the function. Since the model is shared, whenever a worker updates the model parameters it is also updated for all the other workers.

Since each worker is spawned in a new process that has its own memory, all the data the worker should be passed in as an argument to the function explicitly. This also prevents bugs.

Listing 5.7: Running an episode

```
def run_episode(worker_env, worker_model):
    state = torch.from_numpy(worker_env.env.state).float() #A
    values, logprobs, rewards = [],[],[] #B
    done = False
    j=0
    while (done == False): #C
        j+=1
        policy, value = worker_model(state) #D
        values.append(value)
        logits = policy.view(-1)
        action_dist = torch.distributions.Categorical(logits=logits)
        action = action_dist.sample() #E
        logprob_ = policy.view(-1)[action]
        logprobs.append(logprob_)
        state_, _, done, info = worker_env.step(action.detach().numpy())
        state = torch.from_numpy(state_).float()
        if done: #F
            reward = -10
            worker_env.reset()
        else:
            reward = 1.0
        rewards.append(reward)
    return values, logprobs, rewards
```

#A Convert the environment state from a numpy array to a PyTorch Tensor

#B Create lists to store the computed state-values (critic), log-probabilities (actor), and rewards

#C Keep playing the game until the episode ends

#D Compute the state-value and log-probabilities over actions

#E Using the actor's log-probabilities over actions, create and sample from a categorical distribution to get an action

#F If the last action caused the episode to end, set the reward to -10 and reset the environment

The `run_episode` function just runs through a single episode of CartPole and collects the computed state-values from the critic, log-probabilities over actions from the actor, and rewards from the environment. We store these in lists and use them to compute our loss function later. Since this is an actor-critic method and not Q-learning, we take actions by directly sampling from the policy rather than arbitrarily choosing a policy like epsilon-greedy in Q-learning. There's nothing too out of the ordinary in this function, so let's move on to the updating function.

Listing 5.8: Computing and minimizing the loss

```
def update_params(worker_opt, values, logprobs, rewards, clc=0.1, gamma=0.95):
    rewards = torch.Tensor(rewards).flip(dims=(0,)).view(-1) #A
    logprobs = torch.stack(logprobs).flip(dims=(0,)).view(-1)
    values = torch.stack(values).flip(dims=(0,)).view(-1)
    Returns = []
    ret_ = torch.Tensor([0])
    for r in range(rewards.shape[0]): #B
        ret_ = rewards[r] + gamma * ret_
        Returns.append(ret_)
    Returns = torch.stack>Returns().view(-1)
    Returns = F.normalize(Returns, dim=0)
    actor_loss = -1*logprobs * (Returns - values.detach()) #C
    critic_loss = torch.pow(values - Returns, 2) #D
    loss = actor_loss.sum() + clc*critic_loss.sum() #E
    loss.backward()
    worker_opt.step()
    return actor_loss, critic_loss, len(rewards)
```

#A We reverse the order of the rewards, logprobs and values_ arrays and call .view(-1) to make sure they're flat

#B For each reward (in reverse order), we compute the return value and append it to a returns array

#C We need to detach the values_tensor from the graph to prevent backpropagating through the critic head

#D The critic just attempts to learn to predict the return

#E We sum the actor and critic losses to get an overall loss. We scale down the critic loss by the `clc` factor.

The `update_params` function is where all the action is and what sets distributed advantage actor-critic apart from the other algorithms we've learned so far. First we take the lists of rewards, log-probabilities, and state-values and convert them to PyTorch tensors. We then reverse their order because we want to consider the most recent action first, and then we make their they are flattened 1-D arrays by calling the `.view(-1)` method.

The `actor_loss` is computed just we described with math using the advantage (technically baseline since there's no bootstrapping) rather than raw reward. Crucially, we must detach the `values` tensor from the graph when we use in the `actor_loss`, otherwise we will backpropagate through the actor and critic heads, and we only want to update the actor head. The critic loss is a simple squared error between the state-values and the returns and we make sure *not* to detach here since we want to update the critic head. Then we sum the actor and critic losses to get the overall loss. We scale down the critic loss by multiplying by 0.1 because we want the agent to learn faster than the critic. We return the individual losses and the length of the rewards tensor (which indicates how long the episode lasted) to monitor their progress during training.

Put it all together and run it and you'll get a trained CartPole agent within 1 minute on a modern computer running just on a few CPU cores. If you plot the loss over time for this it probably won't be a nice down-trending line like you hope because the actor and critic are in competition with one another. The critic is incentivized to model the returns as best as it can (and the returns depend on what the actor does), but the actor is incentivized to beat the expectations of the critic. If the actor improves faster than the critic, then the critic's loss will be high and vice versa, so there is a somewhat adversarial relationship between the two.

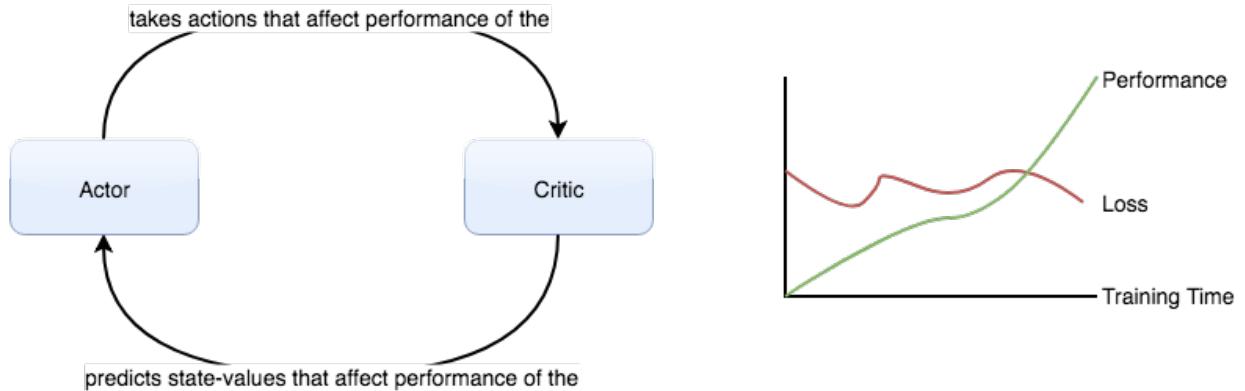


Figure 5.11: The actor and critic have a bit of an adversarial relationship since the actions that the agent take affect the loss of the critic, and the critic makes predictions of state-values that get incorporated into the return that affects the training loss of the actor. Hence the overall loss plot may look chaotic despite the fact that the agent is indeed increasing in performance.

Adversarial training like this is a very powerful technique in many areas of machine learning, not just reinforcement learning. For example, generative adversarial networks (GANs), are an unsupervised method to generate realistic-appearing synthetic samples of data from a training data set using a pair of models that function similarly to an actor and critic. In fact, we will build an even more sophisticated adversarial model in Chapter 8 so you will learn more then. But the take home here is that if you're using an adversarial model, the loss will be largely uninformative (unless it goes to 0 or explodes toward infinity, then something is probably wrong). You have to rely on actually evaluating the objective you care about, in our case how well the agent is performing in the game. Here is the plot of average episode length during the first 45 seconds of training:

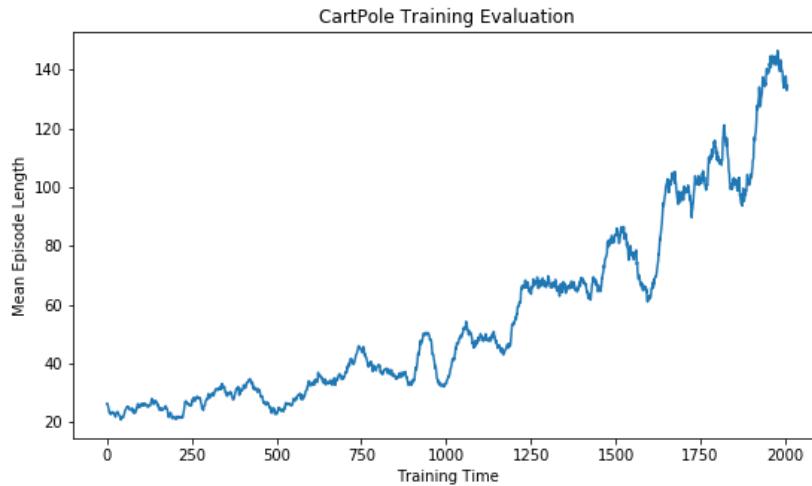


Figure 5.12 The mean episode length over training time for our Monte Carlo distributed advantage actor-critic model. This model is not considered a true critic since the critic is not bootstrapping during training. As a result the training performance has high variance.

5.4 N-Step Actor-Critic

In the last section we implemented distributed advantage actor-critic, except that we trained in “Monte Carlo mode,” i.e. we ran a full episode before updating the model parameters. While that makes total sense for a simple game like CartPole, most of the time we want to be able to make more frequent updates. We briefly touched on N-step learning before, but to re-iterate, it means we simply calculate our loss and update the parameters after N-steps where N is whatever we choose it to be. If N is 1 then it is fully online learning or we could set N to be very large and then it will be Monte Carlo again. The sweet spot is somewhere in-between.

With Monte Carlo full-episode learning, we don’t take advantage of bootstrapping since there’s nothing to bootstrap. We do bootstrap in online learning like we did with DQN, however, with 1-step learning the bootstrap may introduce a lot of bias. This bias may be harmless if it still pushes our parameters in the right direction, but in some cases the bias can be so off that we never move in the right direction.

This is why N-step learning is usually better than 1-step (online) learning, the target value for the critic is more accurate so the critic’s training will be more stable and will be able to produce less biased state-values. With bootstrapping, we’re making a prediction from a prediction, so the predictions will be better if you’re able to collect more data before making them. And we like bootstrapping because it improves sample efficiency since you don’t need to see as much data (e.g. frames in a game) before updating the parameters in the right direction.

So let's see how to modify our code to do N-step learning. The only function we need to modify is the `run_episode` function. We need to change it run for only N-steps rather than wait for the episode to finish. If the episode finishes before N-steps, then the last return value will be set to 0 (since there is no next state when the game is over) as it was in the Monte Carlo case. However, if the episode hasn't finished by N-steps, then we use the last state-value as our prediction for what the return would have been had we kept playing, that's where the bootstrapping happens. Without bootstrapping, the critic is just trying to predict the future returns from a state and it gets the actual returns as training data. With bootstrapping, it is still trying to predict future returns but it is doing so in part by using its own prediction about future returns (since the training data will include its own prediction).

Listing 5.9: N-step training with CartPole

```
def run_episode(worker_env, worker_model, N_steps=10):
    raw_state = np.array(worker_env.env.state)
    state = torch.from_numpy(raw_state).float()
    values, logprobs, rewards = [],[],[]
    done = False
    j=0
    G=torch.Tensor([0]) #A
    while (j < N_steps and done == False): #B
        j+=1
        policy, value = worker_model(state)
        values.append(value)
        logits = policy.view(-1)
        action_dist = torch.distributions.Categorical(logits=logits)
        action = action_dist.sample()
        logprob_ = policy.view(-1)[action]
        logprobs.append(logprob_)
        state_, _, done, info = worker_env.step(action.detach().numpy())
        state = torch.from_numpy(state_).float()
        if done:
            reward = -10
            worker_env.reset()
        else: #C
            reward = 1.0
            G = value.detach()
        rewards.append(reward)
    return values, logprobs, rewards, G
```

#A The variable `G` refers to the return. We initialize to 0

#B Play game until N-steps or when episode is over

#C If episode is not done, set return to the last state-value

The only things we've changed are the conditions for the while loop (exit by N-steps) and we've set the return to be the state-value of the last step if the episode is not over, thereby enabling bootstrapping. You might be surprised at how much more efficient N-step learning is, here's the plot of episode length over the first 45 seconds of training for this model:

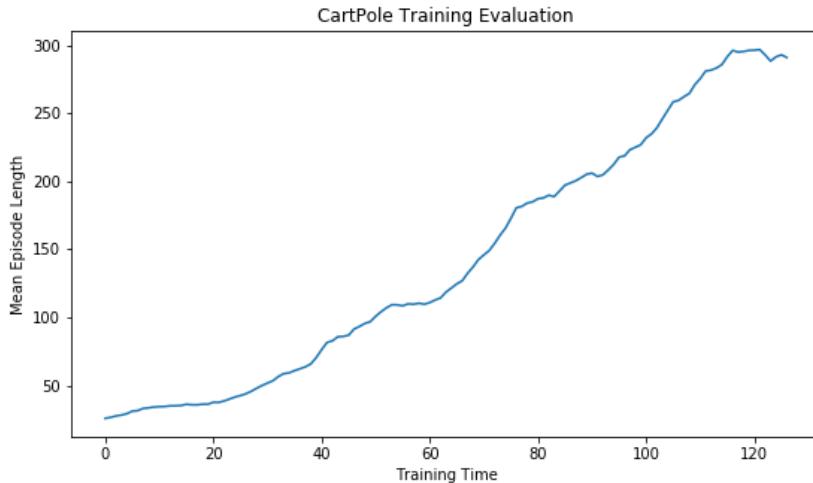


Figure 5.13: Performance plot for distributed advantage actor-critic with true N-step bootstrapping. Compared to our previous Monte Carlo algorithm, the performance is much smoother due to the more stable critic.

Notice that the N-step model starts getting better right away and reaches an episode length of 300 after just 45 seconds, compared to only about 140 for the Monte Carlo version. Also notice that this plot is much smoother than the Monte Carlo one. Bootstrapping reduces the variance in the critic and allows it to learn much more rapidly than Monte Carlo.

As a concrete example, imagine the case where you get 3-step rewards of [1,1,-1] for episode 1 and then [1,1,1] for episode 2. The overall return for episode 1 is 0.01 (with $\gamma=0.9$) and 1.99 for episode 2; that's two orders of magnitude difference in return just based on the random outcome of the episode early in training. That's a lot of variance. Compare that to the same case except with (simulated) bootstrapping so that the return for each of those episodes also includes the bootstrapped predicted return. With a bootstrapped return prediction of 1.0 for both (hence assuming the states are similar), the calculated returns are 0.99 and 2.97, which are much closer than without bootstrapping. You can reproduce this toy example with the following code:

Listing 5.10: Returns with and without bootstrapping

```
#Simulated rewards for 3 steps
r1 = [1,1,-1]
r2 = [1,1,1]
R1,R2 = 0.0,0.0
#No bootstrapping
for i in range(len(r1)-1,0,-1):
    R1 = r1[i] + 0.99*R1
for i in range(len(r2)-1,0,-1):
    R2 = r2[i] + 0.99*R2
print("No bootstrapping")
print(R1,R2)
```

```
#With bootstrapping
R1,R2 = 1.0,1.0
for i in range(len(r1)-1,0,-1):
    R1 = r1[i] + 0.99*R1
for i in range(len(r2)-1,0,-1):
    R2 = r2[i] + 0.99*R2
print("With bootstrapping")
print(R1,R2)
>>> No bootstrapping
0.0100000000000009 1.99
With bootstrapping
0.9901 2.9701
```

5.5 Summary and what's next

In this chapter we covered the advantage actor-critic algorithm and made it run on multiple processes, hence we called it distributed advantage actor-critic (DA2C). In the plain policy gradient method of the previous chapter, we only trained a policy function that would output a probability distribution over all the actions such that the predicted best action would be assigned the highest probability. Unlike Q-learning where a target value is learned, the policy function is directly reinforced to increase or decrease the probability of the action taken depending on the reward. Many times the same action may produce opposite results in terms of reward, causing high variance in the training.

To mitigate this, we introduce a critic model (or in this chapter we used a single, two-headed model) that reduces the variance of the policy function updates by directly modeling the state-value. This way, if the actor (policy) takes an action and gets an unusually big or small reward, the critic can moderate this big swing and prevent an unusually large (and possibly destructive) parameter update to the policy). This also leads to the notion of advantage where instead of training the policy based on raw return (average accumulated rewards), we train based on how much better (or worse) the action was compared to what we predicted it would be from the critic. This is helpful since if two actions both lead to the same positive reward, we will naively assume their equivalent actions, but if we compare to what we expected to happen and one reward performed much better than anticipated, that action should be reinforced more.

As with the rest of deep learning methods, we generally must use batches of data in order to effectively train. Training a single example, a time introduces too much noise and the training will likely never converge. To introduce batch training with Q-learning we used an experience replay buffer that we could randomly select batches of previous experiences. We could have used experience replay with actor-critic, but it is more common to use distributed training with actor-critic (and to be clear, Q-learning can also be distributed). One reason is that in many cases we want to use a recurrent neural network (RNN) layer as part of our reinforcement learning model in cases where keeping track of prior states is necessary or helpful in achieving the goal. But RNNs need a sequence of temporally related examples, and experience replay relies on a batch of independent experiences. We could store entire trajectories (sequences of experiences) in a replay buffer, but that just adds additional

complexity. Instead, with distributed training with each process running online with its own environment, the models can easily incorporate RNNs.

While not covered here, there's another way to train an online actor-critic algorithm besides distributed training and that's by simply utilizing multiple copies of your environment and then batching together the states from each independent environment, feeding it into a single actor-critic model that will then produce independent predictions for each environment. This is a viable alternative to distributed training when the environments are not expensive to run. If your environment is a complicated, high-memory and computer intensive simulator, then it's probably going to be very slow to run multiple copies of it in a single process, so in that case use a distributed approach.

After this chapter, we have covered what we consider to be the most foundational parts of reinforcement learning today. You should be comfortable with the basic mathematical framework of reinforcement learning as a Markov decision process (MDP) and you should be able to implement Q-learning, plain policy gradient, and actor-critic models. If you've followed so far, you should have a good base to be able to tackle many other reinforcement learning domains. In the rest of the book, we cover more advanced reinforcement learning methods with the aim of teaching you

6

Alternative Optimization Methods: Evolutionary Strategies

This chapter covers:

- What are evolutionary strategies
- Pros and cons of evolutionary approaches vs previous algorithms
- Implementing the CartPole game without backpropagation
- Why Evolutionary Strategies scale better than other algorithms

6.1 A Different Approach to Reinforcement Learning

Our next algorithm is a bit different from the previous approaches we took. For DQN and Policy Gradient, we created one agent whose policy depended on a neural network to approximate the Q-function or policy function. The agent would interact with the environment, collect experiences, and then use backpropagation to improve the accuracy of its neural network and hence, it's policy. We needed to carefully tune several hyperparameters ranging from selecting the right optimizer function, picking an initial learning rate along with a learning rate schedule such that the agent would learn within a reasonable amount of time, minibatch size (and replay buffer if needed) to name a few. Since training DQN and policy gradient algorithms both rely on stochastic gradient descent, which as the name suggests, relies on noisy gradients, there is no guarantee that these models will successfully learn (i.e. converge on a local or global optimum).

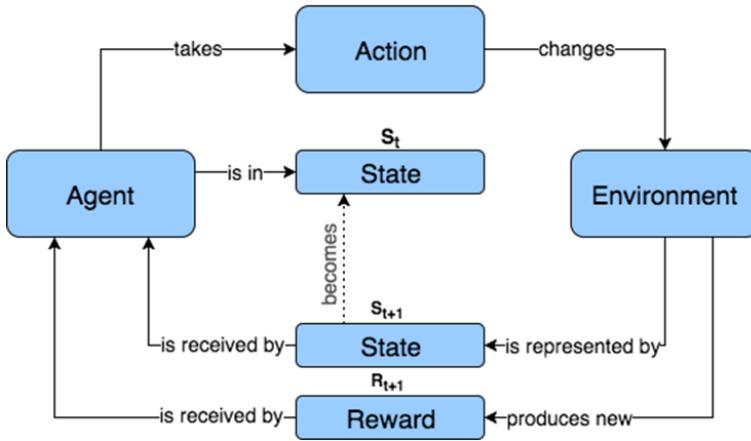


Figure 6.1: For the past algorithms that we covered, our agent interacted with environment, collected experiences, and then learned from those experiences. We repeated the same process over and over for each epoch until the agent stopped learning.

Depending on the environment and complexity of the network, creating an agent with the right hyperparameters may be incredibly difficult. Moreover, in order to use gradient descent and backpropagation we need a model that is differentiable. There are certainly models you could construct that might be interesting useful models but are impossible to train with gradient descent due to the lack of differentiability. But instead of creating one agent and improving it, what if we instead took a page from Charles Darwin and relied on evolution by (un)natural selection. We could spawn multiple different agents with different parameters (weights), observe which ones did the best, and breed the best agents such that the descendants could inherit their parents desirable traits – just like in natural selection. We could emulate biological emulation using algorithms. We would not need to struggle to tune hyperparameters and wait the multiple epochs to see if an agent is learning “correctly” – we would just pick the agents that are already performing better.

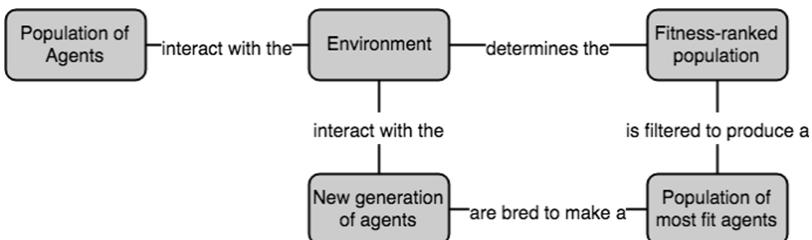


Figure 6.2: Evolutionary algorithms are different from gradient descent-based optimization techniques. With Evolutionary Strategies, we generate agents and pass the most favorable weights down to the subsequent agents.

This class of algorithms does not require an individual agent to learn - it does not rely on gradient descent - and is aptly called a **gradient-free algorithm**. But just because individual agents are not being nudged toward some objective directly, does not mean that we are relying on pure chance. The renowned evolutionary biologist Richard Dawkins once said, "Natural selection is anything but random." Similarly, in our quest to build, or more accurately discover, the best agent, we will not be relying on pure chance, but instead selecting for the fittest amongst a population with variance in traits.

6.2 Reinforcement Learning with Evolution Strategies

In this section, we'll talk about how fitness plays into evolution strategies, and we'll briefly cover the task of selecting for the fittest agents. Next, we'll work on how to recombine those agents into new agents and show what happens when we introduce mutations. This evolution is a multiple-generation process, so we'll discuss that and recap the full training loop.

6.2.1 Fitness

If you remember from your high school biology class, natural selection selects for the "most fit" individuals from each generation. In biology this represents the individuals that had the greatest reproductive success, and hence passed on their genetic information to subsequent generations. Birds with beak shapes more adept at procuring seeds from trees would have more food and thus be more likely to survive to pass that beak-shape gene to its children and grandchildren. But remember, "most fit" is relative to an environment. A polar bear is well adapted to the polar ice caps but would be very unfit in the Amazonian rainforests. You can think of the environment as determining an objective or fitness function that assigns individuals a fitness score based on their performance within that environment, and their performance is determined solely by their genetic information.

In evolutionary reinforcement learning we are selecting for traits that give our agents the highest reward in a given environment, and by traits, we mean model parameters (e.g. the weights of a neural network) or entire model structures. An RL agent's fitness can be determined by the expected reward it would receive if it were to perform in the environment. Let's say Agent A played the Atari game Breakout is able to achieve on average a score of 500 while Agent B is only able to obtain 300 points. We would say that Agent A is more fit than Agent B and that we want our optimal agent to be more similar to Agent A than B. And remember, the only reason why Agent A would be more fit than Agent B is because its model parameters are slightly more optimized to the environment.

The objective in evolutionary reinforcement learning is exactly the same as what we're used to. The only difference is we use this evolutionary process, which is often referred to as a genetic algorithm, to optimize the parameters of a model such as a neural network. The process is quite simple, but let's run through the steps of a genetic algorithm in more detail. We'll keep the description general but later we'll apply these specifically to a reinforcement learning problem.

Let's say we have some function $f(x, \text{params})$, which may be a neural network model or some other machine learning model, which takes some input x and a vector of parameters (`params`) and we want to find the set of parameters where the output of the function f given x takes on some maximum or minimum value. If f were the cost function of a neural network, then we'd want to find the set of parameters that minimizes the cost given the input. With gradient descent, we'd compute the gradient of the function with respect the parameters and use that gradient information to take small, stochastic steps toward a minimum of the function (stochastic gradient descent). Let's see how this same problem is solved with a genetic algorithm.

- We generate an initial population of random potential solutions (i.e. a population of parameter vectors). We refer to each parameter vector in the population as an individual. Let's say this initial population has 100 individuals.
- Then we iterate through this population and assess the fitness of each individual by running the model with that parameter set and recording the model output. Each individual is assigned a fitness score based on its performance on the training data.
- We randomly sample a pair of individuals ("parents") from the population weighted according to their relative fitness score (individuals with higher fitness have a higher probability of being selected) to create a "breeding population".

NOTE: There are many different methods of selecting "parents" for the next generation. One way is to simply map a probability of selection onto each individual based on their relative fitness score, and then sample from this distribution. In this way, the most fit will be selected most often, but still leaving a small chance of poor performers to mate. This may help maintain population diversity. Another way is to simply rank/sort all the individuals and take the top N individuals and use those to mate to fill the next generation. Just about any method that preferentially selects the top performers to mate will work.

- The individuals in this breeding population will then "mate" to produce "offspring" that will form a new, full population of 100 individuals. For example, if the individuals are simply vectors of real numbers (e.g. parameter vectors), then mating vector 1 with vector 2 involves taking a subset from vector 1 and combining it with a complementary subset of vector 2 to make a new offspring vector of the same dimensions. For example, Vector 1: [1 2 3], Vector 2: [4 5 6]. Vector 1 mates with Vector 2 to produce [1 5 6] and [4 2 3]. We simply randomly pair up individuals from the breeding populations and recombine them to produce 2 new offspring until we fill up a new population.
- So now we have a new population with the top solutions from the last generation along with new offspring solutions, at this point, we will iterate over our solutions and randomly mutate some of them to make sure to introduce new "genetic diversity" into every generation to prevent premature convergence on a local optimum. Mutation simply means adding a little random noise to the parameter vectors. If these were binary vectors, mutation would be randomly flipping bits. Importantly, the mutation

- rate needs to be fairly low otherwise we risk ruining the already present good solutions.
- Repeat this process for N number of generations or until we reach convergence (i.e. the average population fitness has stopped improving significantly).

Before we dive into the reinforcement learning application, we'll run a super simple genetic algorithm on a toy problem for illustrative purposes. We will create a population of a random strings and try to evolve them toward a target string of our choosing, such as "Hello World!" So we'll start out with random strings like "gMIgSkybXZyP" and "adIBOM XIrBH," then we use a function that can tell us how similar these strings are to the target string "Hello World!" to give us the fitness scores. So strings that are more similar to "Hello World!" are more likely to be selected to be in the next generation.

We score all the initial random strings in the population and then we sample pairs of parents from the population weighted according to their relative fitness scores such that individuals with higher fitness scores are more likely to be chosen to become parents. We then "mate" these parents (also called crossing or recombining) to produce two offspring strings and add them to the next generation. We also mutate the offspring by randomly flipping a few characters in the string. We iterate this problem and eventually we expect that the population will become enriched with strings very close to our target, and probably at least one will hit our target exactly (at which point we stop the algorithm). Admittedly, we're unable to think of how this particular example might be useful in the real world, but it's one of the simplest examples of a genetic algorithm and the concepts will directly apply to our reinforcement learning tasks.

Listing 6.1 Evolving Strings

```
import random
from matplotlib import pyplot as plt

alphabet = "abcdefghijklmnopqrstuvwxyzABCDEFGHIJKLMNOPQRSTUVWXYZ,.!" #A
target = "Hello World!" #B

class Individual: #C
    def __init__(self, string, fitness=0):
        self.string = string
        self.fitness = fitness

from difflib import SequenceMatcher

def similar(a, b): #D
    return SequenceMatcher(None, a, b).ratio()

def spawn_population(length=26, size=100): #E
    pop = []
    for i in range(size):
        string = ''.join(random.choices(alphabet, k=length))
        individual = Individual(string)
        pop.append(individual)
    return pop
```

#A This is the list of characters we sample from to produce random strings

```
#B This is the string we're trying to evolve from a random population
#C We set up a simple class to store information about each member of the population
#D This method will compute a similarity metric between two strings, giving us a fitness score
#E This method will produce an initial random population of strings
```

So far this code will create an initial population of individuals which are class objects composed of a string field and a fitness score field. We create the random strings by sampling from a list of alphabetic characters. After we have a population, we need to evaluate the fitness of each individual. As we'll see later, this is going to be a function of our loss function when we're using a machine learning model, but for strings, we can compute a similarity metric using a built-in Python function.

Listing 6.1 (continued)

```
def recombine(p1_, p2_): #A
    p1 = p1_.string
    p2 = p2_.string
    child1 = []
    child2 = []
    cross_pt = random.randint(0,len(p1))
    child1.extend(p1[0:cross_pt])
    child1.extend(p2[cross_pt:])
    child2.extend(p2[0:cross_pt])
    child2.extend(p1[cross_pt:])
    c1 = Individual(''.join(child1))
    c2 = Individual(''.join(child2))
    return c1, c2

def mutate(x, mut_rate=0.01): #B
    new_x_ = []
    for char in x.string:
        if random.random() < mut_rate:
            new_x_.extend(random.choices(alphabet,k=1))
        else:
            new_x_.append(char)
    new_x = Individual(''.join(new_x_))
    return new_x
```

```
#A This function recombines two parent strings into two new offspring
#B This function will mutate a string by randomly flipping characters
```

The recombination function simply takes two parent strings like “hello there” and “fog world” and randomly recombines them by generating a random integer up to the length of the strings and taking the first piece of parent 1 and the second piece of parent 2 to create an offspring, such as “fog there” and “hello world” if the split happened in the middle. This means if we have evolved a string that contains part of what we want like “hello” and another string that contains another part of what we want like “world” then the recombination process might give us all of what we want.

The mutation process takes a string like “hellb” and with some small probability (the mutation rate) will replace a character in the string with a random one. For example, if the

mutation rate was 20% (0.2) then it is probably that at least one of the 5 characters in "hellb" will be mutated to a random character, hopefully it will be mutated into "hello" if that was our target. The purpose of mutation is to introduce new information (variance) into the population. If all we did was recombine then it is likely all the individuals in the population would become too similar too fast and we wouldn't find the solution we want because information gets lost each generation if there is no mutation. Note that the mutation rate is critical. If it's too high then the fittest individuals will lose their fitness by mutation and if it's too low we won't have enough variance to find the optimal individual. Unfortunately, you just have to find the right mutation rate empirically.

Listing 6.1 (continued)

```
def evaluate_population(pop, target): #A
    avg_fit = 0
    for i in range(len(pop)):
        fit = similar(pop[i].string, target)
        pop[i].fitness = fit
        avg_fit += fit
    avg_fit /= len(pop)
    return pop, avg_fit

def next_generation(pop, size=100, length=26, mut_rate=0.01): #B
    new_pop = []
    while len(new_pop) < size:
        parents = random.choices(pop,k=2, weights=[x.fitness for x in pop])
        offspring_ = recombine(parents[0],parents[1])
        child1 = mutate(offspring_[0], mut_rate=mut_rate)
        child2 = mutate(offspring_[1], mut_rate=mut_rate),
        offspring = [child1, child2]
        new_pop.extend(offspring)
    return new_pop

#A This function assigns a fitness score to each individual in the population
#B This function generates a new generation by recombination and mutation
```

These are the last two functions we need to complete the evolutionary process. We have a function that evaluates each individual in the population and assigns a fitness score, which is just how similar the individual's string is to the target string. The fitness score will vary depending on what the objective is for a given problem. Lastly, we have a function to generate a new population by sampling the most fit individuals in the current population, recombining them to produce offspring and mutating them.

Listing 6.1 (continued)

```
num_generations = 100
population_size = 3000
str_len = len(target)
mutation_rate = 0.001 #A

pop_fit = []
pop = spawn_population(size=population_size, length=str_len) #initial population
```

```

for gen in range(num_generations):
    pop, avg_fit = evaluate_population(pop, target)
    pop_fit.append(avg_fit) #record population average fitness
    new_pop = next_generation(pop, \
        size=population_size, length=str_len, mut_rate=mutation_rate)
    pop = new_pop

```

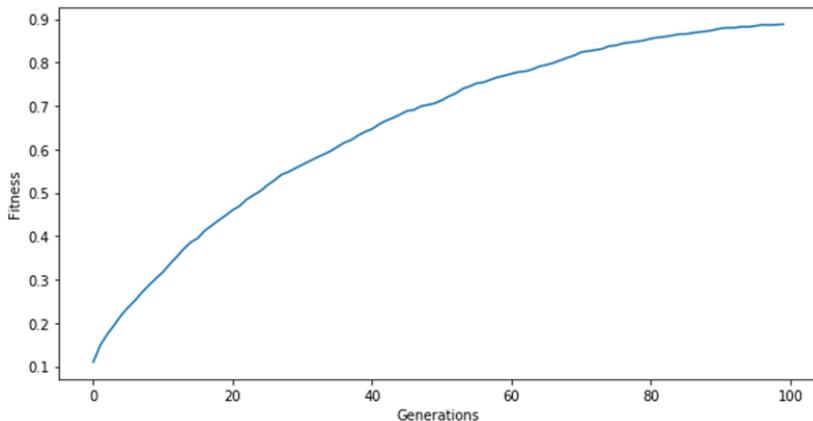


Figure 6.3: This is a plot of the average population fitness over the generations. The average population fitness increases fairly monotonically and then plateaus, which looks promising. If the plot was very jagged, then the mutation rate might be too high or the population size too low. If the plot converged too quickly, then the mutation rate might be too low.

If you run the algorithm, it should take a few minutes on a modern CPU and you can find the highest rank individual in the population using:

```

>>> pop.sort(key=lambda x: x.fitness, reverse=True) #sort in place, highest fitness
      first
>>> pop[0].string
"Hello World!"

```

It worked! This is actually a more difficult problem to optimize using an evolutionary strategy because the space of strings is not continuous, so it is hard to take small, incremental steps in the right direction since the smallest step is flipping a character. Hence, if you try making a longer target string it will take much more time and resources to evolve. When we're optimizing real-valued parameters in a model, even a small increase in value might improve the fitness and we can exploit that.

Let's see how this evolution strategy works in a simple reinforcement learning example. We're going to use an evolutionary process to optimize an agent to play Cartpole. We can represent an agent as a neural network that approximates the policy function – it accepts a state and outputs an action. Below we have an example of a three-layer network initiated with random weights.

Listing 6.2 Defining an Agent

```

import numpy as np
import torch

agent_weights = [
    torch.rand(self.state_space, 10), # fc1 weights
    torch.rand(10), # fc1 bias
    torch.rand(10, 10), # fc2 weights
    torch.rand(10), # fc2 bias
    torch.rand(10, self.action_space), # fc3 weights
    torch.rand(self.action_space), # fc3 bias
]

def get_action_from_agent_weights(agent_weight, state):
    x = F.relu(torch.add(torch.mm(state, weights[0]), weights[1]))
    x = F.relu(torch.add(torch.mm(x, weights[2]), weights[3]))
    act_prob = F.softmax(torch.add(torch.mm(x, weights[4]), weights[5]))
    action = np.random.choice(range(len(act_prob)), p=act_prob)
    return action

```

Note that we are not using PyTorch's nn.Sequential module like we did in the previous section. Although PyTorch's module provides useful abstractions, it does not easily allow us to set the default weights of our model, which we will need to do later in the chapter. All we need to do is initiate some weights, run our input through the model, and then select an action from the output.

To determine the fitness of the agent, we just need to run its policy through the environment and calculate the total reward that it would accrue. We should run it for multiple trials and average the runs to reduce the variance and get more accurate measurements. Just keep in mind that the more trials that we run, the longer it will take to generate determine the fitness.

Listing 6.3 Determining Fitness

```

def get_fitness(self, env, agent_weights, max_episode_length, trial=5):
    total_reward = 0
    for _ in range(trials):
        observation = env.reset()
        for i in range(max_eps_length):
            action = agent(weights, observation)
            observation, reward, done, info = env.step(action)
            total_reward += reward
            if done: break
    return total_reward / trials

```

6.2.2 Selecting for the Fittest Agents

Okay, now we know how to determine when one agent is more fit than another. We will first create a set of agents (we'll call them the first generation) and evaluate the fitness of each of the agents.

Listing 6.4 Creating our first generation of agents

```
first_generation = [init_random_agent_weights() for _ in range(generation_size)]
```

Once we have our first generation we can then select for the top two agents with the highest fitness but having each agent run through the environment. We can call these our parents.

Listing 6.5 Selecting the fittest agents

```
top_agents_weights = sorted(agents_weights, reverse=True, key=lambda a:
    get_fitness(env, a))[:2]
```

6.2.3 Recombining Agents to Produce New Agents

Now that we have determined the most agents, we need to recombine them to pass down their favorable weights to the next generation. We touched on recombination previously, but let's go over it again. Note that recombination is also called "crossing" or "mating" and we will use these terms interchangeably. In biological terms, each agent being recombined, or parent, has a set of genes made of DNA that they will pass down to their offspring. Each parent cannot pass down their entire genes or else their offspring will have twice as many genes as the parents did. Humans for example have 23 pairs of chromosomes (bundles of DNA) for a total of 46. If each parent passed all 46 of their chromosomes to their children then they would have $46+46=92$ chromosomes. And if they have children their children will have more than that. This obviously is not the case (when too many chromosomes are passed on, it is generally not compatible with life). What instead happens is that each parent provides half of their genes, one chromosome per set. The child then will have half of its genes from one parent and the other.

Our artificial agents will follow a similar pattern. The genes in this case will be the weights of our network and each layer can be considered a chromosome. And we do not need to pass exactly half of each parents' genes to their children – we could pass down 1/3 from Parent A and 2/3 from Parent B, 4/5 from Parent A and 1/5 from Parent B, and so on. The problem is that we do not know which genes from each parent to pass down to their children, and so therefore we have to essentially randomly select them. Each parent has a chance of giving a set of weights to its offspring.



Figure 6.4: We will be passing the weights of each parent of each parent down to each child. Each child will receive a random amount of weights from each parent. In the above case, the child received the first two "genes" (FC1 and B1) from parent 1 and the remaining four from parent two, but this could be random permutation.

Below is the code implementation of mating (crossing) two agents. We randomly generate a random number between 0 and the total number of weights called a crossover_idx and the child will inherit all genes before the crossover_idx from Parent A and all genes after the crossover_idx from Parent B.

Listing 6.6 Crossing

```
def cross(agent1_weights, agent2_weights, agent_config):
    num_params = len(agent1_weights)
    crossover_idx = np.random.randint(0, num_params)
    new_weights = agent1.weights[:crossover_idx] + agent2.weights[crossover_idx:]
    num_params_to_update = np.random.randint(0, num_params) # num of params to change
    return new_weights
```

6.2.4 Introducing Mutations

Mutations are critical in evolution. In biology, mutations are random changes in an organism's DNA. This sometimes leads to new traits that have not been exhibited before in any previous generations. Without mutation we would just be shuffling around the same genes of our ancestors. For example, let's say there are two parents where parent 1 held genes FC1 and B1 and parent 2 held genes FC2 and B2. When they bred, and mutations are not possible, no matter how many children they have the children could have only four distinct sets of genes. Mutations add variance to a population, allowing novel information to be created.

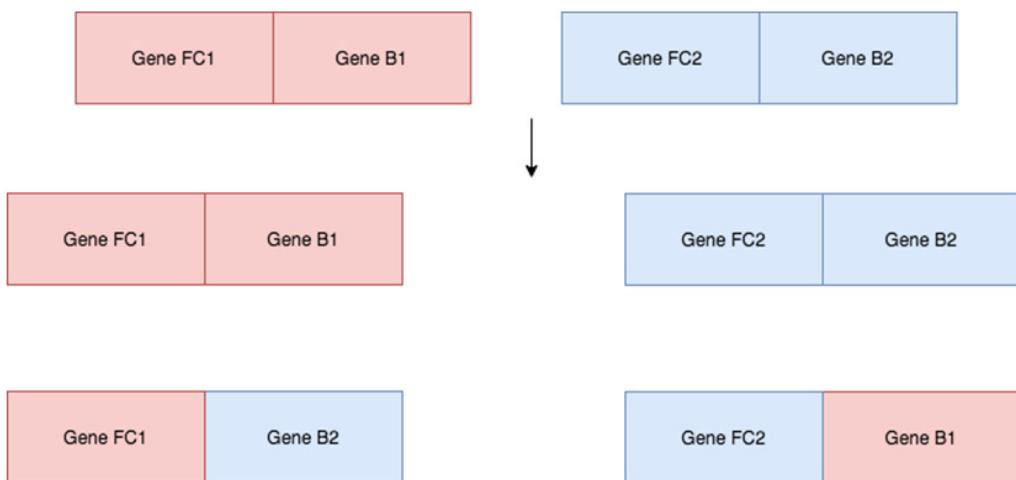


Figure 6.5: If two parents had only two genes, there would be only four different types of descendants that could

form.

There would be no point in breeding for more generations as well, as the same genes present in all the children were present in the parent. We could increase the number of genes to say 6 like we showed in Figure 6.4 and there would be 64 (2^6) different children that could be produced. However, unless we start with a huge population size, it will be very difficult to produce enough variance in each generation such that some are significantly more adept than others.

Mutations allow us to generate a lot more variety in our populations. So when two parents cross to produce a child, they will not always produce an agent that can be predictably determined after the mutation process.

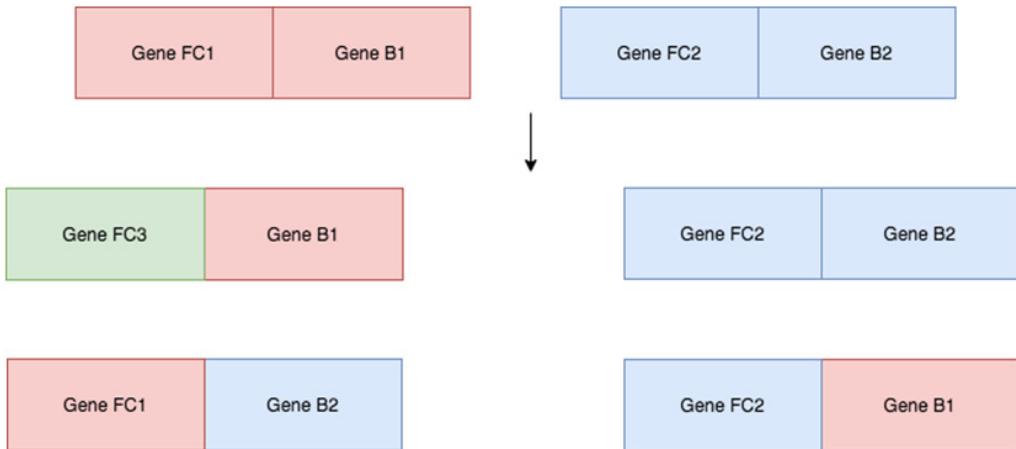


Figure 6.6: Mutations introduce randomly into each generation. Without mutations the combinations of children can easily be determined.

As shown in Figure 6.6, when mutations are introduced, there is a chance that a new variation of a gene may be formed, one that we may not have anticipated. This can then be passed on to future generations. And remember, each future generation has a chance to introduce even more mutations! Importantly, however, mutations happen at a low rate and only introduce small changes. A single mutation is not going to take a random set of parameters and transform them into perfectly optimized ones. But a few small mutations may add up and push the parameters slightly closer to the optimum.

Let's see how this would look in code. The way we will do this is by taking an agent's weights, and randomly generate the number of weights we want to modify. For each weight that we want to modify, we will add some random noise to the weights.

Listing 6.7 Mutation

```
def mutate(new_weights):
    num_params_to_update = np.random.randint(0, num_params) # num of params to
    change
    for i in range(num_params_to_update):
        n = np.random.randint(0, num_params)
        new_weights[n] = new_weights[n] + torch.rand(new_weights[n].size())
    return new_weights
```

6.2.5 Evolution takes multiple generations

In biology, each mutation very subtlety changes the characteristics of the organism such that it may be difficult to discern one generation from another. However, it is the process of crossing multiple generations, allowing these mutations and variations to accumulate that allow for perceptible changes. Let's use the bird beak example we talked about briefly before. At first all birds would have roughly the same beak shape. But as generations occurred, random mutations were introduced into the population. Again, most of these mutations probably did not impact the birds at all or even had a deleterious effect. But with a large enough population and enough generations, random mutations would occur that would affect beak shape favorably. Those birds would have an advantage getting food over the other birds and therefore have a higher likelihood of passing down their genes. Therefore, the next generation would have an increased frequency of the favorably shaped beak gene.

Enough about birds, now back to our reinforcement learning agents. Mutations increase the variance in performance of a population of agents. Because the mutations are random and the environment requires methodical navigation, most of these changes will not impact the fitness of the agent much or even cause the agent to perform worse than its parents.

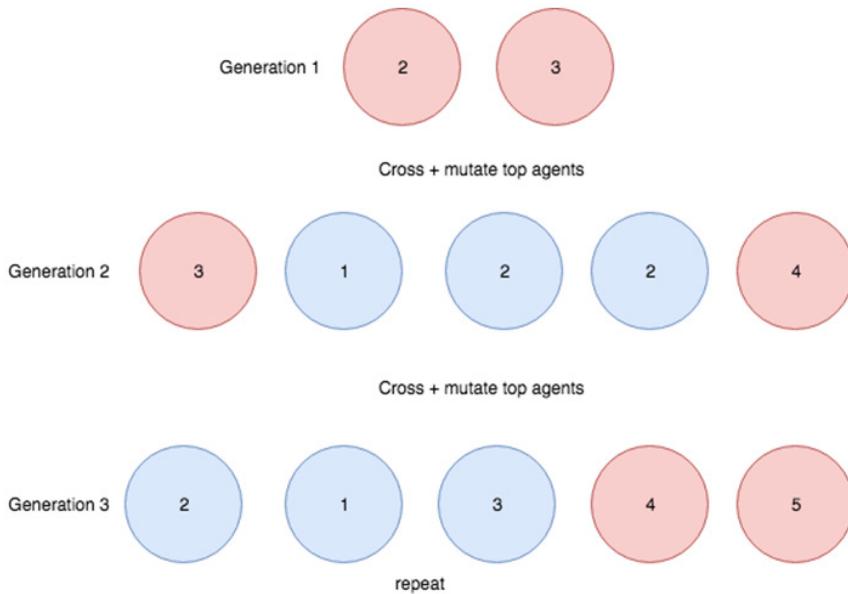


Figure 6.7: A diagram showing the principles of evolution by natural selection. The number represents the fitness of the agent and red agents are the parents that are selected to produce the subsequent generation. Each generation produces descendants with recombined characteristics derived from their parents. Since the crossing and mutations are random, not all descendants are more fit than their parents. It is the process of more fit individuals being more likely to cross that increases the overall population fitness from generation to generation.

However, with large enough population size and generation, there are bound to be descendants that perform slightly better than their parents.

6.2.6 Full training loop

Let's review all the steps. We first need to initiate our first generation of agents. We then select the top two agents, cross them while introducing mutations to produce the next generation. From that next generation we select the top two parents and repeat this until the top agents are produced.

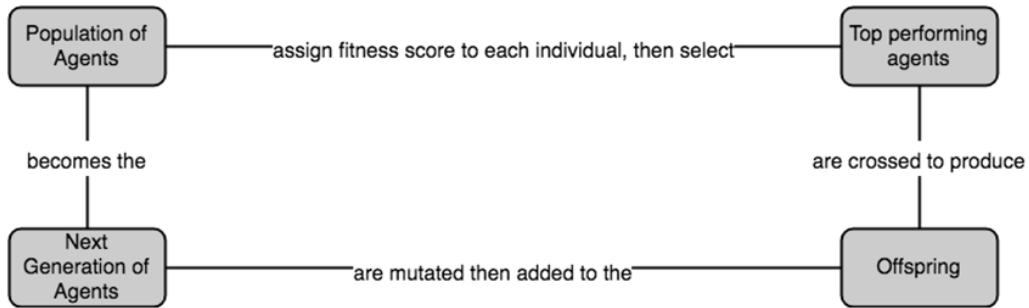


Figure 6.8: Full training loop for evolutionary optimization of reinforcement learning agents.

Below is the entire training loop. We will repeat this loop until an agent of desired fitness is obtained.

Listing 6.8 Full Training Loop

```

n_generations = 100
generation_size = 20
generation_fitness = []

env = gym.make('CartPole-v1')
max_fitness = 0

agents = [init_random_agent_weights(), init_random_agent_weights()]
for i in range(n_generations):
    next_generation = reproduce(env, agents, generation_size)
    ranked_generation = sorted([get_fitness(env, a) for a in next_generation],
                               reverse=True)
    avg_fitness = (ranked_generation[0] + ranked_generation[1]) / 2
    generation_fitness.append(avg_fitness)
    agents = next_generation
  
```

Let's give the above code a run and see how it turns out.

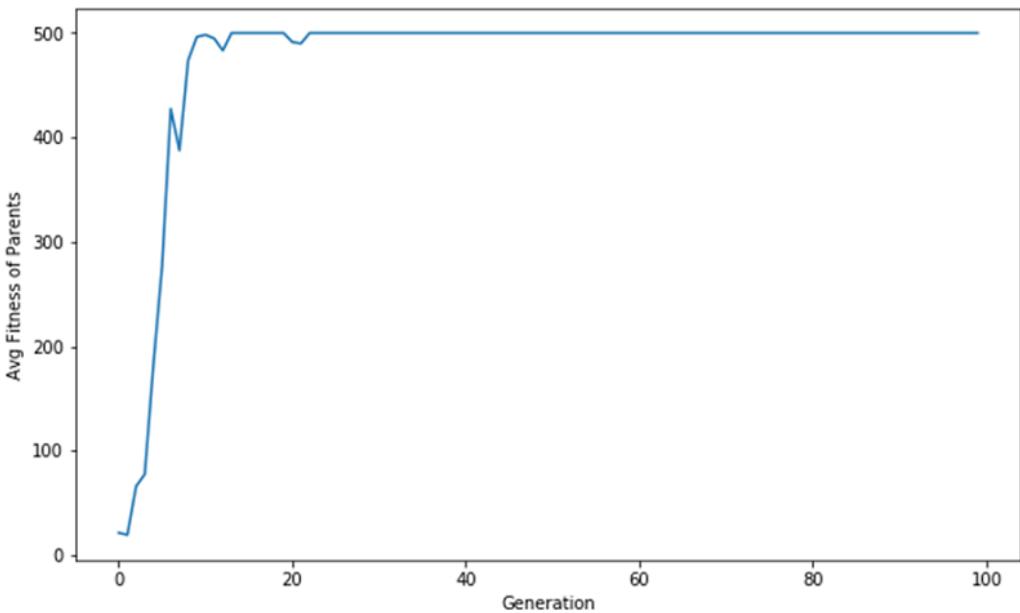


Figure 6.9. Figure caption.

Sweet, we just created an algorithm that mimics natural selection. As you can see from above, after creating a few generations of agents, we produced one that is able to maximize its reward in the environment. One of the drawbacks of evolutionary strategies is that we have to run our agent through the environment a lot more times than if we just used a gradient-based optimization algorithm. We will discuss a few pros and cons of this approach in the next section.

6.3 Pros and Cons of Evolutionary Algorithms

As you probably have seen, the algorithm we implemented above is a bit different the previous approaches. There are circumstances where an ES approach works better and others that make it impractical.

6.3.1 Evolutionary Algorithms Explore More

One advantage of gradient-free approaches is that they tend explore more than their gradient-based counter parts. Both DQN and PG followed a similar strategy – collect experiences and nudge our agent to take actions that led to more reward. As we discussed before, this tends to cause our agents to abandon exploring new states if it knows it prefers an action already. We addressed this with DQN by incorporating an epsilon-greedy strategy, meaning there's a small chance we will take a random action even if we have a preferred action. With stochastic policy

gradient we relied on drawing a variety of actions from the action probability vector output by our model.

The agents in the genetic algorithm on the other hand are not nudged toward any direction. We are producing a lot of agents in each generation, and with so much random variation between them, most of them will have different policies between each other.

6.3.2 Evolutionary algorithms are incredibly sample intensive

As you could probably see from the above code, we need each agent to run through the environment 5 times to determine its fitness. We also have 10 agents per generation. That means that we need to run through the environment 50 times to produce an incrementally improved agent. Compared with gradient-based methods, evolutionary algorithms tend to be more sample hungry since we aren't strategically adjusting the weights of our agents, we are just creating lots of agents and hoping that the random mutations / crossing we introduce are beneficial. We will say that evolutionary algorithms are less **data-efficient** than DQN or PG methods.

We could lower the number of episodes we need to determine fitness from 5 to a smaller number. However, there will be a lot more variance in the fitness value that is calculated from a lower number of runs. Remember, we want our agents to generalize well to being in different states in its environment and having it run through the environment multiple times is a more accurate way of doing so. For example, if we were only requiring the agent to run through the environment one time, we are depending on that single trial to provide us its expected fitness. It could be a bad agent that generalizes poorly but was initiated in a starting position that it was very familiar with leading to a high fitness. We would then falsely believe that the agent was more fit in general, select it as a parent, and pass its poor and overfitted weights to the next generation. This may mean that we need more generations in order to produce a better agent, requiring us to run through the environment more time in the end.

Let's say that want to decrease the size of the population so our parents will need to produce less agents. If you decrease the population size, there are less agents to select from when we are picking our two parents. This will make it likely that less fit individuals will make it into the next generation. We rely on a large number of agents being produced in hopes of finding a combination that leads to a better fitness. Additionally, as in biology, mutations most of the time have a negative impact and will lead to worse fitness. Having a larger population size increases the probability that a mutation we introduce will have a beneficial effect.

Being data-inefficient is a problem if collecting data is expensive, such as in robotics or with autonomous vehicles. Having a robot collect one episode of data usually takes a couple of minutes and we know from our past algorithms that training a simple agent takes hundreds if not thousands of episodes. Imagine how many episodes an autonomous vehicle would need to sufficiently explore its state space (the world). In addition to taking considerably more time, training with physical agents is much more expensive since you need to purchase the robot and account for any maintenance. Ideally, we could train such agents without having to give them physical bodies.

6.3.3 Simulators

Simulators address the concerns listed above. Instead of using an expensive robot or building a car with the necessary sensors, we could instead use a computer software that would emulate the experiences the environment would provide. For example, when training agents to drive autonomous cars, instead of equipping cars with the necessary sensors and deploying their model on physical cars, we can just train the agents inside software environments such as the driving game Grand Theft Auto (or ideally a more realistic driving simulator). The agent would receive as input the images of its surroundings and would be trained to output driving actions that would get their vehicle to the programmed destination as safely as possible.

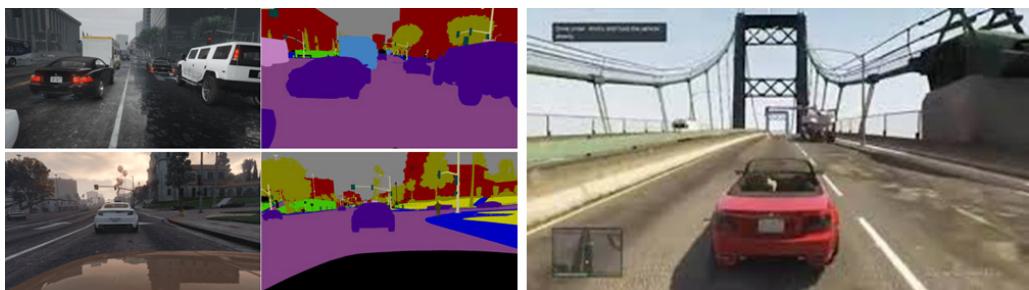


Figure 6.10: The video game Grand Theft Auto was initially used by autonomous driving engineers to test their models. The models would receive images of its surroundings and would output driving actions.

In addition to being significantly cheaper to train agents with, agents are able to train much more quickly since they can interact with environment much faster than in real life. If you need to watch and understand a 2-hour movie, it will require...2 hours of your time. If you focus more intensely, you could probably increase the playback speed by 2 or 3, dropping the amount of time needed to 1 hour or a bit less. A computer on the other hand can be finished before you finish the first act. Depending on the size of your computer, an 8 GPU computer (p3.16x large on Amazon AWS) running ResNet-50 can process over 700 images per second. In a 2-hour movie running at 24 frames per second (standard in Hollywood), there are 172,800 frames that need to be processed. This will require 4 minutes to finish. We could also effectively increase the playback speed for our deep learning model as well by dropping every few frames, which will drop our processing time to under 2 minutes. We could also throw more computers at the problem to increase processing power. For a more recent reinforcement learning example, the OpenAI Five bots were able to play 180 years of Dota 2 games each day. You get the picture...computers can process faster than we can, and that's why simulators are valuable.

6.3.4 Gradient-Free Algorithms could faster to train

So back to Evolutionary Strategies. If a simulator is present, the time and financial cost of collecting samples with ES is less of an issue. In fact, producing a viable agent with ES can sometimes be faster than gradient-based approaches because we do not have to compute the gradients via backpropagation. Depending on the complexity of the network, this will cut down the computation time by roughly 2-3 times. But there is another advantage of ES that can allow them to train faster than their gradient counter-parts – they can scale incredibly well. We will discuss this in detail in the next section.

6.4 Evolutionary Strategies are Parallelizable

Here we'll dive into Evolutionary Strategies as a scalable alternative, discussing parallel v serial processing, scaling efficiency, communication between nodes, and a variety of scaling approaches.

6.4.1 ES as a scalable alternative

Another reason that training an ES agent could be faster is that the algorithm can be scaled very efficiently. OpenAI in 2017 released a paper called *Evolutionary Strategies as a Scalable Alternative to Reinforcement Learning*, where they could train agents incredibly quickly efficiently by adding more machines. On a single machine with 18 CPU cores, they were able to make a 3D Humanoid learn to walk in 11 hours. But with 80 machines (1440 CPU cores) they were able to produce an agent in under 10 minutes!



Figure 6.11: The 3D Humanoid environment provided by the gym library. This is high dimensional problem where the objective is for the humanoid to walk forward. With just one machine an ES was able to “solve” this problem in 11 hours, but by using 80 computers they were able to produce an agent in 10 minutes.

You may be thinking...well that's obvious, they just threw more machines and money at the problem. But this is actually trickier than it sounds, and other gradient-based approaches struggle to scale to that many machines. Before we dive the differences for how these methods scale, let's take a moment to demonstrate in detail what it means for a machine learning algorithm to scale.

6.4.2 Parallel vs Serial Processing

For our above example, when determining the fittest agent in each generation, we had to wait for each agent to run through the environment completely before starting the next run. If the agent takes 30 seconds to run through the environment, and we have 10 agents we are determining the fitness for, this will take 5 minutes.

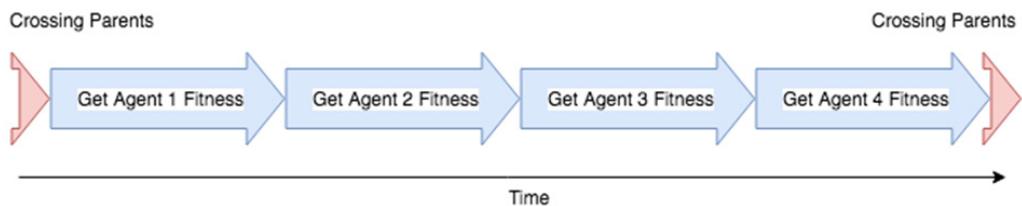


Figure 6.12: Our current computational complexity. Determining the fitness of our agent is often the slowest step in our training loop and requires that we run our agent through the environment (possibly many times). If we are doing this on single computer, we will be doing this in serial – that is we have to wait for one to finish running through the environment before we can start determining the agent of the second agent.

This is known as running a program in **serial**. Determining each agent's fitness will generally be the longest running task in an ES strategy, but each agent can evaluate its own fitness independent of each other. We could instead run each agent in the generation on multiple computers at the same time. Each of the 10 agents would go on 10 machines and we can determine their fitness simultaneously. This means that completing one generation will take ~30 seconds as opposed to 5 minutes when running on one machine, a 10x speed up. This will be known as running our process in **parallel**.

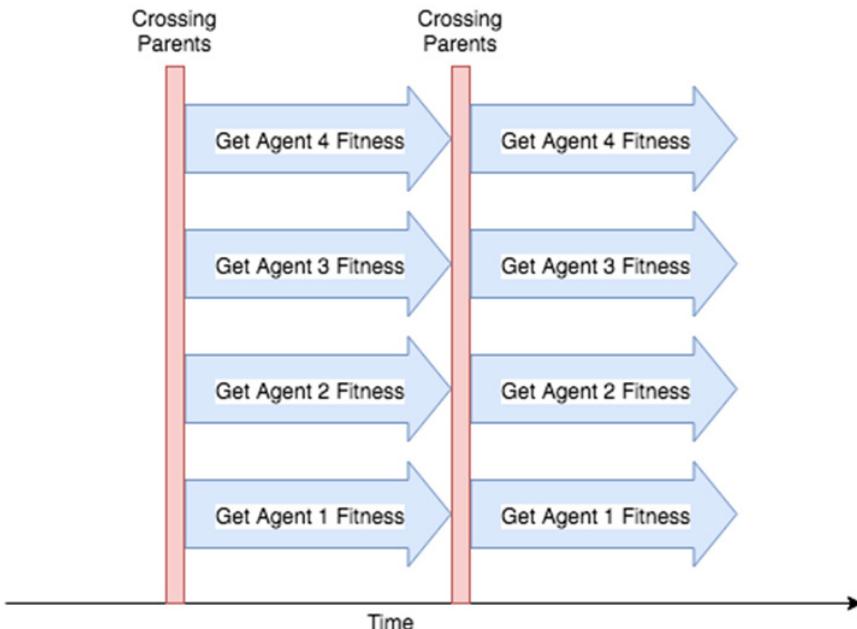


Figure 6.13: If we have multiple machines at our disposal, we can determine the fitness of each agent on its own machine in parallel with each other. We would not have to wait for one agent to finish running through the environment before starting the next one. This will provide us huge speed up if we are training agent with a long episode length.

6.4.3 Scaling Efficiency

So we can just throw more machines and money at the problem and we don't have to wait nearly as long. In the hypothetical example above where we added 10 machines and got a 10x speedup up. This is known as having a scaling efficient of 1.0. **Scaling efficiency** is a term used to describe how a particular approach improves as more resources are thrown at it and can be calculated as below.

$$\text{Scaling Efficiency} = \frac{\text{Multiple of Performance Speed up after adding resources}}{\text{Multiple of Resources Added}}$$

However, in the real world, processes never have a scaling efficiency of 1. There is always some additional cost to adding more machines that decreases its efficiency. More realistically adding 10 more machines will only give us a 9x speed up. Using the scaling efficiency equation above we can calculate the scaling efficiency as 0.9 (which is actually pretty good in the real world). Now back to our evolutionary example. We could implement it such that one machine is responsible for selecting the best agents and the other machines determine the fitness as shown in Figure 6.13.

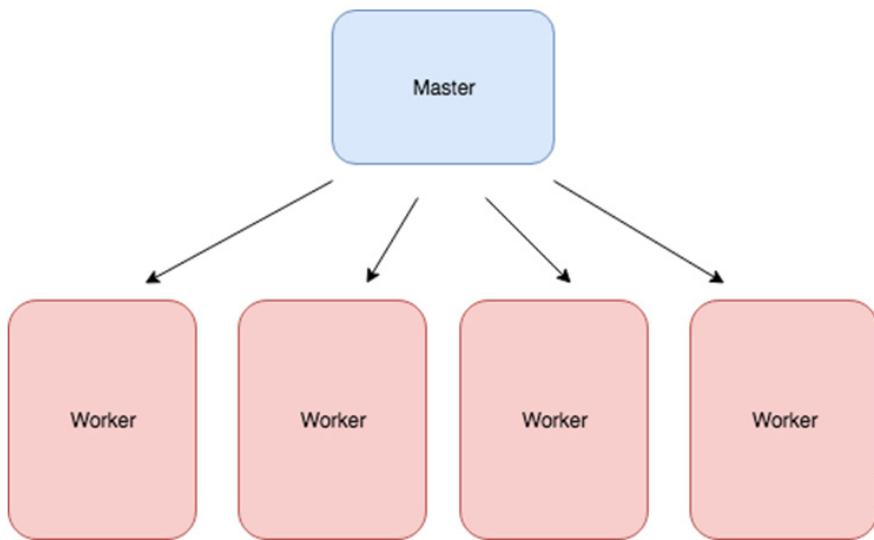


Figure 6.14: The topology for how we can distribute our ES algorithm onto many machines. We have one machine that does the selection process (we will call it the “master” node) and n-machines that determine the fitness of our agent.

Every step does take a little bit of network time to communicate between machines, which is something that we would not encounter if we were running everything on a single machine. Additionally, in order for the “crossing parents” step to begin in the master node, we need all our workers to complete calculating the fitness for each of their agents. If there is just one machine that is slower than the others, the other workers will need to wait.

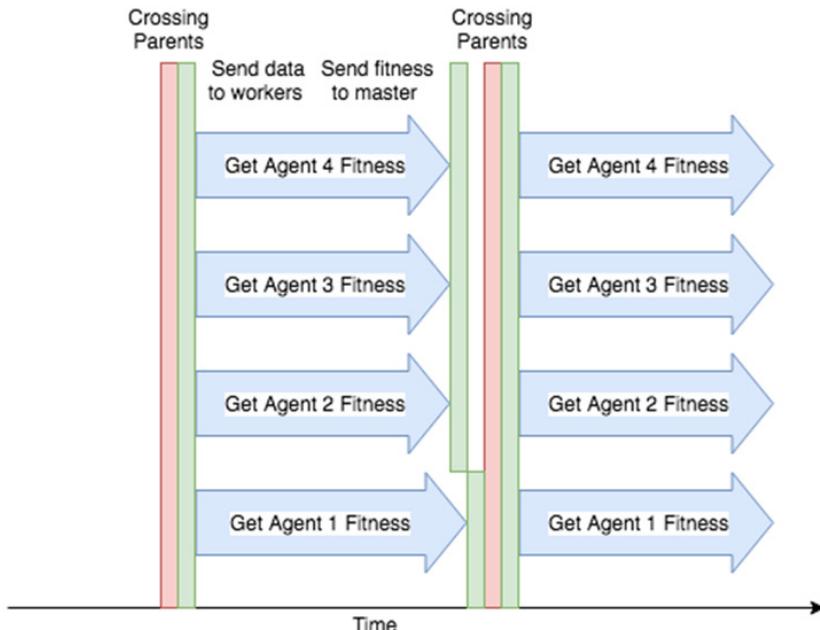


Figure 6.15: A revised view of Figure 6.12 that accounts that introduces real world inefficiencies. The green bars represent network time it takes in order for the master and workers machines to communicate with one another. Additionally, if any of the workers are slower than the others, such as Agent 1, the other workers have to wait for it.

6.4.4 Communicating Between Nodes

So far we have not talked about what data we are sending from the master node to the worker node, but you can imagine that the more data that you are sending between machines the longer it takes. The researchers at OpenAI developed this nifty strategy where each node sends only one number to each other node. We have modified their variation, and have simplified it such that the master to sends two numbers to each worker and each worker only needs to send one number back to the master.

Let's first take a naïve approach. So the master node is in charge of aggregating the fitness scores of the population and determining which agents are going to be the two new parents of the next generation. The workers on the other hand are responsible for determining the fitness of one agent and then sending that fitness to the master. We could have the master node produce the next generation and then send each worker the one agent's weights. However, this is incredibly expensive. Without our very small network with 3 layers of 10 hidden nodes each, there are over 1000 parameters each represented as a float32 (4 bytes of data). That means we would need to send 4 kB per worker. We can definitely do better than that.

6.4.5 Sending only two numbers

Okay, so only the master node knows which agents are the parents and that information is necessary in order to produce the next generation. What if each worker had all the same agents on them and the master node was only responsible for communicating which agents were the parents.

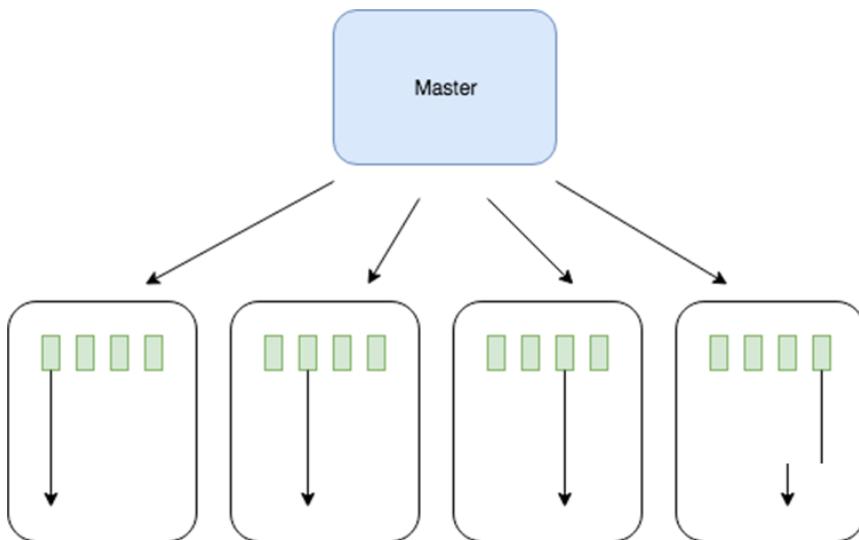


Figure 6.16: The architecture derived from OpenAI's distributed ES paper. Each worker contains all the weights of all the agents but is responsible for evaluating the fitness of only a subset of the population. The fitness scores of the agents can then be sent to the master and the master can send the positions of the most fit agents (the parents) back to the workers. The workers can then produce the next generation and repeat this process.

We would only need to send two numbers to each worker, the identification of parent 1 and parent 2. The workers, now knowing the identity of the parents, would be responsible of producing the next generation, which is a relatively computationally cheap task. There's a catch though. Each worker would need to produce the exact same generation as each other. Even though they have both parents' weights, as we mentioned throughout this chapter, there is a lot of randomness involved. For each descendant in the next generation we randomly generate a `crossover_idx`, the number of genes we want to mutate, and then add random noise to mutate the genes. Luckily, there is solution to this already.

6.4.6 Seeding

Seeding allows us to consistently generate the same random numbers every time, even on different machines. If you run the following code you will get the same output as we've shown below above even though these numbers should be generated "randomly."

Listing 6.9 Seeding

```
import numpy as np
np.random.seed(10)
np.random.rand(4)
>>> array([0.77132064, 0.02075195, 0.63364823, 0.74880388])

np.random.seed(10)
np.random.rand(4)
>> array([0.77132064, 0.02075195, 0.63364823, 0.74880388])
```

Seeding is important so that experiments involving random numbers could be replicated again for other researchers to reproduce. If you do not supply an explicit seed, then usually the system time or some other sort of variable number is used. If we came up with a novel new RL algorithm, we would want others to be able to verify our work on their own machines. We would want the agent that another lab generated to be identical to eliminate any source of error (and therefore doubt) and that's why it's important we provide as much detail about our algorithm as possible – the architecture, the hyperparameters used, and sometimes the random seed we used. However, we hope we've developed an algorithm that is robust to the particular set of random numbers generated.

Now back to scaling our ES problem. If each worker is initially seeded with the same number, the crossing and mutating steps will be exactly the same, and each generation produced on each worker will be identical to each other, which was exactly what we were looking to accomplish. All the workers need to do next is to figure out which subset of agents they will be evaluating the fitness for and we can send those numbers back to the master server and repeat this process over again. We can just have each worker communicate to each other which agents in the generation they are going to evaluate.

But does that even need to be communicated amongst the workers? We can structure it such that each node always evaluates the fitness of the same subsets of agents. In Figure 6.15 we show that each worker node houses a generation of agents of size 4. The first node could always be responsible for evaluating the fitness of the agent at index 0, the second node responsible for the agent at index 1 and so on.

6.4.7 Scaling Linearly

This approach we showed above is a simplified version of the real architecture that the researchers at OpenAI did.

As you may have noticed, the master node does not seem like it has that large of a responsibility and the OpenAI engineers actually removed it and just had the workers communicate directly with each other. The workers would calculate the fitness of its specified

agents, then send over the fitness scalar to every other worker. At the end of the episode, each worker would have all the finesse of the generation, can determine which should be bred, and then cross its subset and repeat this process. By reducing the volume of data sent between the nodes, adding an additional node did not affect the network significantly, and they were able to scale to over a thousand workers linearly.

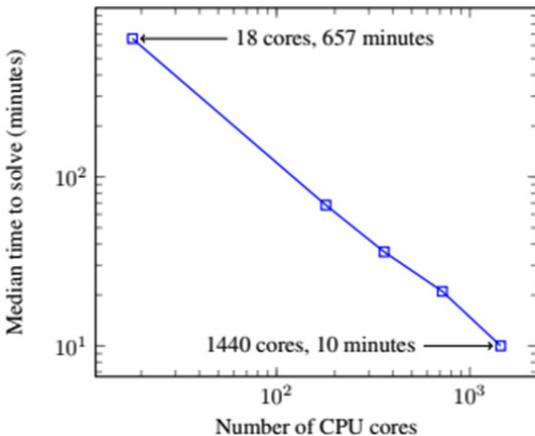


Figure 6.17. Figure taken from the *OpenAI Evolutionary Strategies as a Scalable Alternative to Reinforcement Learning* paper. The figure demonstrates that as more compute resources were added, the time improvement remained constant.

Scaling linearly means that for every machine added, we receive roughly the same performance boost as we did with adding the previous machine. This is denoted by a straight line on a performance over resources graph as seen in Figure 6.16.

6.4.8 Scaling Gradient Based Approaches

Gradient-based approaches can be trained on multiple machines as well. However, they do not scale nearly as well as ES. Currently, most approaches for distributed training of gradient-based approaches involve training the agent on each worker and then passing the gradients back to a central machine to be aggregated. All the gradients must be passed for each epoch or update cycle which requires a lot of network bandwidth and strain on the single central machine. Eventually the network is saturated and adding more workers does not improve training speed as well.

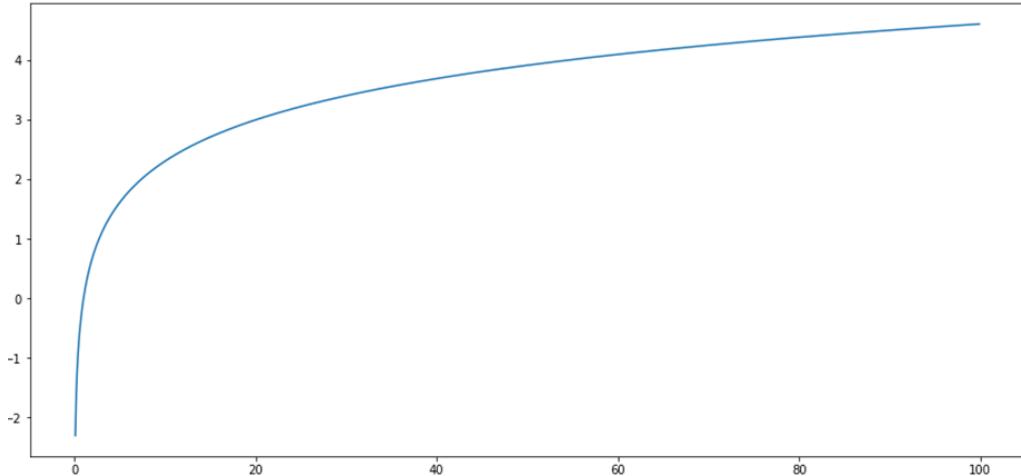


Figure 6.18. The performance of current gradient-based approaches resembles graph like this. In the beginning there is seemingly linear trend because the network has not been saturated. But eventually as more resources are added, we get less and less of a performance boost.

Evolutionary approaches on the other hand, since it does not require backpropagation, does not need to send gradient updates to a central server. And with smart techniques like the ones that OpenAI developed, it may only need to send a single number.

6.5 Summary

- Evolutionary Strategies provide us another powerful toolkit in our arsenal. Adapting from how we humans have evolved:
 - 1.1 we produce individuals
 - 1.2 select the best from the current generation
 - 1.3 shuffle their genes around
 - 1.4 mutate them to introduce some variation
 - 1.5 and mate them to create new generations for the next population
- We were able to code an evolutionary algorithm to fit our reinforcement learning task. We calculated how to determine the fitness of an agent, how to shuffle parameters around to produce new agents, and how to introduce mutations to produce new variation.
- ES algorithms tend to be more data hungry and less data-efficient than gradient-based approaches and that in some circumstances this may be fine, notably if you have a simulator. For some problems though, we may not have access to a simulator and we need to be frugal with our data, such as when we are trying to train a robot.

- In the next section, we will discuss a class of algorithms notable for being more data-efficient than both ES and gradient-base algorithms.

7

Distributional DQN: Getting the full story

In this chapter we learn...

- Why knowing a full probability distribution is better than a single number
- How to extend ordinary Deep Q-networks to output full probability distributions over Q-values
- How to implement a distributional variant of DQN to play Atari Freeway
- To understand the ordinary Bellman equation and its distributional variant
- How to prioritize experience replay to improve training speed

We introduced Q-learning back in Chapter 3 as a way to learn the value of taking each possible action in a given state, called action-values or Q-values. This allowed us to apply a policy to these action-values and choose actions associated with the highest action-values. In this chapter we will learn to extend Q-learning to not just learn a point-estimate of the action-values, but an entire distribution of action-values for each action, which is called Distributional Q-learning. Distributional Q-learning has been shown to result in dramatically better performance on standard benchmarks, and it also allows for more nuanced decision-making, as we will see. Distributional Q-learning algorithms, combined with some other techniques covered in this book, is currently considered a state-of-the-art advance in reinforcement learning.

Most environments we wish to apply reinforcement learning to involve some amount of randomness or unpredictability, where the rewards we observe for a given state-action pair will have some variance. In ordinary Q-learning, which we might call expected-value Q-learning, we only learn the average of the noisy set of observed rewards. But by taking the average, we throw away valuable information about the dynamics of the environment. In some cases the rewards observed may have a more complex pattern than just being clustered

around a single value. There may be two or more clusters of different reward values for a given state-action, for example, sometimes the same state-action will result in a large positive reward and sometimes in a large negative reward. If we just take the average we will get something close to 0, which is actually never an observed reward in this case.

Distributional Q-learning seeks to get a more accurate picture of the distribution of observed rewards. One way to do this would be to just keep an exact record of all the rewards observed for a given state-action pair. Of course this would require a lot of memory and for state spaces of high-dimensionality would be computationally impractical. This is why we must make some approximations. But first, let's delve deeper into what expected-value Q-learning is missing and what distributional Q-learning offers.

7.1 What's wrong with Q-learning?

The expected value version of Q-learning we're familiar with is flawed, and to illustrate this we consider a real-world medical example. Imagine we are a medical company and we want to build an algorithm to predict how a patient with high blood pressure (hypertension) will respond to 4-week course of a new anti-hypertensive drug called Drug X , and thus decide whether or not to prescribe this drug to an individual patient. We gather a bunch of clinical data by running a randomized clinical trial (RCT) in which we take a population of patients with hypertension and randomly assigned them to a treatment group (those who will get the real drug) and a control group (those who will get a placebo, an inactive drug). We then record blood pressures over time while the patients in each group are taking their respective drugs and at the end we can see which patients responded to the drug and how much better compared to placebo (Figure 7.1).

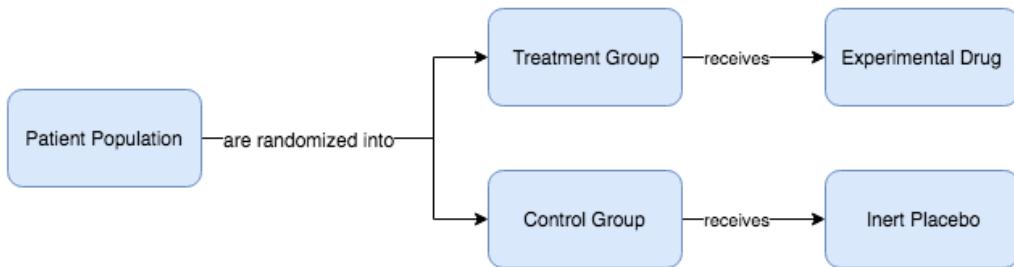


Figure a.: In a randomized control trial (RCT), we wish to study the effect of some treatment compared to a placebo (a non-active substance). We want to only isolate the effect we are trying to treat, so we take a population with some condition and randomly sort them into two groups, a treatment group and a control group. The treatment group gets the experimental drug we are aiming to test, and the control group gets the placebo. After some duration of time, we can measure the outcome we are interested in for both groups of patients and see if the treatment group, on average, had a better response than placebo.

Now we've collected our dataset and we can plot a histogram of the change in blood pressure after 4 weeks on the drug for the treatment and control groups. Let's suppose we see something like the results in Figure 7.2.

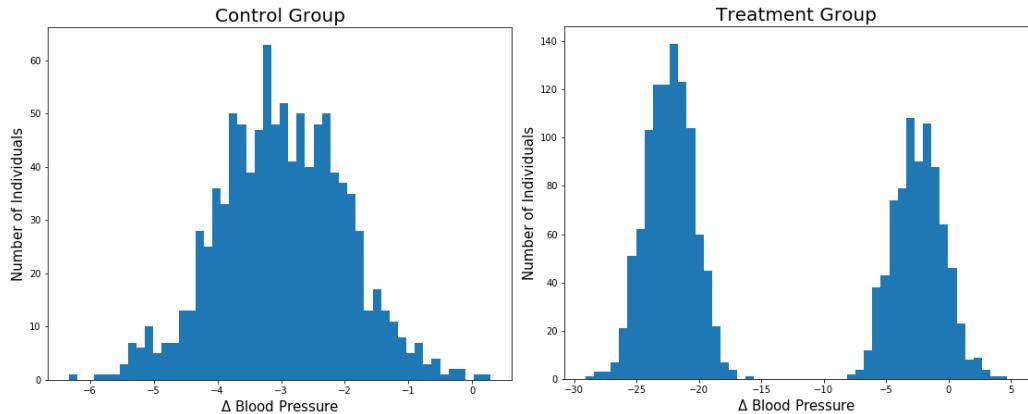


Figure 7.2: These are the simulated histogram results of the measure blood pressure change for the control and treatment groups in a simulated randomized control trial. The x-axis is the change in blood pressure from start (before treatment) to after treatment. We want blood pressure to decrease, so negative numbers are good. We count the number of patients who have each value of blood pressure change, so the highest park at -3 means that most patients had a blood pressure drop of 3 mmHg in the control group. You can see there are two subgroups of patients in the treatment group, one group that had a significant reduction blood pressure, and another group that had a minimal to no effect. We call this a bi-modal distribution, where a mode is another word for "peak" in the distribution.

If you first look at the control group histogram for Figure 7.2, it appears to be a normal-like distribution centered around

-3.0 mmHg (a unit of pressure), which is a fairly insignificant reduction in blood pressure, as you would expect from a placebo. So our algorithm would be correct to predict, that for any patient given a placebo their expected blood pressure change would be -3.0 mmHg on average, all placebo patients had a -3.0 mmHg blood pressure change even though individual patients had greater or lesser changes than that average value.

Now look at the treatment group histogram. You see distribution of blood pressure change is bi-modal, meaning there are two peaks, as if we had added together two separate normal distributions. The right-most mode is centered at -2.5 mmHg, very similar to the control group, suggesting that this sub-group within the treatment group did not benefit from the drug compared to placebo. However, the left-most mode is centered at -22.3 mmHg, which is a very significant reduction in blood pressure, in fact greater than any currently existing anti-hypertensive drug. So this again indicates there is a sub-group within the treatment group except this time it strongly benefits from the drug.

If you're a physician and a patient with hypertension walks in your office, all else being equal, should you prescribe them this new drug? If you take the expected value (i.e. average)

of the treatment group distribution, you only get about -13 mmHg change in blood pressure, which is intermediate between the two modes in the distribution. This is still significant compared to placebo, but worse than many existing anti-hypertensives on the market. If you use the expected value of the change in blood pressure for each drug to make your decision, then this new drug will not appear to be very effective despite the fact that a decent number of patients get tremendous benefit from it. Moreover, the expected value of -13 mmHg is very poorly representative of the distribution since very few patients actually had that level of blood pressure reduction. Patients either had almost no response to the drug or a very robust response, there were very few moderate responders.

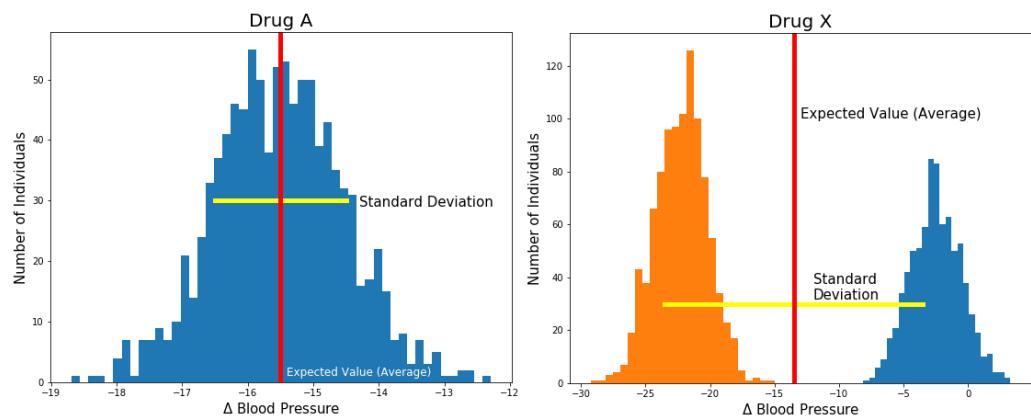


Figure 7.3: Here we compare simulated Drug A to Drug X to see which lowers blood pressure the most. Drug A has a lower average (expected) value of -15.5 mmHg and a lower standard deviation, but Drug X is bi-modal with one mode that is centered at -22.5 mmHg. Notice that for Drug X, virtually no patients had a blood pressure change that falls near the average value.

This should illustrate the limitations of expected values compared to seeing the full distribution. On a population level, if you just use the expected values of the distribution of blood pressure changes for each drug and pick the drug with the lowest expected value (ignoring patient specific complexity such as side effects, etc.) in terms of blood pressure change, then you will be acting optimally at the population level.

More concretely, if drug A, drug B and drug C have average blood pressure changes of -5.1 mmHg, -15.2 mmHg and -9.5 mmHg, you would be acting optimally at the population level by always prescribing drug B since it has the largest effect **on average**. Of course, doctors don't actually do this for a variety of complex reasons we ignore here, but one reason to not use expectation values in prescribing drugs with multi-modality is that multi-modality makes us assess risk differently. Consider Figure 7.2 where we compared an imaginary Drug X with a single mode and Drug A with two modes. If drug X has a probability to reduce a patient's blood pressure by -22.3 mmHg but it also has the possibility of doing nothing, then the healthcare system (or patient in some cases) that has to pay for the drug, may not want to

tolerate the risk of buying the drug when some proportion of patients will not benefit at all as opposed to choosing a drug that has a single mode of moderate efficacy and thus it is less risky.

Another reason the full distribution is important is that a patient may have a particular blood pressure goal. For example, a patient with severe hypertension may *need* to have their blood pressure reduced by at least 20 mmHg. If drug X works for them, then they only need to use one drug. Without drug X they would have to take multiple different drugs. So if you just considered the expected value of drug X of -9 mmHg, you would miss the fact that drug X might actually be the only drug a patient needs if they're the type of patient that has a robust response.

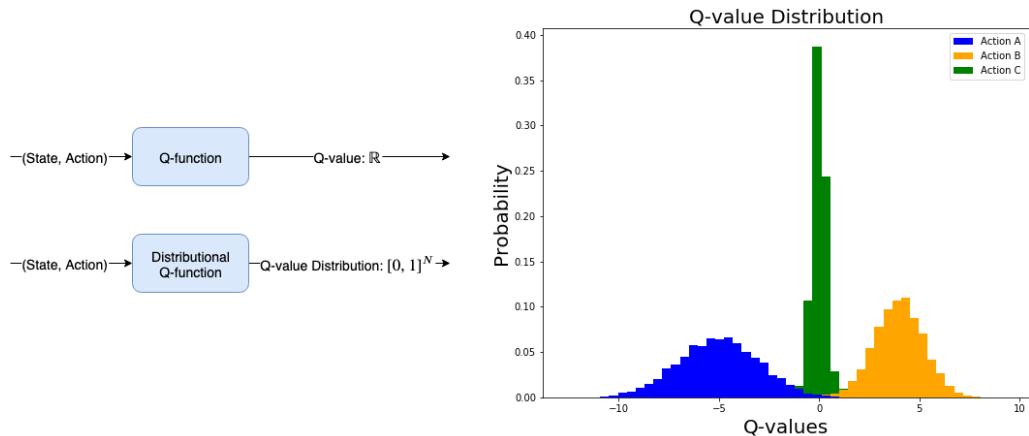


Figure 7.4 : Top-left: An ordinary Q-function takes a state-action pair and computes the associated Q-value.
Bottom-left: A distributional Q-function takes a state-action pair and computes a probability distribution over all possible Q-values. Probabilities are bounded in the interval $[0,1]$ so it returns a vector with all elements in $[0,1]$ and their sum is 1. **Right:** Example Q-value distribution for 3 different actions for some state. Action A is likely to lead to an average reward of -5, whereas Action B is likely to lead to an average reward of +4.

So what does this have to do with deep reinforcement learning? Well, Q-learning as we've learned gives us the expected (average, time-discounted) state-action values, and as you might imagine this can lead to the same limitations we've been discussing with the case of drugs with multi-modal distributions of effects. Learning a full probability distribution over state-action values would give us a lot more power than just learning the expected value as in ordinary Q-learning. With the full distribution we can see if there is multi-modality in the state-action values and how much variance there is in the distribution. Looking at Figure 7.4, which models the action-value distributions for 3 different actions, we can see that some actions have more variance than others. With this additional information we can employ risk-sensitive policies, i.e. policies that aim to not merely maximize expected rewards but to also control the amount of risk we take in doing so.

Most convincingly, an empirical study was done ("Rainbow: Combining Improvements in Deep Reinforcement Learning" by Hessel et al 2017) that evaluated several popular variants and improvements to the original DQN algorithm including a distributional variant of DQN to see which were most effective alone and which were most important in combination. It turns out that distributional Q-learning was the best performing algorithm overall among all the individual improvements to DQN that they tested. They combined all the techniques together into a "Rainbow" DQN, which was shown to be far more effective than any individual technique. They then tested to see which components were most crucial to the success of Rainbow and the results were that distributional Q-learning, multi-step Q-learning (covered in Chapter 5) and prioritized replay (briefly covered in this chapter) were the most important to the Rainbow algorithm's performance.

In this chapter we will learn how to implement a Distributional Deep Q-Network (Dist-DQN) that outputs a probability distribution over state-action values for each possible action given a state. We saw some probability concepts in the policy gradients chapter where we employed a deep neural network as a policy function that directly output a probability distribution over actions, but we will review these concepts again and go into even more depth here as it is important to understand in order to implement Dist-DQN. This may seem a bit too academic, but it will become clear why it is necessary for a practical implementation.

This chapter is the most conceptually difficult chapter in the whole book as it contains a fair amount of probability concepts that are difficult to grasp at first. There is also more math than any other chapter. Getting through this chapter is a big accomplishment and you will have learned or reviewed a lot of very fundamental topics in machine learning and reinforcement learning that will give you a greater grasp of these fields.

7.2 Probability and Statistics Revisited

While the mathematics behind probability theory is consistent and uncontroversial, the interpretation of what it means to say something as trivial as "the probability of a fair coin turning up heads is 0.5" is actually somewhat contentious. The two major camps are called *frequentists* and *Bayesians*. A frequentist says the probability of a coin turning up heads is whatever proportion of heads are observed if one could flip the coin an infinite number of times. A short sequence of coin flips might yield a proportion of heads as high as 0.8, but as you keep flipping it will tend toward 0.5 exactly in the infinite limit. Hence, probabilities are just frequencies of events. In this case, there are two possible outcomes, heads or tails, and each outcome's probability is its frequency after an infinite number of trials (coin flips). This is of course why probabilities are values between 0 (impossible) and 1 (certain) and the probabilities for all possible outcomes must sum to 1.

This is a simple and straightforward approach to probability, but it has significant limitations. In the frequentist setting, it is difficult or perhaps impossible to make sense of a question like "what is the probability that Jane Doe will be elected to city council?" since it is impossible in practice and theory for such an election to happen an infinite number of times. Frequentist probability doesn't make much sense for these kinds of one-off events. We need a

more powerful framework to handle these situations, and that is what Bayesian probability gives us.

In the Bayesian framework, probabilities represent degrees of belief about various possible outcomes. You can certainly have a belief about something that can only happen once, like an election, and your belief about what is likely to happen can vary depending on how much information you have about a particular situation and new information will cause you to update your beliefs (Table 7.1).

Table 7.1: Frequentist versus Bayesian Probabilities

Frequentist	Bayesian
Probabilities are frequencies of individual outcomes	Probabilities are degrees of belief
Compute the probability of the data given a model	Compute the probability of a model given the data
Hypothesis testing	Parameter estimation
Computationally easy	Computationally difficult

In any case, the basic mathematical framework consists of a **sample space** Ω which is the set of all possible outcomes for a particular question. In the case of an election, the sample space is the set of all candidates eligible to win the election. Then there is a probability distribution (or measure) function $P:\Omega\rightarrow[0,1]$, i.e. P is a function from the sample space to real numbers in the interval from 0 to 1. So you could plug in $P(\text{candidate } A)$ and it will spit out a number between 0 and 1 indicating the probability of candidate A winning the election.

PROBABILITY THEORY NOTE:

Technically probability theory is more complicated than we've articulated here and involves a branch of mathematics called measure theory. For our purposes we do not need to delve any deeper into probability theory than what we articulate here. We will stick with an informal and mathematically non-rigorous introduction to the probability concepts we need.

Another term we will use is the **support** of a probability distribution. The support is just the subset of outcomes that are assigned non-zero probabilities. For example, since temperatures can't be less than 0 Kelvin, negative temperatures would be assigned probability 0, so the support of the probability distribution over temperatures would be only from 0 to positive infinity. Since we generally don't care about outcomes that are impossible, you'll often see support or sample space used interchangeably, even though they may not be the same.

7.2.1 Priors and Posteriors

If we were to ask you "what is the probability of each candidate in a 4-way race winning?" without specifying who the candidates were or what the election was about, you might just refuse to answer, citing insufficient information. If we really pressed you, you might say, given

that you know nothing else, each candidate has a $\frac{1}{4}$ chance of winning. With that answer, you've established a **prior probability distribution** that is uniform (each possible outcome has the same probability) over the candidates. Since in the Bayesian framework probabilities represent beliefs, and beliefs are always tentative in situations when new information can become available, a prior probability distribution is just the distribution you start with before receiving some new information. After you receive some new information, such as some biographical information about the candidates, you might update your prior distribution based on that new information and this updated distribution is now called your **posterior probability distribution**. But the distinction between prior and posterior distribution is contextual, since your posterior distribution will become a new prior distribution right before you receive another set of new information. Your beliefs are continually updated as a succession of prior distributions to posterior distributions (Figure 7.5).

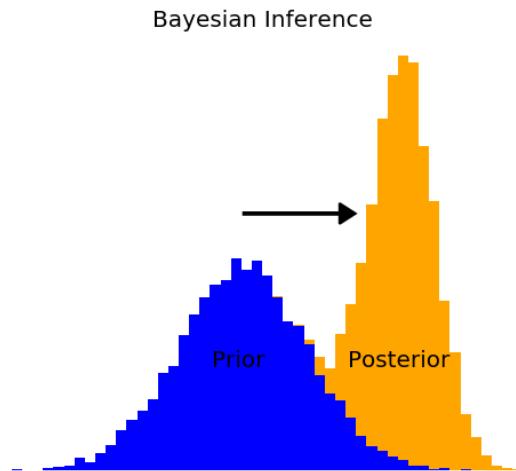


Figure b.: Bayesian inference is the process of starting with a prior distribution, receiving some new information, and using that to update the prior into a new, more informed distribution called the posterior distribution.

7.2.2 Expectation and Variance

There are a number of questions we can ask a probability distribution (i.e. your beliefs about something). We can ask what the single “most likely” outcome is, which we commonly think of as the mean or average of the distribution. You’re probably familiar with the calculation of the mean of something as just taking the sum of all the results and dividing by the number of results. For example, the mean of the 5-day temperature forecast of $[18, 21, 17, 17, 21]^\circ\text{C}$ is $([18+21+17+17+21]) / 5 = 94/5 = 18.8^\circ\text{C}$. This is the average predicted temperature over a sample of 5 days in Chicago, Illinois, USA.

Consider if instead we asked 5 people to give me their prediction for tomorrow's temperature in Chicago and they happened to give me the same numbers, [18,21,17,17,21]°C. If we wanted the average temperature for tomorrow we would do the same procedure, add the numbers up and divide by the number of samples (5) to get the average predicted temperature for tomorrow. However, what if person 1 was a meteorologist and thus we had a lot more confidence in her prediction compared to the other 4 people that we randomly polled on the street? We would probably want to weight her prediction higher than the others. Let's say we think that her prediction is 60% likely to be true, and the other 4 are merely 10% likely to be true (notice $0.6+4*0.1=1.0$), then this is a weighted average and is computed by multiplying each sample by its weight, in this case $[(0.6*18)+0.1*(21+17+17+21)]=18.4^{\circ}\text{C}$.

Each possible temperature is a possible outcome for tomorrow, but not all outcomes are equally likely in this case, so we multiply each possible outcome by its probability (weight) and then sum. If all the weights are equal and sum to 1 then it is equivalent to an ordinary average calculation, but many times it is not. This more general weighted average is called the **expectation value** of a distribution.

The expected value of a probability distribution is its "center of mass," the value that is most likely on average. Given a probability distribution $P(x)$, where x is the sample space, the expected value for discrete distributions is calculated as Table 7.2.

Table 1.1: Computing an expected value from a probability distribution

Math	Python
$\mathbb{E}[P] = \sum x \cdot P(x)$	<pre>>>> x = np.array([1,2,3,4,5,6]) >>> p = np.array([0.1,0.1,0.1,0.1,0.2,0.4]) >>> def expected_value(x,p): ... return x @ p >>> expected_value(x,p) 4.4</pre>

The expected value operator is denoted \mathbb{E} , and is a function that takes in a probability distribution and returns its expected value. It works by just taking a value x , multiplying by its associated probability $P(x)$, and summing for all possible values of x .

In Python, if $P(x)$ is represented as a numpy array of probabilities `probs` and another numpy array of `outcomes` (the sample space), then the expected value is

```
>>> import numpy as np
>>> probs = np.array([0.6, 0.1, 0.1, 0.1, 0.1])
>>> outcomes = np.array([18, 21, 17, 17, 21])
>>> expected_value = 0.0
>>> for i in range(probs.shape[0]):
...     expected_value += probs[i] * outcomes[i]
>>> expected_value
18.4
```

Alternatively, the expected value can be computed as the inner (dot) product between the `probs` array and the `outcomes` array since the inner product does the same thing, it multiplies each corresponding element in the two arrays and sums them all.

```
>>> expected_value = probs @ outcomes
>>> expected_value
18.4
```

A discrete probability distribution means that its sample space is a finite set, or in other words, only a finite number of possible outcomes can occur. A coin can only be one of two outcomes, however, tomorrow's temperature could be any real number (if measured in Kelvin, it would be any real number 0 to infinity), and the real numbers or any subset of the real numbers is infinite, since we can continually divide them, e.g. 1.5 is a real number and so is 1.500001, and so forth.

When the sample space is infinite, then this is a **continuous probability distribution**. In this case, the probability distribution does not tell you the probability of a particular outcome, because with an infinite number of possible outcomes, each individual outcome must have an infinitely small (infinitesimal) probability in order for the sum to be 1. Thus a continuous probability distribution tells you the **probability density** around a particular possible outcome. The probability density is the sum of probabilities around a small interval of some value, or in other words, the probability that the outcome will fall within some small interval. That's all we'll say about continuous distributions for now because in this book we really only deal with discrete probability distributions.

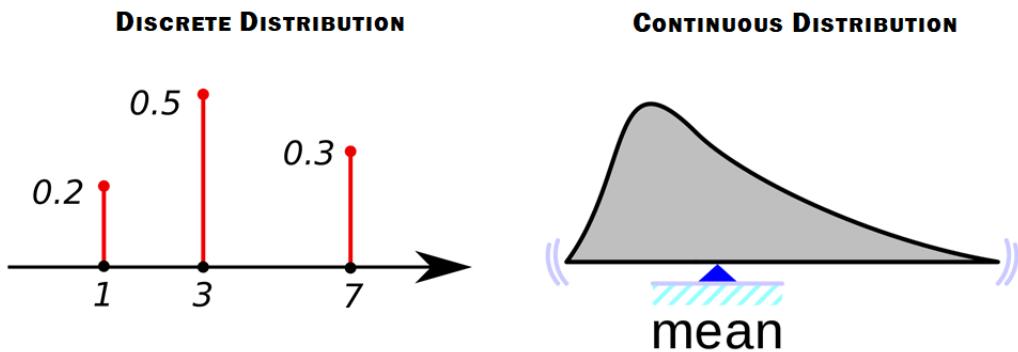
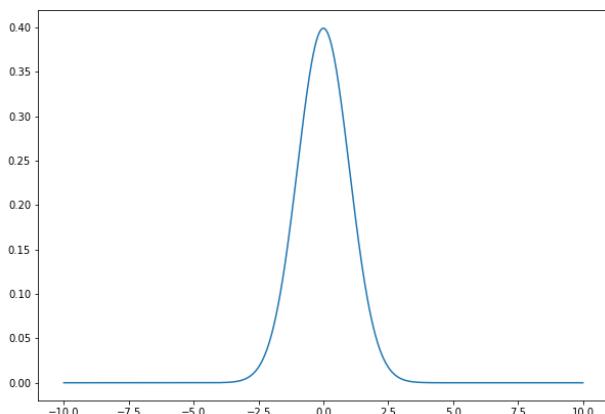
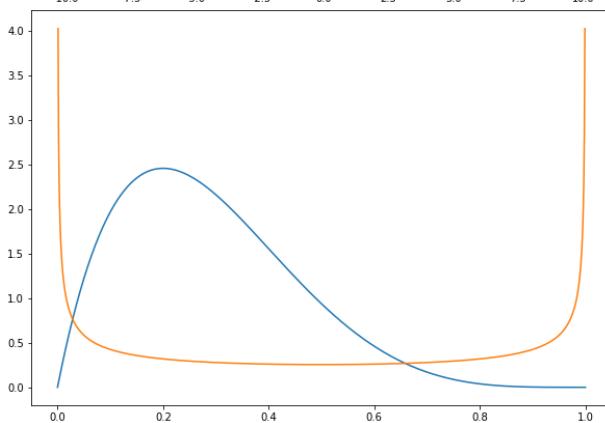
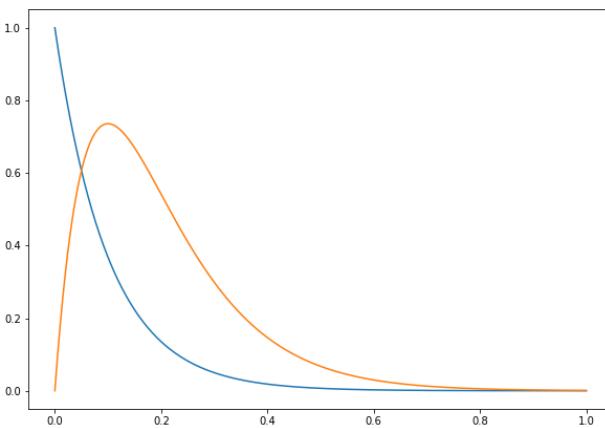


Figure 7.6: Left: A discrete distribution is like a numpy array of probabilities associated with another numpy array of outcome values, i.e. a finite set of probabilities and outcomes. Right: A continuous distribution represents an infinite number of possible outcomes and the y-axis is the probability density (which is the probability that the outcome takes on a value within a small interval).

Another question we can ask of a probability distribution is its spread or variance. Our beliefs about something can be more or less confident, and hence a probability distribution can be narrow or wide, respectively. The calculation of variance uses the expectation operator and is defined as $Var(X)=\sigma^2=\mathbb{E}[(X-\mu)^2]$, but don't worry about remembering this equation as we will just use built-in numpy functions to compute variance. Variance is either denoted $Var(X)$ or σ^2 (sigma squared) where $\sqrt{\sigma^2}=\sigma$ is the standard deviation, so the variance is the standard

deviation squared. The μ in this equation is the standard symbol for mean, which again is $\mu = \mathbb{E}[X]$, where X is a **random variable** of interest.

For example, if we think tomorrow's temperature is just going to be today's temperature plus some random noise, then we can model this as $T = t_0 + e$ where e is a random variable of noise. The noise might have normal (Gaussian) distribution centered around 0 and with a variance of 1. Thus T will be a new normal distribution with mean t_0 (today's temperature) but will still have a variance of 1. A normal distribution is the familiar bell-shaped curve. Table 7.3 shows a few common distributions. The normal distribution just gets wider or narrower depending on the variance parameter, but otherwise looks the same for any set of parameters. In contrast, the beta and gamma distributions can look quite different depending on their parameters. Two different versions of each is shown.

Table 1.2: Common Probability Distributions**Normal Distribution****Beta Distribution****Gamma Distribution**

Random variables are typically denoted with a capital letter like X . In Python, we might setup a random variable using numpy's random module:

```
>>> t0 = 18.4
>>> T = lambda: t0 + np.random.randn(1)
>>> T()
array([18.94571853])
>>> T()
array([18.59060686])
```

Here we made T an anonymous function that accepts no arguments and just adds a small random number to 18.4 every time it is called. So the variance of T is 1, which means that most of the values that T is likely to return will be within 1 degree of 18.4. If the variance was 10, then the spread of the likely temperatures will be greater. Generally we start with a prior distribution that has high variance, and as we get more information the variance decreases. However, it is possible for new information to actually increase the variance of the posterior if the information we get is very unexpected and makes us less certain.

7.3 The Bellman Equation (Optional)

We mentioned Bellman in Chapter 1, but here we will learn about the Bellman equation, which underpins much of reinforcement learning. The Bellman equation shows up everywhere in the reinforcement literature so we thought it is important to at least include a section on it, but if all you want to do is write Python then you can do that without an understanding of the Bellman equation, so this section is optional for those interested in a bit more mathematical background.

Remember, the Q-function tells us the value of a state-action pair, and value is defined as the expected sum of time-discounted rewards. In the Gridworld game, for example, $Q_\pi(s,a)$ tells us the average rewards we will get if we take action a in state s and follow policy π from then forward. The optimal Q -function is denoted Q^* and is the Q -function that is perfectly accurate. When we first start playing a game with a randomly initialized Q -function, it is going to give us very inaccurate Q -value predictions, but the goal is to iteratively update the Q -function until it gets close to the optimal Q^* . The Bellman equation tells us how to update the Q -function when rewards are observed.

$$Q_\pi(s_t, a_t) \leftarrow r_t + \gamma \cdot V_\pi(s_{t+1}),$$

Where

$$V_\pi(s_{t+1}) = \max[Q_\pi(s_{t+1}, a)]$$

So the Q -value of the current state $Q_\pi(s_t, a)$ should be updated to be the observed reward r_t plus the value of the next state $V_\pi(s_{t+1})$ multiplied by the discount factor γ (the left-facing arrow means “assign the value on the right side to the variable on the left side”). The value of the next state is simply whatever the highest Q -value is for the next state (since we get a different Q -value for each possible action). If we use neural networks to approximate the Q -function, then we try to minimize the error between the predicted $Q_\pi(s_t, a)$ on the left-side of

the Bellman equation and the quantity on the right-side by updating the neural network's parameters.

THE DISTRIBUTIONAL BELLMAN EQUATION

The Bellman equation implicitly assumes that the environment is deterministic and thus observed rewards are deterministic, i.e. the observed reward will be always the same if you take the same action in the same state. In some cases this is true, but in other cases it is not. All the games we have used and will use (except for Gridworld) have at least some amount of randomness involved, in some cases just because when we down-sample the frames of a game then some two originally different states will get mapped into the same down-sampled states, leading to some unpredictability in observed rewards. So in this case, we can make the deterministic variable r_t into a random variable $R(s,a)$ that has some underlying probability distribution. If there is randomness in how states evolve into new states, then the Q-function must be a random variable as well. The original Bellman equation from above can now be represented as:

$$Q(s_t, a_t) \leftarrow \mathbb{E}[R(s_t, a_t)] + \gamma \cdot \mathbb{E}[Q(s_{t+1}, A_{t+1})]$$

Again, the Q -function is a random variable because we interpret the environment as having stochastic transitions. That is, taking an action may not lead to the same next state. So we get a probability distribution over next states and actions. So the expected Q -value of the next state-action pair is the most likely Q -value given the most likely next state-action pair. If we get rid of the expectation operator, we get a full distributional Bellman equation.

$$Z(s_t, a_t) \leftarrow R(s_t, a_t) + \gamma \cdot Z(s_{t+1}, A_{t+1})$$

Where we use Z to denote the distributional Q -value function (which we will also refer to as the **value distribution**). When we do Q-learning with the original Bellman equation, our Q -function will learn the expected value of the value distribution because that is the best it can do, but in this chapter we will use a slightly more sophisticated neural network that will return a value distribution and thus can actually learn the distribution of observed rewards rather than just the expected value. This is useful for the reasons we described in the first section, namely that by learning a distribution we have a way to utilize risk-sensitive policies that take into consideration the variance and possible multi-modality of the distribution.

7.4 Distributional Q-learning

Okay, now we have covered all the preliminaries necessary to actually implement a distributional deep Q -network (Dist-DQN). If you didn't completely understand all of the material in the previous sections, don't worry, it will become more clear when we start writing the code. In this chapter we are going to use one of the simplest Atari games in the OpenAI Gym, Freeway, so that we can train the algorithm on a laptop CPU. Unlike other chapters, we're also going to use the RAM version of the game. If you look at the available game

environments at <https://gym.openai.com/envs/#atari> you will see each game has two versions where one is labeled with "RAM."

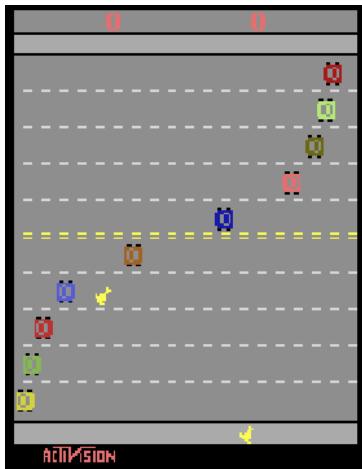


Figure 7.8: Screenshot from the Atari game Freeway. The objective is to move the chicken across the freeway, avoiding oncoming traffic.

Freeway is a game where you control a chicken with actions of UP, DOWN, or NOOP ("no-operation" or do nothing). The objective is to move the chicken across the freeway, avoiding the oncoming traffic, to get to the other side where you get a reward of +1. If you don't get all 3 chickens across the road in a limited amount of time, then you lose the game and get a negative reward.

In most cases in this book we train our DRL agents using the raw pixel representation of the game and thus we use convolutional layers in our neural network, but since we're introducing a new complexity by making a distributional DQN, we want to avoid convolutional layers to keep the focus on the topic at hand and keep training efficient. The RAM version of each game is essentially a compressed representation of the game (e.g. the positions and velocities of each game character, etc.) in the form of a 128-element vector. A 128-element vector is small enough to process through a few fully-connected (dense) layers. Once you are comfortable with the simple implementation we use here, you can use the pixel version of the game and upgrade the Dist-DQN to use convolutional layers.

7.4.1 Representing a probability distribution in Python

If you didn't read the previous optional section, the only important thing you missed is that instead of using a neural network to represent a Q -function $Z_\pi(s,a)$ that returns a single Q -value, we instead denote a value distribution $Z_\pi(s,a)$ that represents a random variable of Q -values given a state-action pair.

Let's first start with how we're going to represent and work with value distributions. As we did in the section on probability theory, we will represent a discrete probability distribution over rewards using two numpy arrays. One numpy array will be the possible outcomes (i.e. the *support* of the distribution) and the other will be an equal-sized array storing the probabilities for each associated outcome. Recall, if we take the inner product between the support array and the probability array then we get the expected reward of the distribution.

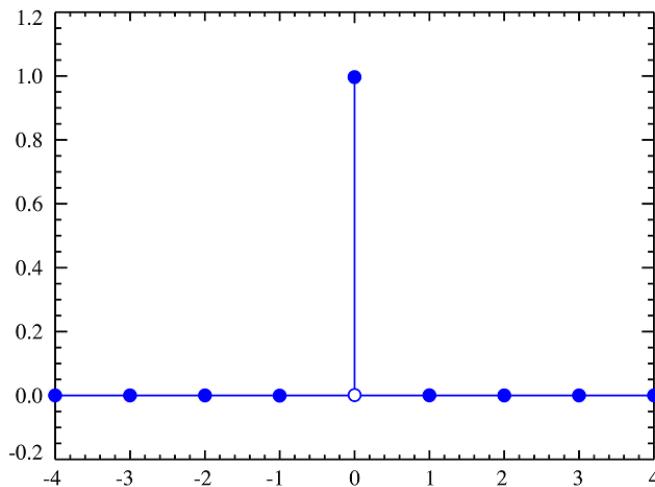


Figure 7.9: This is a **degenerate distribution**, since all the possible values are assigned a probability of 0 except for one value (zero). The outcome values that are *not* assigned to 0 probability are called the probability distribution's **support**. The degenerate distribution has support of 1 element (the value 0).

One problem with the way we're representing the value distribution $Z_n(s,a)$ is that since our array is a finite size, we can only represent a finite number of outcomes. In some cases, the rewards are usually restricted within some fixed, finite range, however, in the stock market the amount of money you make or lose is theoretically unlimited. But with our method we have to choose a minimum and maximum value that we can represent. This limitation has been solved in the follow up paper "Distributional Reinforcement Learning with Quantile Regression" by Dabney et al 2017. We will briefly discuss their approach at the end of the chapter.

For Freeway, we restrict the support to be between -10 and +10. We make all time-steps that are non-terminal (i.e. not a winning or losing state) result in a reward of -1 to penalize taking too much time crossing the road. We reward +10 if the chicken successfully crosses the road and -10 if the game is lost (the chicken doesn't cross the road before the timer runs out).

Our Dist-DQN is going to take a state, which is a 128-element vector and will return 3 separate but equally-sized tensors representing the probability distribution over the support for each of the 3 possible actions (UP, DOWN, NO-OP) given the input state. We will use a 51-

element support, thus the support and probability tensors will be 51-elements. If our agent begins the game with a randomly initialized Dist-DQN, takes action "UP" and receives a reward of -1, how do we update our Dist-DQN? What is the target distribution and how do we compute a loss function between two distributions? Well, we use whatever distribution the Dist-DQN returns for the subsequent state s_{t+1} as a prior distribution, and we update the prior distribution with the single observed reward r_t such that a little bit of the distribution gets re-distributed around the observed r_t .

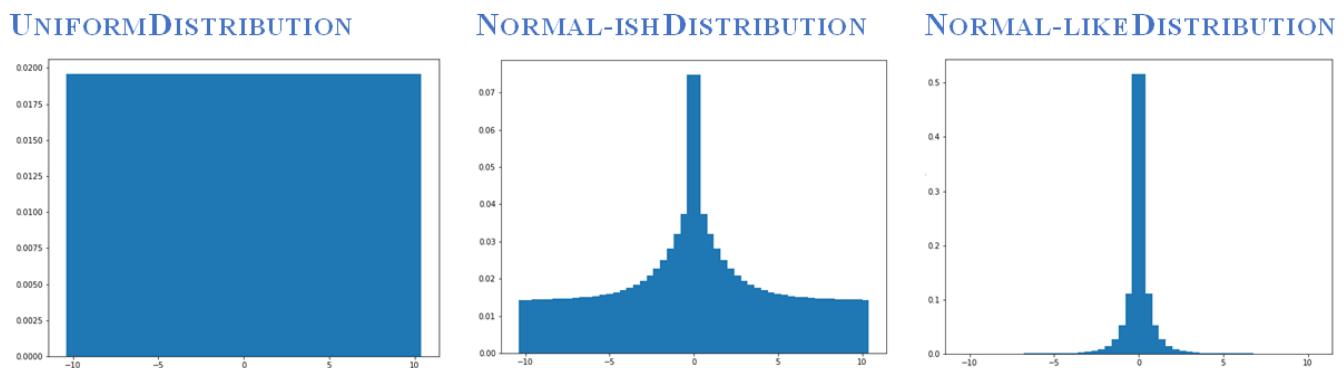


Figure 7.10: We've created a function that takes a discrete distribution and updates it based on observed rewards. This function is performing a kind of approximate Bayesian inference by updating a prior distribution into a posterior distribution. Starting from a uniform distribution on the left, we observe some rewards and we get a peaked distribution at 0 shown in the middle, then we observe even more rewards (all zeros), and the distribution becomes a narrow, normal-like distribution as shown on the right.

If we start with a uniform distribution and observe $r_t = -1$ then the posterior distribution should no longer be uniform but it should still be pretty close. Only if we repeatedly observe $r_t = -1$ for the same state should the distribution start to strongly peak around -1. In normal Q-learning, the discount rate γ (gamma) controlled how much expected future rewards contribute to the value of the current state. In distributional Q -learning, the γ parameter controls how much we update the prior toward the observed reward, which achieves a similar function.

If we discount the future a lot, then the posterior will be strongly centered around the recently observed reward. If we weakly discount the future, then the observed reward will only mildly update the prior distribution $Z(S_{t+1}, A_{t+1})$. Since Freeway has sparse positive rewards in the beginning (e.g. we need to take many actions before we observe our first win) we will set gamma so we only make small updates to the prior distribution.

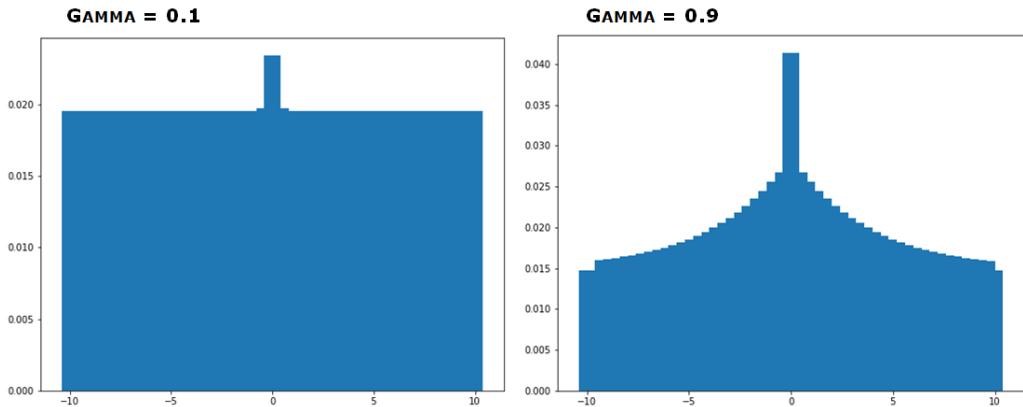


Figure 7.11: This figure shows how a uniform distribution changes with lower or higher values for gamma (the discount factor).

Listing 7.1 Setting up a discrete probability distribution in numpy

```

import torch
import numpy as np
from matplotlib import pyplot as plt

vmin,vmax = -10.,10. #A
nsup=51 #B
support = np.linspace(vmin,vmax,nsup) #C
probs = np.ones(nsup)
probs /= probs.sum()
z3 = torch.from_numpy(probs).float() #D
plt.bar(support,probs)

```

#A Set the minimum and maximum values of the support of the distribution
#B Set the number of elements of the support
#C Create the support tensor, a tensor of evenly-spaced values from -10 to +10
#D Plot the distribution as a bar plot

Now let's see how we update the distribution. We want a function `update_dist(z, reward)` that takes a prior distribution and an observed reward and returns a posterior distribution. Since the support is a vector from -10 to 10:

```

>>> support
array([-10. , -9.6, -9.2, -8.8, -8.4, -8. , -7.6, -7.2, -6.8,
       -6.4, -6. , -5.6, -5.2, -4.8, -4.4, -4. , -3.6, -3.2,
       -2.8, -2.4, -2. , -1.6, -1.2, -0.8, -0.4,  0. ,  0.4,
       0.8,  1.2,  1.6,  2. ,  2.4,  2.8,  3.2,  3.6,  4. ,
       4.4,  4.8,  5.2,  5.6,  6. ,  6.4,  6.8,  7.2,  7.6,
       8. ,  8.4,  8.8,  9.2,  9.6, 10. ])

```

We need to be able to find the closest support element in the support vector to an observed reward. For example, if we observe $r_t = -1$ then we want to map that to either -1.2 or -0.8 .

since those are the closest (equally close) support elements. More importantly, we want the indices of these support elements so that we can get their corresponding probabilities in the probability vector. The support vector is static, we never update it. We only update the corresponding probabilities.

You can see that each support element is 0.4 away from its nearest neighbors. The numpy linspace function creates a sequence of evenly spaced elements, and the spacing is given by $v_{max} - v_{min} / N - 1$, where N is the number of support elements. If you plug 10, -10 and $N=51$ into that formula you get 0.4. We call this value dz (for delta Z), and we use it to find the closest support element index value by the equation $b_j = (r - v_{min}) / dz$, where b_j is the index value. Since b_j may be a fractional number, and indices need to be non-negative integers, we simply round the value to the nearest whole number with `np.round(...)`. We also need to clip any values outside the minimum and maximum support range. For example, if the observed $r_t = -2$, then $b_j = -2 - (-10) / 0.4 = -2 + 10 / 0.4 = 20$. You can see that the support element with index 20 is -2, which in this case exactly corresponds to the observed reward (no rounding needed). We can then find the corresponding probability for the -2 support element using the index.

Once we find the index value of the support element corresponding to the observed reward, we want to redistribute some of the probability mass to that support and the nearby support elements. We have to take care that the final probability distribution is a real distribution and sums to 1. What we will do is simply take some of the probability mass from the neighbors on the left and right and add it to the element that corresponds to the observed reward. Then those nearest neighbors will steal some probability mass from their nearest neighbor, and so on, as shown in Figure 7.11. But the amount of probability mass stolen will get exponentially smaller the farther we go from the observed reward.

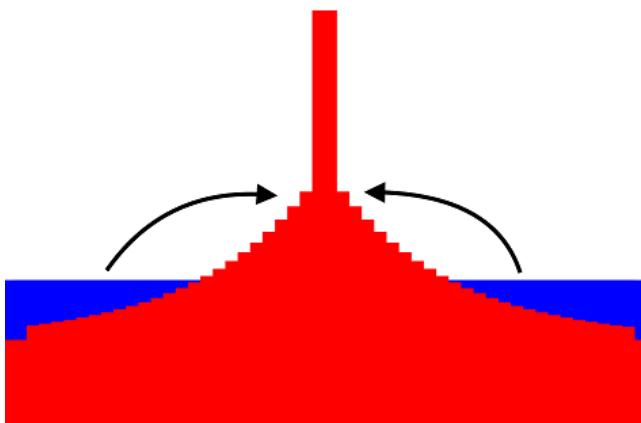


Figure 7.12 : The `update_dist` function re-distributes probability from neighbors toward the observed reward value.

Below we implement the function that takes a set of supports, the associated probabilities, and an observation and returns an updated probability distribution by redistributing the probability mass toward the observed value.

Listing 7.2 Updating a probability distribution

```
def update_dist(r,support,probs,lim=(-10.,10.),gamma=0.8):
    nsup = probs.shape[0]
    vmin,vmax = lim[0],lim[1]
    dz = (vmax-vmin)/(nsup-1.) #A
    bj = np.round((r-vmin)/dz) #B
    bj = int(np.clip(bj,0,nsup-1)) #C
    m = probs.clone()
    j = 1
    for i in range(bj,1,-1): #D
        m[i] += np.power(gamma,j) * m[i-1]
        j += 1
    j = 1
    for i in range(bj,nsup-1,1): #E
        m[i] += np.power(gamma,j) * m[i+1]
        j += 1
    m /= m.sum() #F
    return m
```

#A Calculate the support spacing value

#B Calculate the index value of the observed reward in the support

#C Round and clip the value to make sure it is a valid index value into the support

#D Starting from the immediate left neighbor, steal part of its probability

#E Starting from the immediate right neighbor, steal part of its probability

#F Divide by the sum to make sure it sums to 1

Let's walk through the mechanics of this to see how it works. We start with a uniform prior distribution:

```
>>> probs
array([0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784,
       0.01960784, 0.01960784, 0.01960784, 0.01960784, 0.01960784])
```

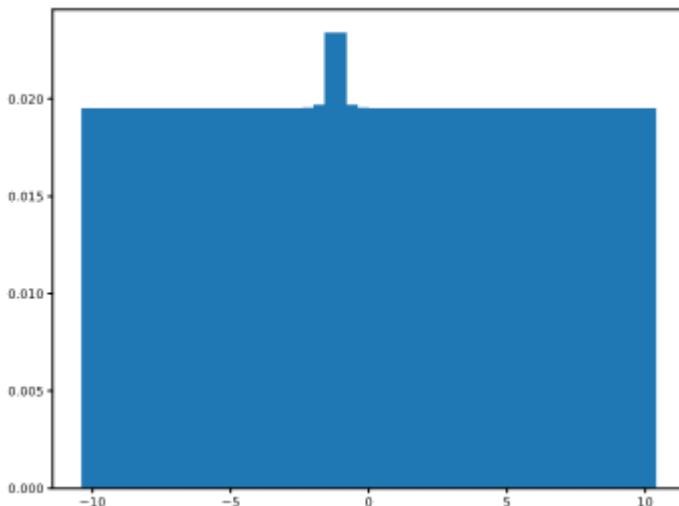
You can see each support has a probability of about 0.02. We observe $r_t = -1$, and we calculate $b_j \approx 22$. We then find the nearest left and right neighbors, denoted m_l and m_r , to be indices 21 and 23, respectively. We then multiply m_l by γ^j where j is a value that we increment by 1 starting at 1, so we get a sequence of exponentially decreasing gammas, e.g. $\gamma^1, \gamma^2, \dots, \gamma^j$.

Remember, gamma must be a value between 0 and 1, so the the sequence of gammas will be 0.5, 0.25, 0.125, 0.0625 if $\gamma=0.5$. So at first we take $0.5*0.02=0.01$ from the left and right neighbor and add it so the existing probability at $b_j=22$, which is also 0.02. So the probability at $b_j = 22$ will become $0.01+0.01+0.02=0.04$.

Now the left neighbor m_l steals probability mass from its own left neighbor at index 20, but it steals less since we multiply by γ^2 . The right neighbor m_r does the same by stealing from its neighbor on the right. Each element in turn steals from either its left or right neighbor until we get to the end of the array. If gamma is close to 1 like 0.99, then a lot of probability mass will be re-distributed to the support close to r_t . Let's test our distribution update function. We'll give it an observed reward of -1 starting from a uniform distribution.

Listing 7.3 Redistributing probability mass after a single observation

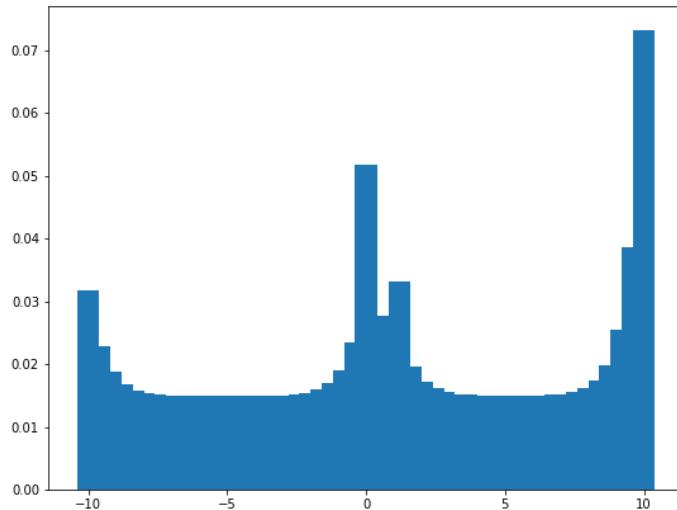
```
ob_reward = -1
Z = torch.from_numpy(probs).float()
Z =
    update_dist(ob_reward,torch.from_numpy(support).float(),Z,lim=(vmin,vmax),gamm
    a=0.1)
plt.bar(support,Z)
```



You can see that the distribution is still fairly uniform but now there is a distinct “bump” centered at -1. We can control how big this bump is with the discount factor γ . On your own, try changing gamma to see how it changes the update. Now let's see how the distribution changes when we observe a sequence of varying rewards. We should be able to observe multi-modality.

Listing 7.4 Redistributing probability mass with a sequence of observations

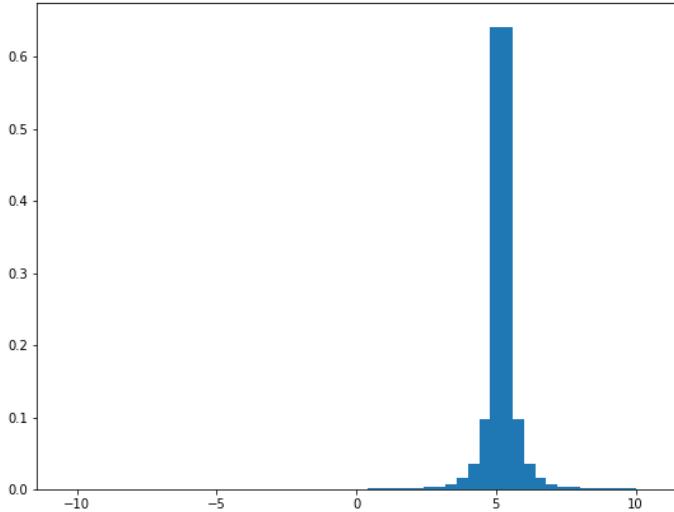
```
ob_rewards = [10,10,10,0,1,0,-10,-10,10,10]
for i in range(len(ob_rewards)):
    Z = update_dist(ob_rewards[i], torch.from_numpy(support).float(), Z,
                    lim=(vmin,vmax), gamma=0.5)
plt.bar(support, Z)
```



You can see there are now 4 peaks of varying heights corresponding the 4 different kinds of rewards observed, namely 10, 0, 1, and -10. The highest peak (mode of the distribution) corresponds to 10 since that was the most frequently observed reward. Now let's see how the variance will decrease if we observe the same reward multiple times starting from a uniform prior.

Listing 7.5 Decreased variance with sequence of same reward

```
ob_rewards = [5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5, 5]
for i in range(len(ob_rewards)):
    Z = update_dist(ob_rewards[i], torch.from_numpy(support).float(), \
                    Z, lim=(vmin,vmax), gamma=0.7)
plt.bar(support, Z)
```



You can see that the uniform distribution transforms into a normal-like distribution centered at 5 with much lower variance. We will use this function to generate the target distribution that we want the Dist-DQN to learn to approximate. Let's build the Dist-DQN now.

7.4.2 Implementing the Dist-DQN

As we briefly discussed earlier, the Dist-DQN will take a 128-element state vector, pass it through a couple of dense feedforward layers, and then we will use a for-loop to multiply the last layer by 3 separate matrices to get 3 separate distribution vectors. We will lastly apply the softmax function to ensure it is a valid probability distribution. So it is a neural network with 3 different output "heads." We collect these 3 output distributions into a single 3×51 matrix and return that as the final output of the Dist-DQN. Thus we can get the individual action-value distributions for a particular action by indexing a particular row of the output matrix. Figure 7.11 shows the overall architecture and tensor transformations.

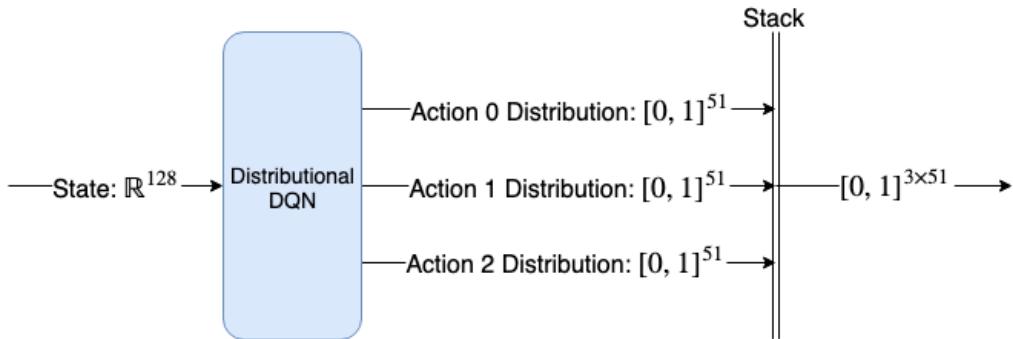


Figure 7.13 : The Distributional DQN (Dist-DQN) accepts a 128-element state vector and produces 3 separate 51-element probability distribution vectors, which then get stacked into a single 3×51 matrix.

Listing 7.6 The Distributional DQN

```

def dist_dqn(x,theta,aspace=3): #A
    dim0,dim1,dim2,dim3 = 128,100,25,51 #B
    t1 = dim0*dim1
    t2 = dim2*dim1
    theta1 = theta[0:t1].reshape(dim0,dim1) #C
    theta2 = theta[t1:t1 + t2].reshape(dim1,dim2)
    l1 = x @ theta1 #D
    l1 = torch.selu(l1)
    l2 = l1 @ theta2 #E
    l2 = torch.selu(l2)
    l3 = []
    for i in range(aspace): #F
        step = dim2*dim3
        theta5_dim = t1 + t2 + i * step
        theta5 = theta[theta5_dim:theta5_dim+step].reshape(dim2,dim3)
        l3_ = l2 @ theta5 #G
        l3.append(l3_)
    l3 = torch.stack(l3,dim=1) #H
    l3 = torch.nn.functional.softmax(l3,dim=2)
    return l3.squeeze()

```

#A `x` is the 128-element vector state, `theta` is the parameter vector, and `aspace` is the size of the action space
#B We define the layer dimensions so we can unpack theta into appropriately sized matrices
#C We unpack the first portion of `theta` into the first layer matrix
#D The dimensions of this computation are $B \times 128 \times 128 \times 100 = B \times 100$, where `B` is batch size
#E The dimensions of this computation are $B \times 100 \times 100 \times 25 = B \times 25$
#F Loop through each action to generate each action-value distribution
#G The dimensions of this computation are $B \times 25 \times 25 \times 51 = B \times 51$
#H The dimensions of the last layer are $B \times 3 \times 51$

In this chapter we will do gradient descent manually, and to make this easier we have our Dist-DQN accept a single parameter vector called 'theta' that we will unpack and reshape

into multiple separate layer matrices of the appropriate sizes. This is easier since we can just do gradient descent on a single vector rather than multiple separate entities. We also will use a separate target network as we did in the DQN chapter, so all we need to do is keep a copy of `theta` and pass that into the same `dist_dqn` function.

The other novelty is the multiple output heads. We're used to a neural network returning a single output vector but in this case we want it to return a matrix. To do that, we setup a loop where we multiply `I2` by each of 3 separate layer matrices, resulting in 3 different output vectors that we stack into a matrix. Other than that, it is a very simple neural network with a total of 5 dense layers.

Now we need a function that will take the output of our Dist-DQN, a reward, and an action and then generate the target distribution we want our neural network to get closer to. This function will use the `update_dist` function we used earlier but it only want to update the distribution associated with the action that was actually taken. Also, as we learned in the DQN chapter, we also need a different target when we've reached a terminal state. At the terminal state, the expected reward is the observed reward since there are no future rewards by definition. That means the Bellman update reduces to $Z(s_t, a_t) \leftarrow R(S_t, A_t)$. Since we only observe a single reward and there is no prior distribution to update, the target becomes what is called a **degenerate distribution**. That's just a fancy term for a distribution where all the probability mass is concentrated at a single value.

Listing 7.7 Computing the target distribution

```
def get_target_dist(dist_batch,action_batch,reward_batch,support,lim=(-10,10),gamma=0.8):
    nsup = support.shape[0]
    vmin,vmax = lim[0],lim[1]
    dz = (vmax-vmin)/(nsup-1.)
    target_dist_batch = dist_batch.clone() #A
    for i in range(dist_batch.shape[0]): #A
        dist_full = dist_batch[i]
        action = int(action_batch[i].item())
        dist = dist_full[action]
        r = reward_batch[i]
        if r != -1: #B
            target_dist = torch.zeros(nsup)
            bj = np.round((r-vmin)/dz)
            bj = int(np.clip(bj,0,nsup-1))
            target_dist[bj] = 1.
        else: #C
            target_dist = update_dist(r,support,dist,lim=lim,gamma=gamma)
        target_dist_batch[i,action,:] = target_dist #D
    return target_dist_batch
```

#A Loop through the batch dimension

#B If the reward is not -1 then it is a terminal state and the target is a degenerate distribution at the reward value

#C If the state is non-terminal, then the target distribution is a Bayesian update of the prior given the reward

#D Only change the distribution for the action that was taken

The `get_target_dist` function takes a batch of data of shape $B \times 3 \times 51$ where `B` is the batch dimension and returns an equal sized tensor. For example, if we only have one example in our batch, i.e. $1 \times 3 \times 51$, and the agent took action 1 and observed a reward of -1 , then this function will return a $1 \times 3 \times 51$ tensor except that the 1×51 distribution associated with index 1 (of dimension 1) will be changed according to the `update_dist` function using the observed reward of -1 . If the observed reward was instead 10 , then the 1×51 distribution associated with action 1 will be updated to be a degenerate distribution where all elements have 0 probability except the one associated with reward of 10 (index 50).

7.5 Comparing Probability Distributions

Now that we have a Dist-DQN and a way to generate target distributions, we need a loss function that will calculate how different the predicted action-value distribution is from the target distribution, and then we can backpropagate and do gradient descent as usual to update the Dist-DQN parameters to be more accurate next time. We often use the Mean Squared Error (MSE) loss function when trying to minimize the distance between two batches of scalars or vectors, but this is not an appropriate loss function between two probability distributions. However, there are in fact many possible choices for a loss function between probability distributions. We want a function that will measure how different or distant two probability distributions are and minimize that distance.

In machine learning, we are usually trying to train a parametric model (e.g. a neural network) to predict or produce data that closely matches empirical data from some dataset. Thinking probabilistically, we can conceive of a neural network as generating synthetic data and trying to train the neural network to produce more and more realistic data, i.e. data that closely resembles some empirical dataset. This is how we train **generative** models, i.e. models that generate data; we train them by updating their parameters so that the data they generate looks very close to some training (empirical) dataset.

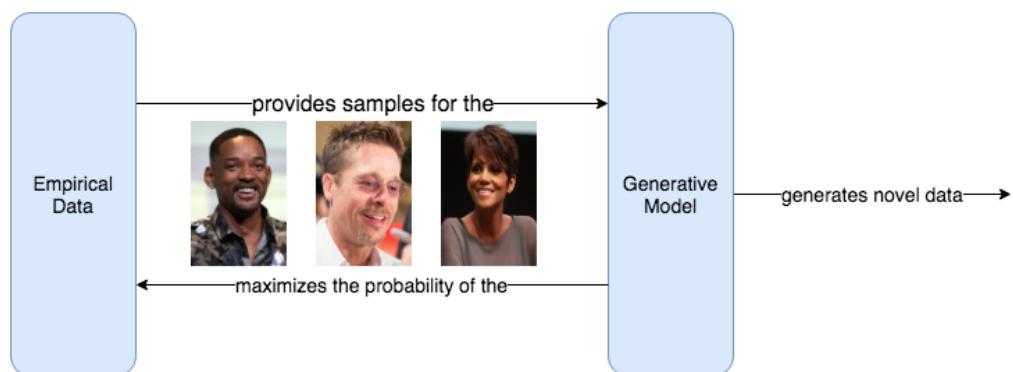


Figure 7.14: A generative model can be a probabilistic model that trains by maximizing the probability that it

generates samples that are similar to some empirical dataset. Before training, the generative model will assign low probability to examples taken from the training data set, and the objective is for the generative model to assign high-probability to examples drawn from the dataset, and thus it will be able to generate novel samples. Training happens in an iterative loop where the empirical data is supplied to the generative model, which tries to maximize the probability of the empirical data. After a sufficient number of iterations, the generative model will have assigned high probability to the empirical data and therefore we can sample from this distribution to generate new, synthetic data.

For example, let's say we want to build a generative model that produces images of celebrities faces. In order to do this, we need some training data, so we use the freely available CelebA dataset that contains hundreds of thousands of high quality photographs of various celebrities such as Will Smith and Britney Spears. Let's call our generative model P and this empirical dataset Q .

Now the images in the dataset Q were sampled from the real world, but they are just a small sample of the infinite number of photographs that already exist but are not in the dataset and the ones that could have been taken but did not. For example, there may just be one headshot photo of Will Smith in the dataset, but another photo of Will Smith taken at a different angle could have just as easily been part of the dataset. However, a photo of Will Smith with a baby elephant on top of his head, while not impossible, would be less likely to be included in the dataset because it is less likely to exist (who would put a baby elephant on their head?).

There are naturally more and less likely photos of celebrities, thus the real world has a probability distribution over images of celebrities. We can denote this true probability distribution of celebrity photos as $Q(x)$, where x is some arbitrary image, and $Q(x)$ tells us the probability of that image existing in world. If x is a specific image in the dataset Q , then $Q(x) = 1.0$ since that image definitely exists in the real world. However, if we plug in an image that's not in the dataset but likely exists in the real world outside of our small sample, then $Q(x)$ might equal 0.9.

When we randomly initialize our generative model P , it will output random-looking images that look like white noise. We can think of our generative model as a random variable, and every random variable has an associated probability distribution that we denote $P(x)$, so we can also ask our generative model what the probability of a specific image is given its current set of parameters. When we first initialize it, it will think all images are more or less equally probable and all will be assigned a fairly low probability. So if we ask $P(\text{"Will Smith photo"})$ it will return some tiny probability, but if we ask $Q(\text{"Will Smith Photo"})$ we get 1.0.

In order to train our generative model P to generate realistic celebrity photos using the dataset Q , we want the generative model to assign high probability to the data in Q and also data that are not in Q but plausibly could be. Mathematically, we want to maximize this ratio:

$$LR = \frac{P(x)}{Q(x)}$$

Which we call the likelihood ratio (LR) between $P(x)$ and $Q(x)$. Likelihood in this context is just another word for probability. If we take the ratio for an example image of Will Smith that exists in Q using an un-trained P , we might get:

$$LR = \frac{P(x = \text{Will Smith})}{Q(x = \text{Will Smith})} = \frac{0.0001}{1.0} = 0.0001$$

This is a tiny ratio. We want to backpropagate into our generative model and do gradient descent to update its parameters so that this ratio is maximized. This likelihood ratio is our objective function to maximize (or minimize its negative). But we don't want to do this just for a single image, we want the generative model to maximize the total probability of all the images in the dataset Q . We can find this total probability by taking the product of all the individual examples (because the probability of A *and* B is the probability of A *times* the probability of B when A and B are independent and come from the same distribution). So our new objective function is the product of the likelihood ratios for each datum in the dataset. Note that we have several math equations coming up but we're just using them to explain the underlying probability concepts, don't spend any time trying to remember them.

Table 1.3: The Likelihood Ratio in Math and Python

Math

$$LR = \prod_i \frac{P(x_i)}{Q(x_i)}$$

Python

```
p = np.array([0.1, 0.1])
q = np.array([0.6, 0.5])
def lr(p,q):
    return np.prod(p/q)
```

One problem with this objective function is that computers have a hard time multiplying a bunch of probabilities since they are tiny floating-point numbers, which when multiplied together to create even smaller floating-point numbers. This results in numerical inaccuracies and ultimately numerical underflow since computers have a finite range of numbers they can represent. To improve this situation, we generally use log-probabilities (equivalently, log-likelihoods) because the logarithm function turns tiny probabilities into large numbers ranging from negative infinity (when the probability approaches 0) up to a maximum of 0 (when the probability is 1).

Logarithms also have the nice property that $\log(a \cdot b) = \log(a) + \log(b)$, so we can turn multiplication into addition, and computers can handle that a lot easier without risking

numerical instability or overflows. We can transform the product log-likelihood ratio equation above into:

Table 1.4: The Log-Likelihood Ratio in Math and Python

Math

$$LR = \sum_i \log\left(\frac{P(x_i)}{Q(x_i)}\right)$$

Python

```
p = np.array([0.1,0.1])
q = np.array([0.6,0.5])
def lr(p,q):
    return np.sum(np.log(p/q))
```

Okay, the log-probability version of the equation is simpler and better for computation, but another problem is that we want to weight individual samples differently. For example, if we sample an image of Will Smith from the dataset then it should have a higher probability than an image of some less famous celebrity since the less famous celebrity probably has fewer photos taken of them. We want our model to put more weight on learning images that are more probable out in the real world, or in other words, with respect to the empirical distribution $Q(x)$. So we will weight each log-likelihood ratio by its $Q(x)$ probability.

Table 1.5: The Weighted Log-Likelihood Ratio in Math and Python

Math

$$LR = \sum_i Q(x_i) \cdot \log\left(\frac{P(x_i)}{Q(x_i)}\right)$$

Python

```
p = np.array([0.1,0.1])
q = np.array([0.6,0.5])
def lr(p,q):
    x = q * np.log(p/q)
    x = np.sum(x)
    return x
```

We now have an objective function that measures how likely a sample from the generative model is compared to the real world distribution of data, weighted by how likely the sample is in the real world. There's one last minor problem. This objective function must be maximized because we want the log-likelihood ratio to be high, but by convenience and convention we prefer to have objective functions that are error or loss functions to be minimized. We can remedy this just by adding a negative sign, so a high-likelihood ratio becomes a small error or loss.

Table 1.6: The Kullback-Leibler divergence**Math**

$$D_{KL}(Q \parallel P) = - \sum_i Q(x_i) \cdot \log\left(\frac{P(x_i)}{Q(x_i)}\right)$$

Python

```
p = np.array([0.1,0.1])
q = np.array([0.6,0.5])
def lr(p,q):
    x = q * np.log(p/q)
    x = -1 * np.sum(x)
    return x
```

You may notice we switched out LR for some strange symbols $D_{KL}(Q \parallel P)$. It turns out the objective function we just created is a very important one in all of machine learning and is called the **Kullback-Leibler divergence** or KL divergence for short. The KL divergence is a kind of error function between probability distributions, i.e. it tells you how different two probability distributions are.

Often times we are trying to minimize the distance between a model generated probability distribution and some empirical distribution from real data, so we want to minimize the KL divergence. As we just saw, minimizing the KL divergence is equivalent to maximizing the joint log-likelihood ratio of the generated data compared to the empirical data. One important thing to note is that the KL divergence is not symmetric, i.e. $D_{KL}(Q \parallel P) \neq D_{KL}(P \parallel Q)$, and this should be clear from its mathematical definition. The KL divergence contains a ratio, and thus no ratio can equal its inverse unless both are 1, i.e. $a/b \neq b/a$ unless $a=b$.

While the *KL* divergence makes a perfect objective function, we can actually simplify it just a bit for our purposes. Recall that $\log(a/b)=\log(a)-\log(b)$ in general. So we can rewrite the *KL* divergence as:

$$D_{KL}(Q \parallel P) = - \sum_i Q(x) \cdot \log(P(x_i)) - \log(Q(x_i))$$

Note that in machine learning, we only want to optimize (update the parameters of the model to reduce the error) the model, we cannot change the empirical distribution $Q(x)$. Therefore, we really only care about the weighted log-probability on the left side, i.e.

$$H(Q, P) = - \sum_i Q(x) \cdot \log(P(x_i))$$

This simplified version is called the **cross-entropy loss** and denoted $H(Q,P)$. This is the actual loss function that we will use in this chapter to get the error between our predicted action-value distribution and a target (empirical) distribution.

Or in Python given a batch of action-value distributions with dimensions $B \times 3 \times 51$:

Listing 7.8 The Cross-Entropy Loss Function

```
def lossfn(x,y):#A
    loss = torch.Tensor([0.])
    loss.requires_grad=True
    for i in range(x.shape[0]): #B
        loss_ = -1 * torch.log(x[i].flatten(start_dim=0)) @
        y[i].flatten(start_dim=0) #C
        loss = loss + loss_
    return loss
```

#A Loss between prediction distribution `x` and target distribution `y`

#B Loop through batch dimension

#C Flatten along action dimension to get a concatenated sequence of the distributions

The `lossfn` function takes a prediction distribution `x` of dimensions $B \times 3 \times 51$ and a target distribution `y` of the same dimensions and then flattens the distribution over the action dimension to get a $B \times 153$ matrix. Then we loop through each 1×153 row in the matrix and compute the cross entropy between the 1×153 prediction distribution and the 1×153 target distribution. Rather than explicitly summing over the product of `x` and `y`, we can combine these two operations and get the result in one shot by using the inner product operator `@`.

We could choose to just compute the loss between the specific action-value distribution for the action that was taken, but we compute the loss for all 3 action-value distributions so that the Dist-DQN learns to keep the other 2 actions not taken unchanged and only updates the action-value distribution that was taken.

7.6 Dist-DQN on Simulated Data

Let's test all the parts so far with a simulated target distribution to see if our Dist-DQN can successfully learn to match the target distribution.

Listing 7.9 Testing with simulated data

```
aspace = 3 #A
tot_params = 128*100 + 25*100 + aspace*25*51 #B
theta = torch.randn(tot_params)/10. #C
theta.requires_grad=True
theta_2 = theta.detach().clone() #D
#
vmin,vmax= -10,10
gamma=0.9
lr = 0.00001
update_rate = 75 #E
support = torch.linspace(-10,10,51)
state = torch.randn(2,128)/10. #F
action_batch = torch.Tensor([0,2]) #G
reward_batch = torch.Tensor([0,10]) #H
losses = []
pred_batch = dist_dqn(state,theta,aspace=aspace) #I
target_dist = get_target_dist(pred_batch,action_batch,reward_batch, \
support, lim=(vmin,vmax),gamma=gamma) #J
```

```

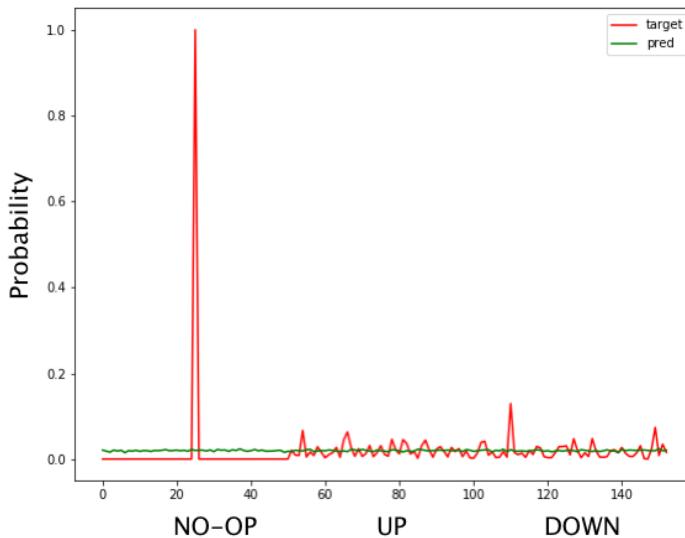
plt.plot((target_dist.flatten(start_dim=1)[0].data.numpy()),color='red',label='target')
plt.plot((pred_batch.flatten(start_dim=1)[0].data.numpy()),color='green',label='pred')
plt.legend()

```

```

#A Define the action space to be of size 3
#B Define the total number of Dist-DQN parameters based on layer sizes
#C Randomly initialize a parameter vector for Dist-DQN
#D Clone `theta` to use as a target network
#E We will synchronize the main and target Dist-DQN parameters every 75 steps
#F Randomly initialize two states for testing
#G Create synthetic action data
#H Create synthetic reward data
#I Initialize a prediction batch
#J Initialize a target batch

```



Concatenated action-values for all actions

Figure 7.15: This shows the predicted action-value distributions produced by an untrained Dist-DQN and the target distribution after observing a reward. There are 3 separate action-value distributions of length 51-elements but here they've been concatenated into one long vector to see the overall fit between the prediction and target. The first 51 elements correspond to the action-value distribution of the NO-OP operation, the second 51 elements correspond to the action-value distribution of the UP action, and the last 51 elements correspond to the DOWN distribution. You can see the prediction is a completely flat (uniform) distribution for all 3 actions, whereas the target distribution has a mode (i.e. peak) for action 0 and some noisy peaks for the other two actions. The goal is to get the prediction to match the target distribution.

Here we're going to test the Dist-DQNs ability to learn the distribution for 2 samples of data. Action 0 is associated with a reward of 0, and action 2 is associated with a reward of 10. We expect the Dist-DQN to learn that state 1 is associated with action 1 and state 2 with action 2 and learn the distributions. You can see with the randomly initialized parameter vector that the prediction distribution for all 3 actions (remember, we flattened it along the action dimension) is pretty much a uniform distribution, whereas the target distribution has a peak at 0 (since we plotted only the first sample). After training, the prediction and target distributions should match fairly well.

The reason why a target network is so important is very clear with Dist-DQN. Remember, a target network is just a copy of your main model that we only update after some lag time. We use the target network's prediction to create the target for learning but we only use the main model parameters to do gradient descent. This stabilizes the training because without a target network, the target distribution will change after each parameter update from gradient descent, yet gradient descent is trying to move the parameters toward being more accurate to the target distribution, so there is a circularity (hence instability) and it can lead to the target distribution dramatically changing as a result of this dance between the Dist-DQN's predictions and the target distribution.

By using a lagged copy of the Dist-DQN prediction (via a lagged copy of the parameters, which is the target network), the target distribution does not change every iteration and is not immediately affected by the continual updates from the main Dist-DQN model. This significantly stabilizes the training. If you reduce the `update_rate` to 1 and try training you will see that the target evolves into something completely wrong. Let's see how to train.

Listing 7.10 Dist-DQN Test Training

```
for i in range(1000):
    reward_batch = torch.Tensor([0,8]) + torch.randn(2)/10.0 #A
    pred_batch = dist_dqn(state,theta,aspace=aspace) #B
    pred_batch2 = dist_dqn(state,theta_2,aspace=aspace) #C
    target_dist = get_target_dist(pred_batch2,action_batch,reward_batch, \
                                    support, lim=(vmin,vmax),gamma=gamma) #D
    loss = lossfn(pred_batch,target_dist.detach()) #E
    losses.append(loss.item())
    loss.backward()
    # Gradient Descent
    with torch.no_grad():
        theta -= lr * theta.grad
    theta.requires_grad = True

    if i % update_rate == 0: #F
        theta_2 = theta.detach().clone()

plt.plot((target_dist.flatten(start_dim=1)[0].data.numpy()),color='red',label='target')
plt.plot((pred_batch.flatten(start_dim=1)[0].data.numpy()),color='green',label='pred')
plt.plot(losses)
```

```
#A Add some random noise to rewards to make it a bit harder
#B Use main model Dist-DQN to make distribution prediction
#C Use target network Dist-DQN to make distribution prediction (using lagged parameters)
#D Use the target network's distributions to create the target distribution for learning
#E Use the main model's distribution prediction in the loss function
#F Synchronize target network parameters with main model parameters
```

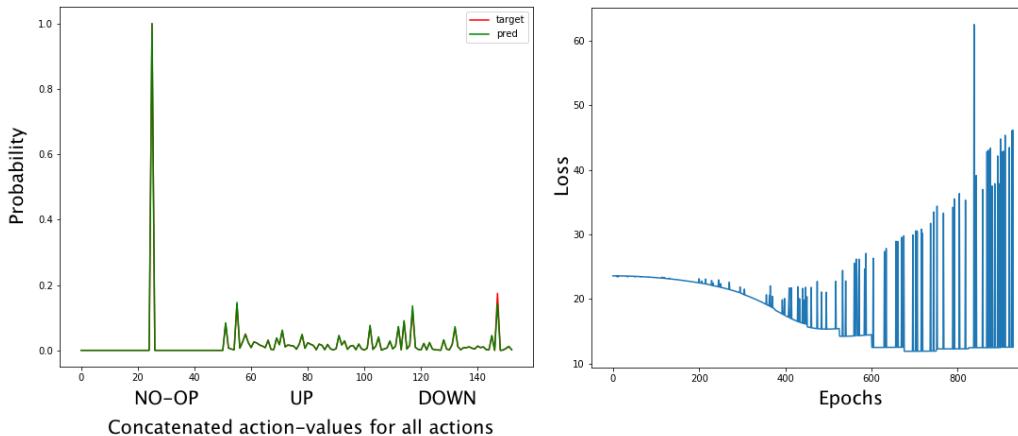


Figure 7.16: Left: The concatenated action-value distributions for all 3 actions after training. Right: Loss plot over training time. The baseline loss is decreasing but we see ever-increasing spikes.

You can see that the target and prediction from Dist-DQN now match almost exactly after training (you may not even be able to see there are two overlapping distributions anymore), it works! The loss plot has those spikes from each time the target network gets synchronized to the main model and thus the target distribution suddenly changes, leading to a higher than normal loss at that time step. We can also look at the learned distributions for each action for each sample in the batch, which we show how to do in Listing 7.11.

Listing 7.11 Visualizing the learned action-value distributions

```
tpred = pred_batch
cs = ['gray','green','red']
num_batch = 2
labels = ['Action {}'.format(i,) for i in range(aspace)]
fig,ax = plt.subplots(nrows=num_batch,ncols=aspace)

for j in range(num_batch): #A
    for i in range(tpred.shape[1]): #B
        ax[j,i].bar(support.data.numpy(),tpred[j,i,:].data.numpy(),\
                     label='Action {}'.format(i),alpha=0.9,color=cs[i])
```

#A Loop through experiences in batch
#B Loop through each action

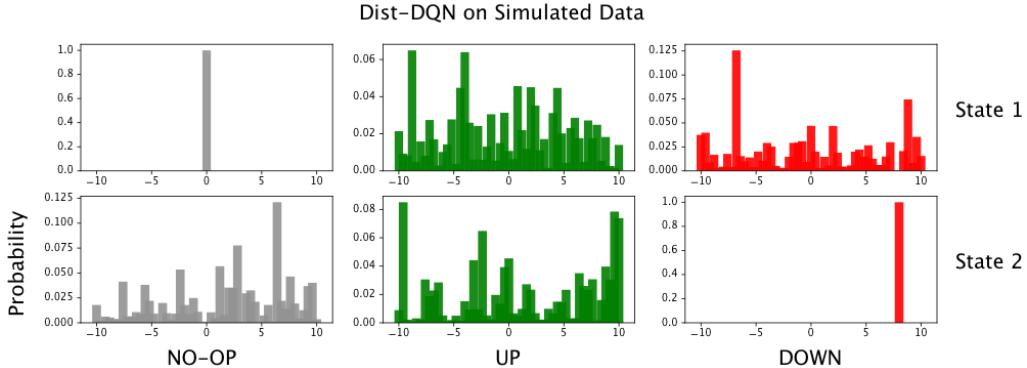


Figure 7.17: Each row contains the action-value distributions for an individual state and each column in a row is the distribution for actions 0, 1, and 2, respectively.

You can see that in the first sample, the distribution on the left, associated with action 0, has collapsed into a degenerate distribution at 0, just like the simulated data. Yet the other 2 actions remain fairly uniform with no clear peaks. Similarly in the second sample in the batch the action 2 distribution is a degenerate distribution at 10, as the data were, and again the other 2 actions remain fairly uniform-like.

This Dist-DQN test has almost everything we will use in a real experiment with Atari Freeway. There are 2 functions we need before we get to playing Freeway. One is to preprocess the states returned from the OpenAI Gym environment. We will get a 128-element numpy array with elements ranging from 0 to 255, but we need to convert it to a PyTorch tensor and normalize the values to be between 0 and 1 to moderate the size of the gradients.

We also need a policy function that decides which actions to take given the predicted action-value distributions. With access to a full probability distribution over action-values, we can utilize more sophisticated risk-sensitize policies. In this chapter, to keep complexity at a minimum, we will use a simple policy of choosing actions based on their expected value. Yes, although we are learning a full probability distribution, we will choose actions based on their expected value just like in ordinary Q-learning.

Listing 7.12 Preprocessing states and action selection

```
def preproc_state(state):
    p_state = torch.from_numpy(state).unsqueeze(dim=0).float()
    p_state = torch.nn.functional.normalize(p_state, dim=1) #A
    return p_state

def get_action(dist,support):
    actions = []
    for b in range(dist.shape[0]): #B
        expectations = [support @ dist[b,a,:] for a in range(dist.shape[1])] #C
        action = int(np.argmax(expectations)) #D
        actions.append(action)
    actions = torch.Tensor(actions).int()
```

```

return actions

#A Normalize state values to be between 0 and 1
#B Loop through batch dimension of distribution
#C Compute the expectation values for each action-value distribution
#D Compute the action associated with the highest expectation value

```

Recall, we can compute the expected (or expectation) value of a discrete distribution by simply taking the inner product of the support tensor with the probability tensor. We do this for all 3 actions and select the one that had the highest expected value. Once you get comfortable with the code here, you can try coming up with a more sophisticated policy, perhaps one that takes into consideration the variance (in other words, confidence) of each action-value distribution.

7.7 Distributional Q-learning to play Freeway

We're finally ready to use the Dist-DQN algorithm to play the Atari game Freeway. We don't need any other major functionality beside what we've already described. We will have a main Dist-DQN model and a copy, the target network to stabilize training. We will use an epsilon-greedy strategy with a decreasing epsilon value over epochs. So with probability epsilon the action selection will be random, otherwise we choose the action using our `get_action` function that chooses based on the highest expected value. We will also use an experience replay mechanism just like with an ordinary DQN.

We also introduce a very basic form of **prioritized replay**. With normal experience replay, we just store all the experiences the agent has in a fixed-size memory buffer, and new experiences displace old ones at random. Then we randomly sample a batch from this memory buffer for training. In a game like Freeway where almost all actions result in a -1 reward and we rarely get a +10 or -10 reward, the experience replay memory is going to be heavily dominated by data that all basically says the same thing, and thus it is not very informative to the agent and the truly significant experiences such as winning or losing the game get strongly diluted, significantly slowing learning.

To alleviate this problem, whenever we take an action that leads to a winning or losing state of the game (i.e. we get a reward of -10 or +10), we add multiple copies of this experience to the replay buffer to prevent it from being diluted by all the -1 reward experiences. Hence, we *prioritize* certain highly informative experiences over other less informative experiences because we really want our agent to learn which agents lead to success or failure rather than just game continuation.

If you access the code for this chapter on this book's GitHub at <https://github.com/DeepReinforcementLearning/DeepReinforcementLearningInAction/> then you will find the code we used to record frames of the live game play during training. We also record the real-time changes in the action-value distributions so you can see how the game play affects the predicted distributions and vice versa. We do not include that code here as it would take too much space.

Listing 7.13 Dist-DQN plays Freeway, preliminaries

```

import gym
from collections import deque
env = gym.make('Freeway-ram-v0')
aspace = 3
env.env.get_action_meanings()

vmin,vmax = -10,10
replay_size = 200
batch_size = 50
nsup = 51
dz = (vmax - vmin) / (nsup-1)
support = torch.linspace(vmin,vmax,nsup)

replay = deque(maxlen=replay_size) #A
lr = 0.0001 #B
gamma = 0.1 #C
epochs = 1300
eps = 0.20 #D starting epsilon for epsilon-greedy policy
eps_min = 0.05 #E ending epsilon
priority_level = 5 #F
update_freq = 25 #G

#Initialize DQN parameter vector
tot_params = 128*100 + 25*100 + aspace*25*51 #H
theta = torch.randn(tot_params)/10. #I
theta.requires_grad=True
theta_2 = theta.detach().clone() #J

losses = []
cum_rewards = [] #K
renders = []
state = preproc_state(env.reset())

```

#A Experience replay buffer using the deque data structure
#B Learning rate
#C Discount factor
#D Starting epsilon for epsilon-greedy policy
#E Ending/minimum epsilon
#F Prioritized-replay; duplicate highly informative experiences in the replay this many times
#G Update the target network every 25 steps
#H The total number of parameters for Dist-DQN
#I Randomly initialize parameters for Dist-DQN
#J Initialize parameters for target network
#K Stores each win (successful freeway crossing) as a 1 in this list

These are all the settings and starting objects we need before we get to the main training loop. All of it is roughly the same as what we did for the simulation test except, we have a prioritized replay setting that controls how many copies of a highly informative experience (e.g. a win) we should add to the replay. We also use an epsilon-greedy strategy and we will start with an initially high epsilon value and then during training decrease it to a minimum value to maintain a minimal amount of exploration.

Listing 7.14 The main training loop

```

from random import shuffle
for i in range(epochs):
    pred = dist_dqn(state,theta,aspace=aspace)
    if i < replay_size or np.random.rand(1) < eps: #A
        action = np.random.randint(aspace)
    else:
        action = get_action(pred.unsqueeze(dim=0).detach(),support).item()
    state2, reward, done, info = env.step(action) #B
    state2 = preproc_state(state2)
    if reward == 1: cum_rewards.append(1)
    reward = 10 if reward == 1 else reward #C
    reward = -10 if done else reward #D
    reward = -1 if reward == 0 else reward #E
    exp = (state,action,reward,state2) #F
    replay.append(exp) #G

    if reward == 10: #H
        for e in range(priority_level):
            replay.append(exp)

    shuffle(replay)
    state = state2

    if len(replay) == replay_size: #I
        idx = np.random.randint(low=0,high=len(replay),size=batch_size)
        exps = [replay[j] for j in idx]
        state_batch = torch.stack([ex[0] for ex in exps],dim=1).squeeze()
        action_batch = torch.Tensor([ex[1] for ex in exps])
        reward_batch = torch.Tensor([ex[2] for ex in exps])
        state2_batch = torch.stack([ex[3] for ex in exps],dim=1).squeeze()
        pred_batch = dist_dqn(state_batch.detach(),theta,aspace=aspace)
        pred2_batch = dist_dqn(state2_batch.detach(),theta_2,aspace=aspace)
        target_dist = get_target_dist(pred2_batch,action_batch,reward_batch, \
                                      support, lim=(vmin,vmax),gamma=gamma)
        loss = lossfn(pred_batch,target_dist.detach())
        losses.append(loss.item())
        loss.backward()
        with torch.no_grad(): #J
            theta -= lr * theta.grad
        theta.requires_grad = True

    if i % update_freq == 0: #K
        theta_2 = theta.detach().clone()

    if i > 100 and eps > eps_min: #L
        dec = 1./np.log2(i)
        dec /= 1e3
        eps -= dec

    if done: #M
        state = preproc_state(env.reset())
        done = False

```

#A Epsilon-greedy action selection

#B Take selected action in the environment

#C Change reward to +10 if environment produced reward of 1 (successful freeway crossing)

```

#D Change reward to -10 if game is over (no crossings after a long time)
#E Change reward to -1 if original reward was 0 (game is just continuing) to penalize doing nothing
#F Prepare experience as a tuple of the starting state, the observed reward, the action taken, and the subsequent state
#G Add experience to replay memory
#H If reward is 10, then that indicates a successful crossing and we want to amplify this experience
#I Once replay buffer is full, begin training
#J Gradient descent
#K Synchronize the target network parameters to the main model parameters
#L Decrement the epsilon as a function of the epoch number
#M Reset the environment if the game is over

```

Almost all of this is the same kind of code we used for the ordinary DQN a few chapters ago. The only changes are the fact that we're dealing with Q-distributions rather than single Q-values and that we use prioritized replay. If you plot the losses you should get something like this:

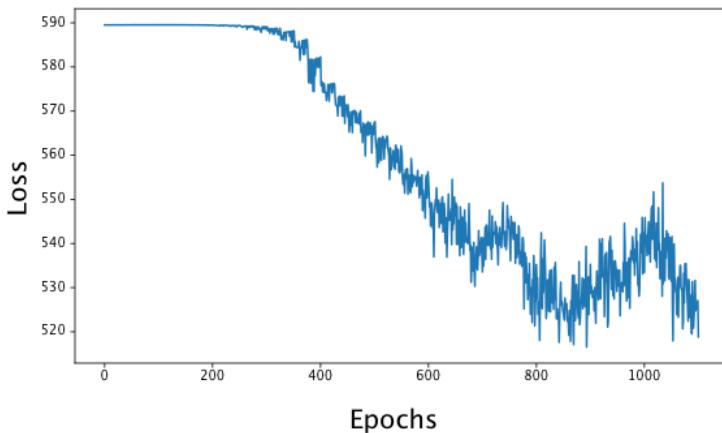


Figure 7.18: The loss plot for training DList-DQN on the Atari game Freeway. The loss gradually declines but has significant “spikiness” due to the periodic target network updates.

It generally goes down but has “spikiness” due to the updates of the target network just like we saw with the simulated example. If you investigate the `cum_rewards` list, you should get a list of ones [1, 1, 1, 1, 1, 1] indicating how many successful chicken crossings occurred. If you’re getting 4 or more, that indicates a successfully trained agent. We can also see a mid-training game screenshot alongside the corresponding predicted action-value distributions (again, refer to the GitHub code to see how to do this).

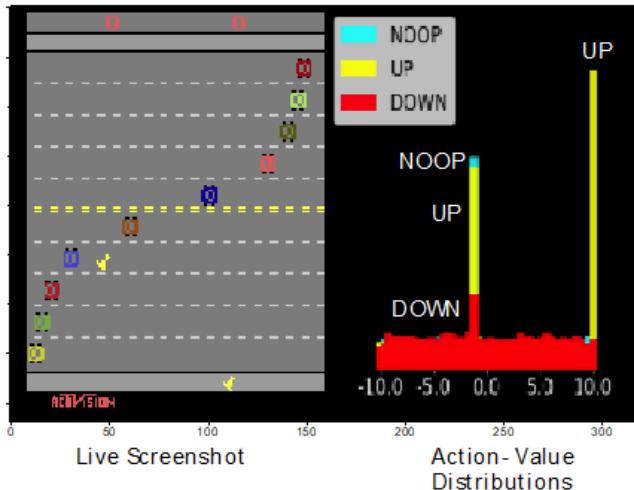


Figure 7.19 : Left: Screenshot of live gameplay in Atari Freeway. **Right:** The corresponding action-value distributions of each of the each actions overlaid. The spike on the right corresponds to action UP and the spike on the left corresponds mostly action NO-OP. Since the right spike is larger, the agent is more likely to take action UP, which seems like the right thing to do in this case. It is difficult to see but the UP action also has a spike that is overlaid on-top of the NO-OP spike on the left, so the UP action-value distribution is bi-modal, suggesting that taking action UP might lead to either a -1 reward or a +10 reward, but the +10 reward is more likely since that spike is taller.

You can see the action-value distribution for the “UP” action has two modes (peaks), one at -1 and the other at $+10.0$. The expectation value of this distribution is much higher than the other actions so this action will be selected. And we can take a peek at a few of the learned distributions in the experience replay buffer to get a better view of the distributions.

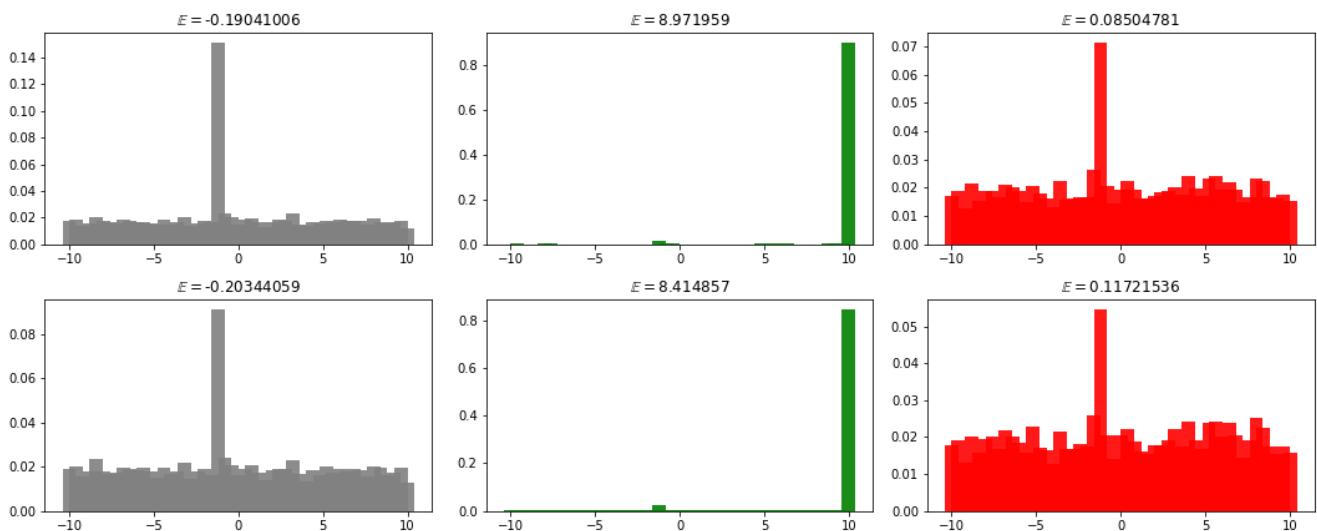


Figure 7.20 : Each column has the action-value distributions for a particular action for a given state (each row). The number above each plot is the expectation-value for that distribution, which is the weighted average value for that distribution. Each distribution looks fairly similar by eye but the expected values are definitely distinct enough to result in significantly different action selections.

Each row of figures is a sample from the replay buffer associated with a single state. Each figure in a row is the action-value distribution for actions “NOOP,” “UP,” “DOWN,” respectively. Above each figure is the expected value of that distribution. You can see that in all samples the “UP” action has the highest expected value and it has two clear peaks, one at -1 and another at +10. The distributions for the other two actions have a lot more variance because once the agent learns that going up is the best way to win, there are fewer and fewer experiences using the other two actions, so they remain relatively uniform. If we continued training for longer, they would eventually converge to a peak at -1 and possibly a smaller peak at -10 since with epsilon greedy we will still be taking a few random actions.

As we mentioned earlier, distributional Q-learning is one of the biggest improvements to Q-learning in the past few years and is still being actively researched. You should compare Dist-DQN to ordinary DQN. You should get better overall performance with Dist-DQN. It is actually not completely well-understood why Dist-DQN performs so much better, especially given that we are only choosing actions based on expected values, but a few reasons are likely. One is that training a neural network to predict multiple things at the same time has been shown to improve generalization and overall performance, and our Dist-DQN is learning to predict 3 full probability distributions rather than a single action-value, so these auxiliary tasks force the algorithm to learn more robust abstractions.

We also discussed a significance limitation of the way we’ve implemented Dist-DQN, namely that we’re using discrete probability distributions with finite support, so we can only

represent action-values within a very small range from -10 to 10. Of course we could make this range wider at the cost of more computational processing, but we can never represent an arbitrarily small or large value with this approach. The way we've implemented it is to use a fixed set of supports but learn the set of associated probabilities. One fix to this problem is to instead use a fixed set of probabilities over a variable (learned) set of supports.



Figure 7.21 : In quantile regression, rather than learning what the probabilities are that are assigned to a fixed set of supports, we learn a set of supports that correspond to a fixed set of probabilities (quantiles). In this figure you can see the median value is 1 since it is at the 50th percentile.

For example, we can fix our probability tensor to range from 0.1 to 0.9, e.g. array([0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9]), and then we instead have our Dist-DQN predict the set of associated supports with these fixed probabilities. That is, we're asking our Dist-DQN to learn what support value has a probability of 0.1, and 0.2, and so on. This is called **quantile regression** because these fixed probabilities end up representing quantiles of the distribution, i.e. we learn the supports at and below the 50th percentile (probability 0.5), the 60th percentile, and so on. With this approach, we still have a discrete probability distribution, but we can now represent any possible action-value, i.e. it can be arbitrarily small or large and we have no fixed range.

7.8 Summary

- The advantages of Distributional Q-learning include improved performance and offer a way to utilize risk-sensitive policies
- Prioritized replay can speed learning by increasing the proportion of highly-informative experiences in the experience replay buffer
- The Bellman equation gives us the precise way to update a Q-function
- The OpenAI Gym includes alternative environments that produce RAM states, rather than raw video frames, which are easier to learn since they are usually of much lower dimensionality.

- Random variables are variables that can take on a set of outcomes weighted by an underlying probability distribution
- The entropy of a probability distribution describes how much information it contains
- The KL-divergence and cross-entropy can be used to measure the loss between two probability distributions
- That the support of a probability distribution is the set of values that have non-zero probability
- Quantile regression is a way to learn a highly flexible discrete distribution by learning the set of supports rather than the set of probabilities

8

Curiosity-Driven Exploration

In this chapter

- Understand the sparse reward problem
- Understand how curiosity can serve as an intrinsic reward
- Play Super Mario Bros. from OpenAI Gym
- Implement an intrinsic curiosity module in PyTorch
- Train a deep Q-network agent to play Super Mario Bros. using just curiosity

Code for this chapter is at this book's GitHub repository under Chapter 8:

<https://github.com/DeepReinforcementLearning/DeepReinforcementLearningInAction/>

The fundamental reinforcement learning algorithms we have studied so far such as Deep Q-learning and policy gradient methods are very powerful techniques in a lot of situations, but fail dramatically in other environments. Google DeepMind pioneered the field of deep reinforcement learning back in 2013 when they used Deep Q-learning to train an agent to play multiple Atari games at superhuman performance levels. But the performance of the agent was highly variable across different types of games. At one extreme their DQN agent played the Atari game Breakout vastly better than a human, but at the other extreme, the DQN was much worse than a human at playing Montezuma's Revenge where it could not even pass the first level.



Figure 8.1: Screenshot from the Montezuma's Revenge Atari game. The player must navigate through obstacles to get a key before any rewards are received.

WANT TO LEARN MORE ?

The paper that brought great attention to the field of deep reinforcement learning was “Human-level control through deep reinforcement learning” by Mnih and collaborators at Google DeepMind in 2015. The paper is fairly readable and contains the details you need to replicate their results.

What’s the difference between the environments that explains these disparities in performance? The games that DQN was successful at all gave relatively frequent rewards during game play and did not require significant long-term planning. Montezuma’s Revenge on the other hand only gives a reward after finding a key in the room, which also contains numerous obstacles and enemies. With a vanilla DQN the agent starts exploring essentially at random. It will take random actions and wait to observe rewards, and then the rewards reinforce which actions are best to take given the environment. But in the case of Montezuma’s Revenge, it is extremely unlikely that the agent will find the key and get a reward with this random exploration policy, so it will never observe a reward and will never learn.

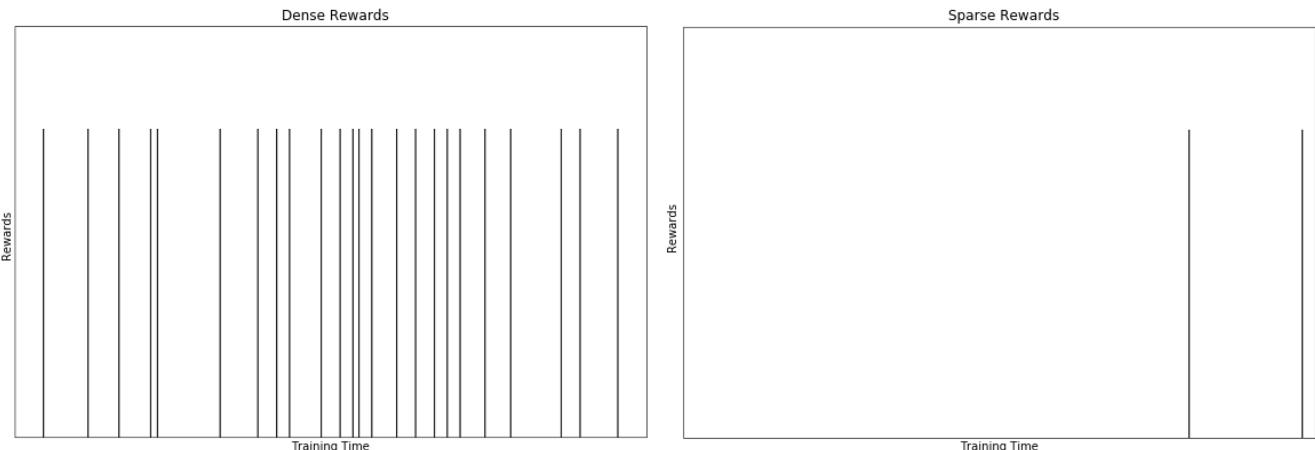


Figure 8.2: In environments with dense rewards, rewards are received fairly frequently during training time making it easy to reinforce actions. In sparse reward environments, rewards may only be received after many sub-goals are completed, making it difficult or impossible for an agent to learn based on reward signals alone.

This problem is called the sparse reward problem since the rewards in the environment are sparsely distributed. If the agent doesn't observe enough reward signals to reinforce its actions, it can't learn. Animal and human learning offer us the only natural examples of intelligent systems and we can turn to them for inspiration. Indeed, researchers trying to tackle this sparse reward problem noticed that humans not only maximize extrinsic (i.e. from the environment) rewards like food and sex, but also demonstrate an intrinsic curiosity, a motivation to explore just for the sake of understanding how things work.

In this chapter we will learn about methods for successfully training reinforcement learning agents in sparse reward environments by using principles from human intelligence, specifically our innate curiosity. We will see how curiosity can drive the development of basic skills that the agent can use to accomplish sub-goals and find the sparse rewards.

8.1 Tackling Sparse Rewards with Predictive Coding

In the world of neuroscience and particularly computational neuroscience, there is a framework for understanding neural systems at a high level called the predictive coding model. In this predictive coding model, the theory says essentially that all neural systems from individual neurons up to large scale neural networks are running an algorithm that attempts to predict inputs, and hence tries to minimize the prediction error. So at a high level, as you're going about your day your brain is taking in a bunch of sensory information from the environment and it's training to predict how the sensory information will evolve, it's trying to stay one step ahead of the actual raw data coming in.

If something surprising (i.e. unexpected) happens, your brain experiences a large prediction error and then presumably does some parameter updating to prevent that from happening again. For example, you might be talking to someone you just met and your brain is constantly trying to predict the next word that person will say before they say it. Since this is someone you don't know, your brain will probably have a relatively high average prediction error but if you become best friends, you'll probably be quite good at finishing their sentences. Similarly, curiosity can be thought of as a kind of desire to reduce the uncertainty in your environment (and hence reduce prediction errors). If you were a software engineer and saw some online posts about this interesting field called machine learning, your curiosity to read a book like this would be to reduce your uncertainty about machine learning.

Using a prediction error mechanism was one of the first attempts to imbue reinforcement learning agents with a sense of curiosity. The idea was that in addition to trying to maximize extrinsic (i.e. environment-provided) rewards, the agent would also just try to predict the next state of the environment given its action and would try to reduce its prediction error. In very familiar areas of an environment, the agent would learn how it works and would have a low prediction error. By using this prediction error as another kind of reward signal, the agent would be incentivized to visit areas of the environment that were novel and unknown. That is, the higher the prediction error is, the more surprising a state is and therefore the agent should be incentivized to visit these high prediction error states. Figure 8.1 shows the basic framework for this approach.

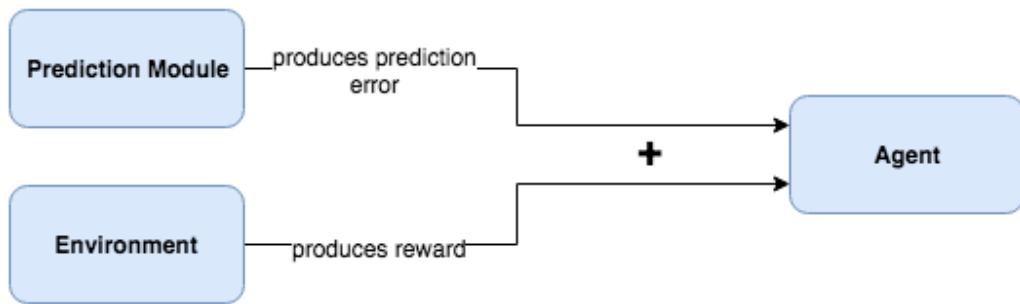


Figure 8.3: Prediction error is summed with the extrinsic environment reward for use by the agent.

The idea is to just sum the prediction error (which we will call the intrinsic reward) with the extrinsic reward and use that as the new reward signal for the environment. Now the agent is incentivized to not only figure out how to maximize the environment reward but also to be curious about the environment. The prediction error is calculated according to Figure 8.2.

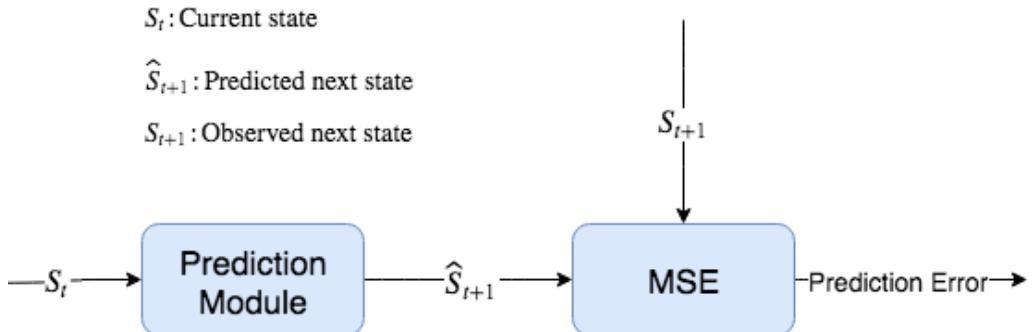


Figure 8.4: The prediction module takes in a state S_t and action a_t and produces a prediction for the subsequent state S_{t+1} . This prediction along with the true next state are passed to a mean-squared error (or some other error) function which produces the prediction error.

So this intrinsic reward is based on the prediction error of states in the environment. It turns out this works fairly well at first pass, however, people eventually realized it runs into another problem often called the “noisy TV problem.” It turns out, if you train these agents in an environment that has a constant source of randomness, such as a TV screen playing random noise, the agent will have a constantly high prediction error and will be unable to reduce it, so it just stares at the noisy TV indefinitely. This is more than just an academic problem since many real-world environments have these kinds of sources of randomness (e.g. a tree’s leaves blowing in the wind).

At this point, it seems like prediction error has a lot of potential, but the noisy TV problem is a big flaw. Perhaps we shouldn’t pay attention to the absolute prediction error but instead to the rate of change of prediction error. When the agent transitions to an unpredictable state, it will experience a transient surge of prediction error, but then it goes away. Similarly, if the agent encounters a noisy TV, at first it is highly unpredictable and therefore high prediction error, but the high prediction error is maintained and thus the rate of change is zero. This formulation is better, but still has some potential issues. Imagine an agent is outside and sees a tree with its leaves blowing in the wind. The leaves are blowing around randomly and hence this is a high prediction error. The wind stops blowing, and now the prediction error goes down since the leaves are not moving anymore. Then the wind starts blowing again and prediction error goes up. In this case, even if we’re using prediction error rate, the rate will be fluctuating along with the wind. We need something more robust.



Figure 8.5: The noisy TV problem is a theoretical and practical problem where a reinforcement learning agent with a naïve sense of curiosity will become entranced by a noisy TV, forever staring at it. This is because it is intrinsically rewarded by unpredictability and white noise is very unpredictable.

We want to use this prediction error idea but don't want it to be vulnerable to randomness or unpredictability in the environment that doesn't matter. How do we add in the "doesn't matter" constraint to the prediction error module? Well when we say something doesn't matter, we mean that it does not affect us or is perhaps uncontrollable. If leaves are randomly blowing in the wind, the agent's actions don't affect the leaves and the leaves don't affect the actions of the agent. It turns out we can implement this idea as a separate module in addition to the state prediction module, and that is the subject of this chapter. This chapter is based on elucidating and implementing the idea from the paper "Curiosity-driven Exploration by Self-supervised Prediction" Pathak et al 2017 which successfully resolves the issues we've been discussing so far.

We will follow this paper pretty closely because it was one of the biggest contributions to solving the sparse reward problem that led to a flurry of related research. It also turns out to be one of the easiest algorithms to implement among the many others in this area. In addition, one of the goals of this book is to not only teach you the foundational knowledge and skills of reinforcement learning, but to give you a solid enough mathematics background to be able to read and understand reinforcement learning papers and implement them on your own. Of course, some papers require advanced mathematics that are outside the scope of this book, many of the biggest papers in the field require only some basic calculus, algebra, and linear algebra understanding, things that you probably know if you have made it this far. So the only barrier is really getting past the mathematical notation, something we hope to make easier here. We want to teach you how to fish rather than just giving you fish, as the saying goes.

8.2 Inverse Dynamics Prediction

Let's start to peer into the inside of the prediction module. The prediction error module from last section is implemented as a function $f: (S_t, a_t) \rightarrow \hat{S}_{t+1}$ that takes a state and the action

taken and returns the predicted next state. It is predicting the dynamics of the environment, and so we call it the **forward prediction model**, since it predicts the future (forward) state.

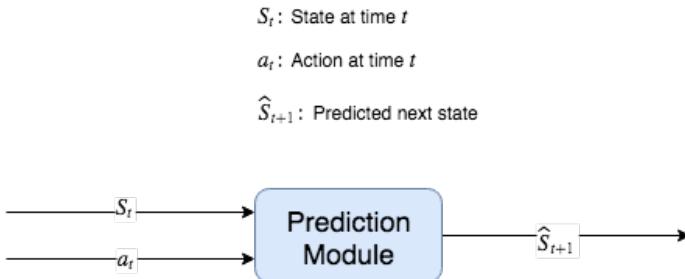


Figure 8.6: Diagram of the forward prediction module function $f:(S_t, a_t) \rightarrow \hat{S}_{t+1}$, that maps a current state and action to a predicted next state.

Remember we want to only predict aspects of the state that actually matter, not parts that are trivial or noise. The way we build in the “doesn’t matter” constraint to the prediction model is to add another model called an **inverse model** $g:(S_t, S_{t+1}) \rightarrow \hat{a}_t$. That is, it is a function g that takes a state and the next state and then returns a prediction for which action was taken that led to that transition S_t to S_{t+1} .

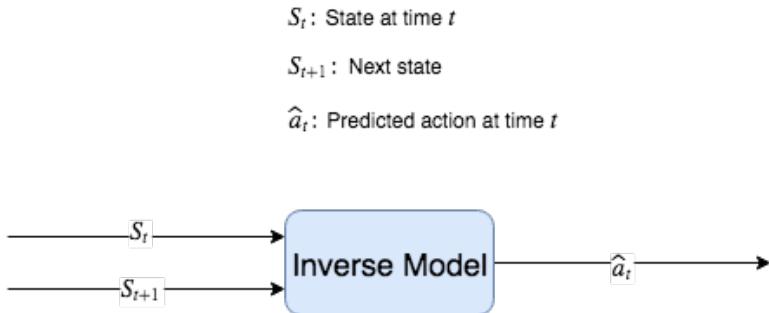


Figure 8.7: The inverse model takes two consecutive states and tries to predict which action was taken.

On its own, this inverse model is not really useful, there’s an additional model that is tightly coupled to the inverse model called the encoder model, denoted ϕ . The encoder is a function, $\phi:S_t \rightarrow \hat{S}_t$, i.e. it takes a state and returns an encoded state \hat{S}_t such that the dimensionality of \hat{S}_t is significantly lower than the raw state S_t . The raw state might be an RGB video frame with height, width and channel dimensions and ϕ will encode that state into a low dimensional vector. For example, a frame might be 100 pixels by 100 pixels by 3 color channels for a total

of 30,000 elements. Many of those pixels will be redundant and not useful, so we want our encoder to encode this state into say a 200-element vector with high level features.

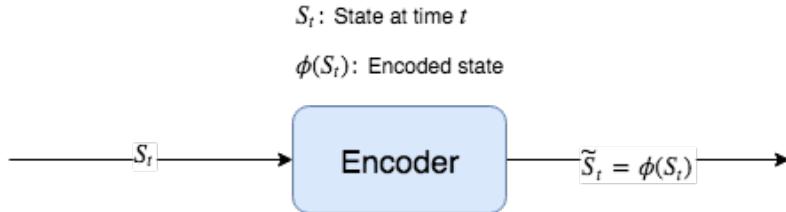


Figure 8.8: The encoder model takes a high-dimensional state representation such as an RGB array and encodes it as a low-dimensional vector.

NOTATION

A variable with the tilde symbol over it such as \tilde{S}_t denotes some sort of transformed version of the underlying variable which may have different dimensionality. A variable with the hat symbol over it such as \hat{S}_t denotes an approximation (or prediction) of the underlying state and is the same dimensionality.

The encoder model is trained via the inverse model because we actually use the encoded states as inputs to the forward and inverse models f and g rather than the raw states. That is, the forward model becomes a function $f: \phi(S_t) \times a_t \rightarrow \hat{\phi}(S_{t+1})$ where $\hat{\phi}(S_{t+1})$ refers to a prediction of the encoded state, and the inverse model becomes a function $g: \phi(S_t) \times \phi(S_{t+1}) \rightarrow (a_t)$.

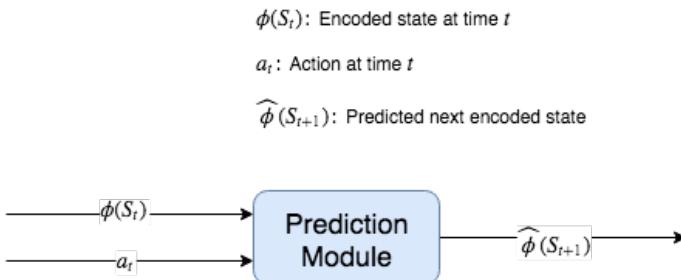


Figure 8.9: The forward prediction module actually uses encoded states, not the raw states. Encoded states are denoted $\phi(S_t)$ or \tilde{S}_t

The encoder model isn't trained directly, it is *not* an autoencoder, it is only trained through the inverse model. The inverse model is trying to predict the action that was taken to transition from one state to the next using the encoded states as inputs, and in order to minimize its own prediction error, its error will backpropagate through to the encoder model as well as itself. The encoder model will then learn to encode states in a way that is useful for the task of

the inverse model. Importantly, although the forward model also uses the encoded states as inputs, we do **not** backpropagate from the forward model to the encoder model. If we did, then the forward model will coerce the encoder model into mapping all states into a single fixed output since that will be the easiest to predict. Figure 8.3 shows the overall graph structure of these components.

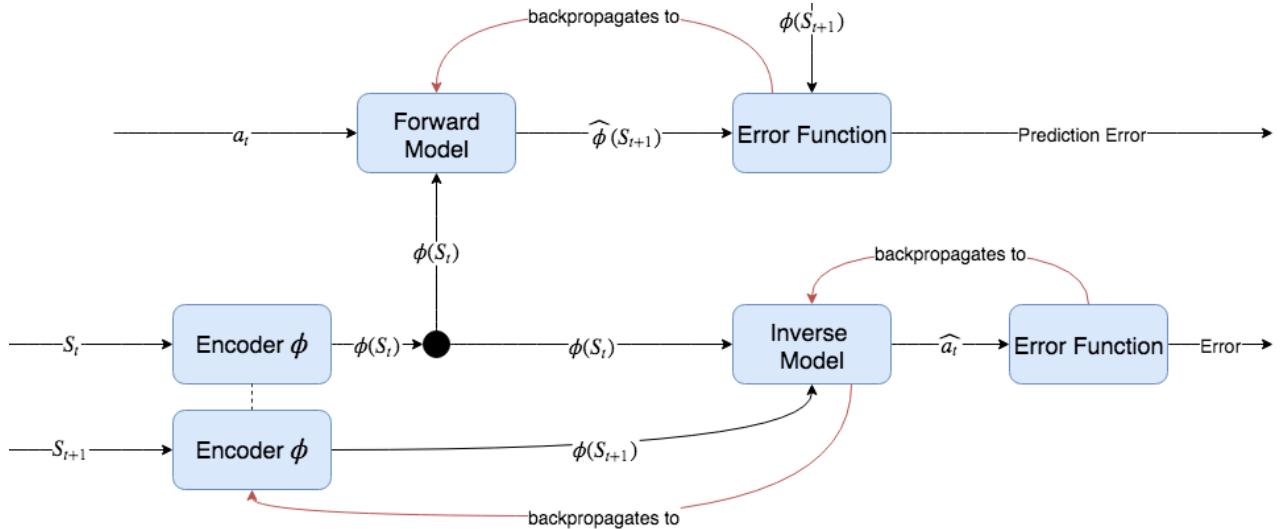


Figure 8.10: The curiosity module. First the encoder will encode states S_t and S_{t+1} into low dimensional vectors, $\phi(S_t)$ and $\phi(S_{t+1})$, respectively. These encoded states are passed to the forward and inverse models. Notice that the inverse model backpropagates to the encoded model thereby training it through its own error. The forward model is trained by backpropagating from its own error function but it does **not** backpropagate through to the encoded like the inverse model does. This ensures that the encoder learns to produce state representations that are only useful for predicting which action was taken. The black circle just indicates a copy operation that copies the output from the encoder and passes the copies to the forward and inverse models.

Figure 8.3 shows the forward pass of all these components and also the backward (backpropagation) pass to update the model parameters. It is worth repeating that the inverse model backpropagates back through to the encoder model and the encoder model is only trained together with the inverse model. We must use PyTorch’s `detach()` method to detach the forward model from the encoder so that it won’t backpropagate into the encoder. The purpose of the encoder is not to give us a low-dimensional input for improved performance, the purpose is to learn to encode the state using a representation that only contains information relevant for predicting actions. This means that aspects of the state that are randomly fluctuating and have no impact on the agent’s actions will be stripped from this encoded representation. This, in theory, should avoid the noisy TV problem.

Notice that for both the forward and inverse models we need access to the data for a full transition, i.e. we need (S_t, a_t, S_{t+1}) , but this is not an issue when we use an experience replay

memory as we did in the Deep Q-learning chapter since the memory will store a bunch of these kinds of tuples.

8.3 Setting up Super Mario Bros.

Together, the forward, inverse and encoder models form the Internal Curiosity Module (ICM), which we will cover in detail later in this chapter. The components of the ICM function together for the sole purpose of generating an intrinsic reward that drives curiosity in the agent. The ICM only generates a new intrinsic reward signal based on information from the environment, therefore it is independent of how the agent model is implemented. We could use whatever agent model implementation we want, such as A3C (the actor-critic policy gradient method we covered in chapter 5) model, however, we will use a Q-learning model here to keep things simple and focus on implementing the ICM. The ICM can be used for any type of environment, but it will be most useful in sparse reward environments. We will use Super Mario Bros as our testbed.

Super Mario Bros. does not really suffer from the sparse reward problem. The particular environment implementation we will use provides a reward in part based on forward progress through the game, so positive rewards are almost continuously provided. However, Super Mario Bros. is still a great choice to test the ICM because we can choose to “turn off” the extrinsic (environment provided) reward signal and see how well the agent explores the environment just based off curiosity. The implementation of Super Mario Bros. has 12 discrete actions that can be taken at each time step including a NO-OP (no-operation, i.e. do nothing) action. The complete action list is below:

Table 8.1: Actions in Super Mario Bros.

Index	Action
0	Do nothing
1	Right
2	Right + A
3	Right + B
4	Right + A + B
5	A
6	Left
7	Left + A
8	Left + B
9	Left + A + B
10	Down

11

Up

```
A = Jump, B = run
```

You can install Super Mario Bros. with pip:

```
>>> pip install gym-super-mario-bros
```

After it is installed, you can test the environment (e.g. try running this code in a Jupyter Notebook) by playing a random agent (taking random actions). All of the code for this chapter is at this book's GitHub repository under Chapter 8:

<https://github.com/DeepReinforcementLearning/DeepReinforcementLearningInAction/>

To review how to use the OpenAI Gym, please refer back to chapter 4.

Listing 8.1: Setting up the Super Mario Bros. Environment

```
import gym
from nes_py.wrappers import BinarySpaceToDiscreteSpaceEnv #A
import gym_super_mario_bros
from gym_super_mario_bros.actions import SIMPLE_MOVEMENT, COMPLEX_MOVEMENT #B
env = gym_super_mario_bros.make('SuperMarioBros-v0')
env = BinarySpaceToDiscreteSpaceEnv(env, COMPLEX_MOVEMENT) #C

done = True
for step in range(2500): #D
    if done:
        state = env.reset()
        state, reward, done, info = env.step(env.action_space.sample())
        env.render()
env.close()
```

#A This a wrapper module that will makes the action-space smaller by combining actions together.

#B There are two sets of action-spaces we can import, one with 5 actions (simple) and one with 12 (complex).

#C Wrap the environment's action space to be 12 discrete actions.

#D Test the environment by taking random actions

If everything went well, a little window should pop-up with Super Marios Bros. but it will be doing random actions and not making any forward progress through the level. By the end of this chapter you will have trained an agent that makes consistent forward progress, has learned to avoid or jump on enemies and jump over obstacles, and only using the intrinsic curiosity-based reward.

Recall that the environment is instantiated as a class object called `env` and that the main method you need to use is its `step(...)` method. The `step` method takes an integer representing the action to be taken. As with all OpenAI Gym environments, this one returns state, reward, done, and info data after each action is taken. The state is a numpy array with dimensions (240, 256, 3) representing an RGB video frame. The reward is bounded between -15 and 15 and is based on the amount of forward progress. The `done` variable is a

Boolean that indicates whether or not the game is over (e.g. Mario dies). The info variable is a Python dictionary with the following metadata:

Table 8.2: Description of the meta-data returned after each action in the *info* variable

Key	Type	Description
coins	int	The number of collected coins
flag_get	bool	True if Mario reached a flag or ax
life	int	The number of lives left, i.e., {3, 2, 1}
score	int	The cumulative in-game score
stage	int	The current stage, i.e., {1, ..., 4}
status	str	Mario's status, i.e., {'small', 'tall', 'fireball'}
time	int	The time left on the clock
world	int	The current world, i.e., {1, ..., 8}
x_pos	int	Mario's x position in the stage

Source: <https://github.com/Kautenja/gym-super-mario-bros>

We will only need to use the `x_pos` key/value. In addition to getting the state after calling the `step` method, you can also retrieve the state at any point by calling `env.render("rgb_array")`. That's basically all you need to know about the environment in order to train an agent to play it.

8.4 Preprocessing and the Q-network

The raw state is an RGB video frame with dimensions (240, 256, 3), which is unnecessarily high-dimensional and would be computationally costly at no advantage. We will convert these RGB states into grayscale and resize to be 42 x 42.

Listing 8.2: Downsample State and Convert to Grayscale

```
import matplotlib.pyplot as plt
from skimage.transform import resize #A
import numpy as np

def downscale_obs(obs, new_size=(42,42), to_gray=True):
    if to_gray:
        return resize(obs, new_size, anti_aliasing=True).max(axis=2) #B
    else:
        return resize(obs, new_size, anti_aliasing=True)
```

#A The scikit-image library has an image resizing function built-in

#B To convert to grayscale we simply take the maximum values across the channel dimension for good contrast

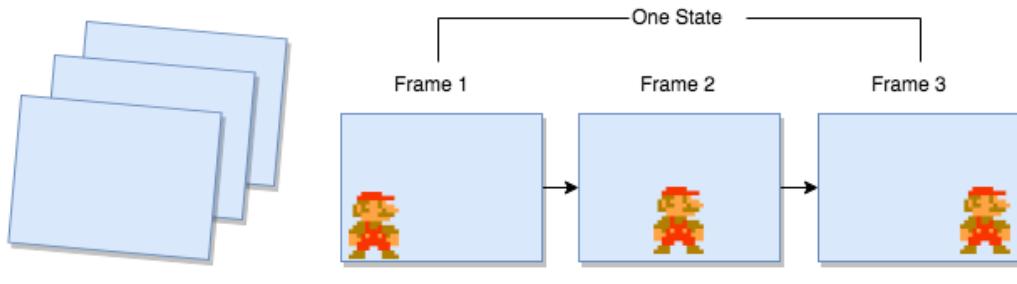
This function accepts the state array (`obs`), a tuple indicating the new size in height and width and a Boolean for whether to convert to grayscale or not. We set it True by default since that is what we want. We use the scikit-image library's `resize` function, so you may need to install it if you don't have it already by following the instructions at <https://scikit-image.org/download>. It's a very useful library for working with image data in the form of multi-dimensional arrays.

You can use matplotlib to visualize a frame of the state.

```
>>> plt.imshow(env.render("rgb_array"))
>>> plt.imshow(downsamp_obs(env.render("rgb_array")))
```

The down-sampled image will look pretty blurry, but it still contains enough visual information to play the game.

We have a few other data processing functions to build to transform these raw states into a useful form. We will not just pass a single 42x42 frame to our models, we will instead pass the last 3 frames of the game (in essence adding a channel dimension) so the states will be 3x42x42. Using the last 3 frames gives our models access to velocity information (i.e. how fast and which direction things are moving) rather than just positional information.



State Representation: 3 Grayscale Frames

Figure 8.11: Each state given to the agent is a concatenation of the 3 most recent (grayscale) frames in the game. This is necessary so that the model can have access to not just the position of objects but also their direction of movement.

When the game first starts, we only have access to the first frame, so we prepare the initial state by just concatenating the same state 3 times to get that 3x42x42 initial state. After this initial copied state, we can just replace the last frame in the state with the most recent frame from the environment, replace the second frame with the old last one, and replace the first frame with the old second. Basically we have a fixed length first-in-first-out data structure where we append to the right and the left automatically pops off. Python has a built in data structure called the `deque` from the `collections` library that can implement this behavior when the `maxlen` attribute is set to 3.

These are the three functions we will use to prepare the raw states into a form that our agent and encoder models will use. The `prepare_state` function just resizes the image, converts to grayscale, converts from numpy to PyTorch Tensor and adds a batch dimension using the `.unsqueeze(dim=)` method. The `prepare_multi_state` takes a tensor of dimensions `Batch x Channel x Height x Width` and updates the channel dimension with new frames. This function will only be used during testing of the trained model, during training we will use a `deque` data structure to continuously append and pop frames.

Listing 8.4: Preparing the states

```
import torch
from torch import nn
from torch import optim
import torch.nn.functional as F

def prepare_state(state): #A
    return torch.from_numpy(downscaled_obs(state,
        to_gray=True)).float().unsqueeze(dim=0)

def prepare_multi_state(state1, state2): #B
    state1 = state1.clone()
    tmp = torch.from_numpy(downscaled_obs(state2, to_gray=True)).float()
    state1[0][0] = state1[0][1]
    state1[0][1] = state1[0][2]
    state1[0][2] = tmp
    return state1

def prepare_initial_state(state,N=3): #C
    state_ = torch.from_numpy(downscaled_obs(state, to_gray=True)).float()
    tmp = state_.repeat((N,1,1))
    return tmp.unsqueeze(dim=0)
```

#A Downscale state and convert to grayscale, then convert to a PyTorch Tensor, then finally add a batch dimension

#B Given an existing 3-frame state1 and a new single frame 2, add the latest frame to the queue

#C Create a state with 3 copies of the same frame and add a batch dimension

8.5 Setting up the Q-network and Policy Function

As we mentioned, we will use a Deep Q-network (DQN) for the agent. Recall that a DQN takes a state and produces action-values, i.e. predictions for the expected rewards for taking each possible action. We use these action-values to determine a policy for action selection. For this particular game there are 12 discrete actions, therefore the output layer of our DQN will produce a vector of length 12, where the first element is the predicted value of taking action 0, and so on.

Remember that action-values are (in general) unbounded in either direction, they can be positive or negative if the rewards can be positive or negative (which they can be in this game) so we do not apply any activation function on the last layer. The input to the DQN is a

tensor of shape `Batch x 3 x 42 x 42`, where, remember the channel dimension (3) is for the most recent 3 frames of game play.

For the DQN, we use an architecture consisting of 4 convolutional layers and 2 linear layers. The exponential linear unit (ELU) activation function is used after each convolutional layer and the first linear layer (but no activation function after the last linear layer). The architecture is diagrammed in Figure 8.4. As an exercise you can add an LSTM or GRU layer that can allow the agent to learn from long-term temporal patterns.

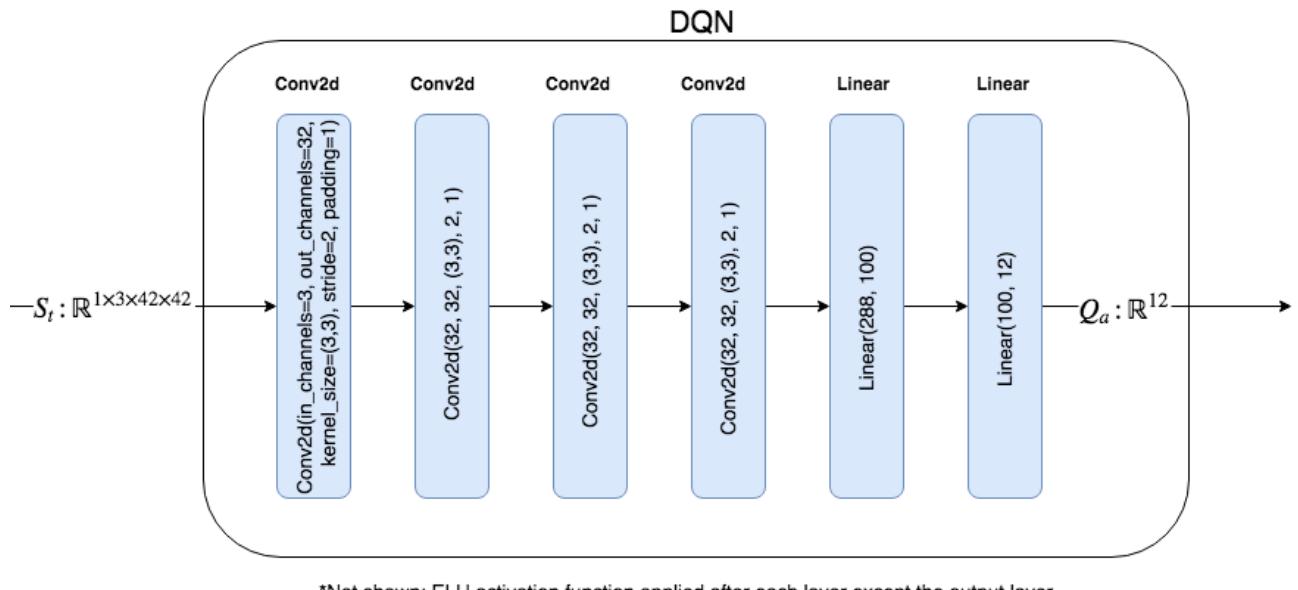


Figure 8.12: This is the diagram of the DQN architecture we will use. The state tensor is the input and is passed through 4 convolutional layers then two linear layers. The ELU activation function is applied after the first 5 layers but not the output layer because the output needs to be able to produce arbitrarily scaled Q-values.

So our DQN will learn to predict the expected rewards for each possible action given the state (i.e. action-values or Q-values), and we use these action-values to decide which action to take. Naïvely we should just take the action associated with the highest value, however, our DQN will not produce accurate action-values in the beginning, so we need to have a policy that allows for some exploration so the DQN can learn better action-value estimates.

Earlier we discussed using the epsilon-greedy policy where we take a random action with probability ϵ and take the action with the highest value with probability $1-\epsilon$. We usually set ϵ to be some reasonably small probability like 0.1, and often we'll slowly decrease ϵ during training so that it becomes more and more likely to just choose the highest value action.

We also discussed sampling from a softmax function as our policy. The softmax function essentially takes a vector input with arbitrary real numbers and then outputs a same-sized

vector where each element is a probability and all elements sum to 1. If the input vector is action-values, then the softmax will return a discrete probability distribution over the actions based on their action-values, such that the action with the highest action-value will be assigned the highest probability. If we sample from this distribution then the actions with the highest values will be chosen more often, however, other actions will also be chosen. The problem with this approach is that if the best action (according to action-value) is only slightly better than other options, then the worse actions will still be chosen with fairly high frequency. For example, below we take an action-value tensor for 5 actions and apply the softmax function from PyTorch's functional module.

```
>>> torch.nn.functional.softmax(th.Tensor([3.6, 4, 3, 2.9, 3.5]))
tensor([0.2251, 0.3358, 0.1235, 0.1118, 0.2037])
```

As you can see the best action (index 1) is only slightly better than the others, so all the actions have pretty high probability and this policy is not that much different from a uniformly random policy. We will use a policy that begins with a softmax policy to encourage exploration and after a fixed number of game steps we will switch to an epsilon-greedy strategy which will continue to give us some exploration capacity but mostly just takes the best action.

Listing 8.5: The policy function

```
def policy(qvalues, eps=None): #A
    if eps is not None:
        if torch.rand(1) < eps:
            return torch.randint(low=0,high=7,size=(1,))
        else:
            return torch.argmax(qvalues)
    else:
        return torch.multinomial(F.softmax(F.normalize(qvalues)), num_samples=1) #B
```

#A The policy function takes a vector of action-values and an epsilon (eps) parameter.

#B If eps is not provided, use a softmax policy. We sample from the softmax using the multinomial function.

The other big component we need for the DQN is an experience replay memory. Gradient-based optimization does not work well if you only pass one sample of data at a time because the gradients are too noisy. In order to average over the noisy gradients, we take sufficiently large samples (called batches or mini-batches) and average or sum the gradients over all the samples. Since we only see one sample of data at a time when playing a game, we instead store the experiences in a "memory" store and then sample minibatches from the memory for training. We will build an experience replay class that contains a list to store tuples of experiences, where each tuple is of the form (S_t, a_t, r_t, S_{t+1}) . The class will also have methods to add a memory and sample a minibatch.

Listing 8.6: Experience Replay

```
from random import shuffle
import torch
```

```

from torch import nn
from torch import optim
import torch.nn.functional as F

class ExperienceReplay:
    def __init__(self, N=500, batch_size=100):
        self.N = N #A
        self.batch_size = batch_size #B
        self.memory = []
        self.counter = 0

    def add_memory(self, state1, action, reward, state2):
        self.counter += 1
        if self.counter % 500 == 0: #C
            self.shuffle_memory()

        if len(self.memory) < self.N: #D
            self.memory.append( (state1, action, reward, state2) )
        else:
            rand_index = np.random.randint(0,self.N-1)
            self.memory[rand_index] = (state1, action, reward, state2)

    def shuffle_memory(self): #E
        shuffle(self.memory)

    def get_batch(self): #F
        if len(self.memory) < self.batch_size:
            batch_size = len(self.memory)
        else:
            batch_size = self.batch_size
        if len(self.memory) < 1:
            print("Error: No data in memory.")
            return None
        #G
        ind = np.random.choice(np.arange(len(self.memory)),batch_size,replace=False)
        batch = [self.memory[i] for i in ind] #batch is a list of tuples
        state1_batch = torch.stack([x[0].squeeze(dim=0) for x in batch],dim=0)
        action_batch = torch.Tensor([x[1] for x in batch]).long()
        reward_batch = torch.Tensor([x[2] for x in batch])
        state2_batch = torch.stack([x[3].squeeze(dim=0) for x in batch],dim=0)
        return state1_batch, action_batch, reward_batch, state2_batch

```

#A N is the maximum size of the memory list
#B batch_size is the number of samples to generate from the memory with the get_batch(...) method
#C Every 500 iterations of adding a memory, shuffle the memory list to promote a more random sample
#D If the memory is not full, add to the list, otherwise replace a random memory with the new one
#E Use Python's built-in shuffle function to shuffle the memory list
#F Randomly samples a minibatch from the memory list
#G Create an array of random integers representing indices

The experience replay class essentially wraps a list with extra functionality. We want to be able to add tuples to the list but only up to a maximum number and we want to be able to sample from the list. When we sample with the `get_batch(...)` method we create an array of

random integers representing indices in the memory list. We index into the memory list with these indices, retrieving a random sample of memories. Since each sample is a tuple (S_t, a_t, r_t, S_{t+1}) , we want to separate out the different components and stack them together into a S_t tensor, a_t tensor and so on where the first dimension of the array is the batch size. For example, the S_t tensor we want to return should be of dimension `batch_size × 3 (channels) × 42 (height) × 42 (width)`. PyTorch's `stack(...)` function will concatenate a list of individual tensors into a single tensor. We also make use of the `squeeze(...)` and `unsqueeze(...)` methods to remove and add dimensions of size 1.

With all of that setup, we have just about everything we need to train a vanilla DQN besides the training loop itself. So in the next section we will implement the intrinsic curiosity module (ICM).

8.6 Intrinsic Curiosity Module

As we described earlier, the ICM is composed of 3 independent neural network models: the forward model, inverse model, and encoder. The forward model is trained to predict the next (encoded) state given the current (encoded) state and an action. The inverse model is trained to predict the action that was taken given two successive (encoded) states $\phi(S_t)$ and $\phi(S_{t+1})$. The encoder simply transforms a raw 3 channel state into a single low-dimensional vector. The inverse model acts indirectly to train the encoder to encode states in a way that only preserves information relevant to predicting the action.

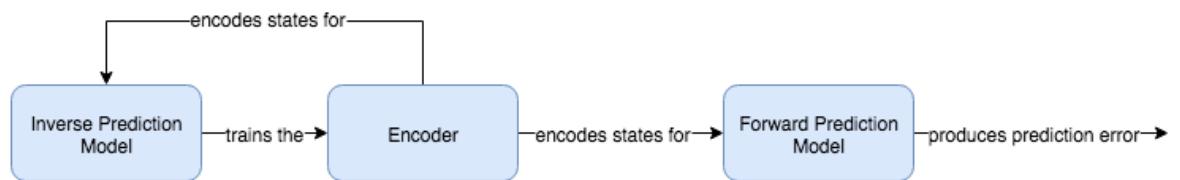


Figure 8.13: High-level overview of the intrinsic curiosity module (ICM). The ICM has 3 components that are each separate neural networks. The encoder model encodes states into a low-dimensional vector and it is trained indirectly through the inverse model that tries to predict the action that was taken given two consecutive states. The forward model predicts the next encoded state and its error is the prediction error that is used as the intrinsic reward.

The forward model is a simple two layer neural network with linear layers. The input to the forward model is constructed by concatenating the state $\phi(S_t)$ with the action a_t . The encoded state $\phi(S_t)$ is a tensor $B \times 288$ and the action $a_t : B \times 1$ is a batch of integers indicating the action index, so we make a one-hot encoded vector by just creating a vector of size 12 and setting the respective a_t index to 1. Then we concatenate these two tensors to create a $Batch \times 288 + 12 = Batch \times 300$ dimensional tensor. We use the rectified linear unit (ReLU) activation unit after the first layer but we do not use an activation function after the output layer. The output layer produces a $B \times 288$ tensor.

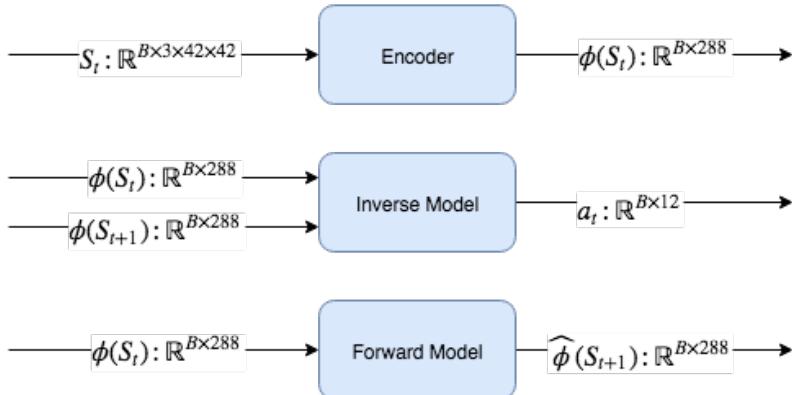


Figure 8.14: This figure shows the type and dimensionality of the inputs and outputs of each component of the ICM.

The inverse model is also a simple two layer neural network with linear layers. The input is two encoded states S_t and S_{t+1} concatenated together to form a tensor of dimension Batch x 288 + 288 = Batch x 576. We use a ReLU activation function after the first layer. The output layer produces a tensor of dimension Batch x 12 with a softmax function applied resulting in a discrete probability distribution over actions. When we train the inverse model, we compute the error between this discrete distribution over actions and a one-hot encoded vector of the true action taken.

The encoder is a neural network composed of 4 convolutional layers (with an identical architecture to the DQN) with the ELU activation function after each layer. The final output is then flattened to get a flat 288 dimensional vector output.

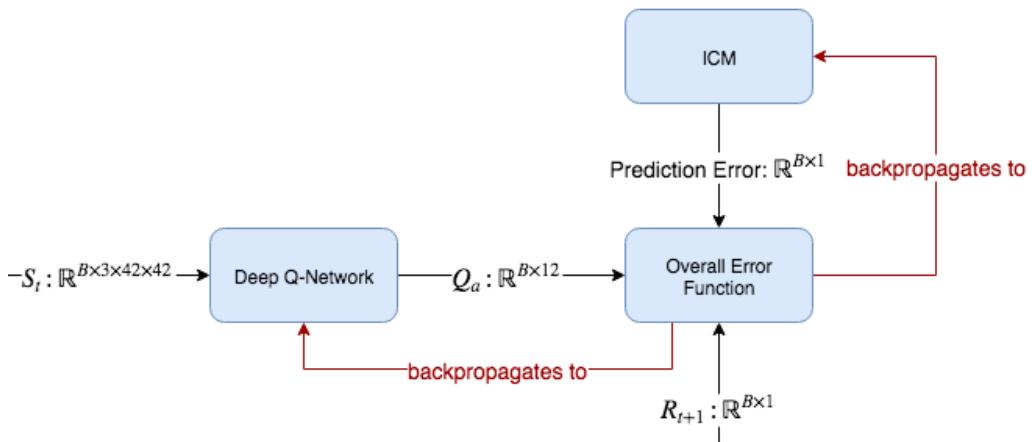


Figure 8.15: The DQN and the ICM contribute to a single overall loss function that is given to the optimizer to

minimize with respect to the DQN and ICM parameters. The DQN's q-value predictions are compared to the observed rewards. The observed rewards, however, are summed together with the ICM's prediction error to get a new reward value.

The whole point of the ICM is to produce a single quantity, the forward model prediction error. We literally take the error produced from the loss function and use that as the intrinsic reward signal for our DQN. We can add this intrinsic reward to the extrinsic reward to get the final reward signal $r_t = r_i + r_e$... We can scale the intrinsic or extrinsic rewards to control the proportions of the total reward.

Below is a figure of the ICM with more detail and including the agent model (DQN).

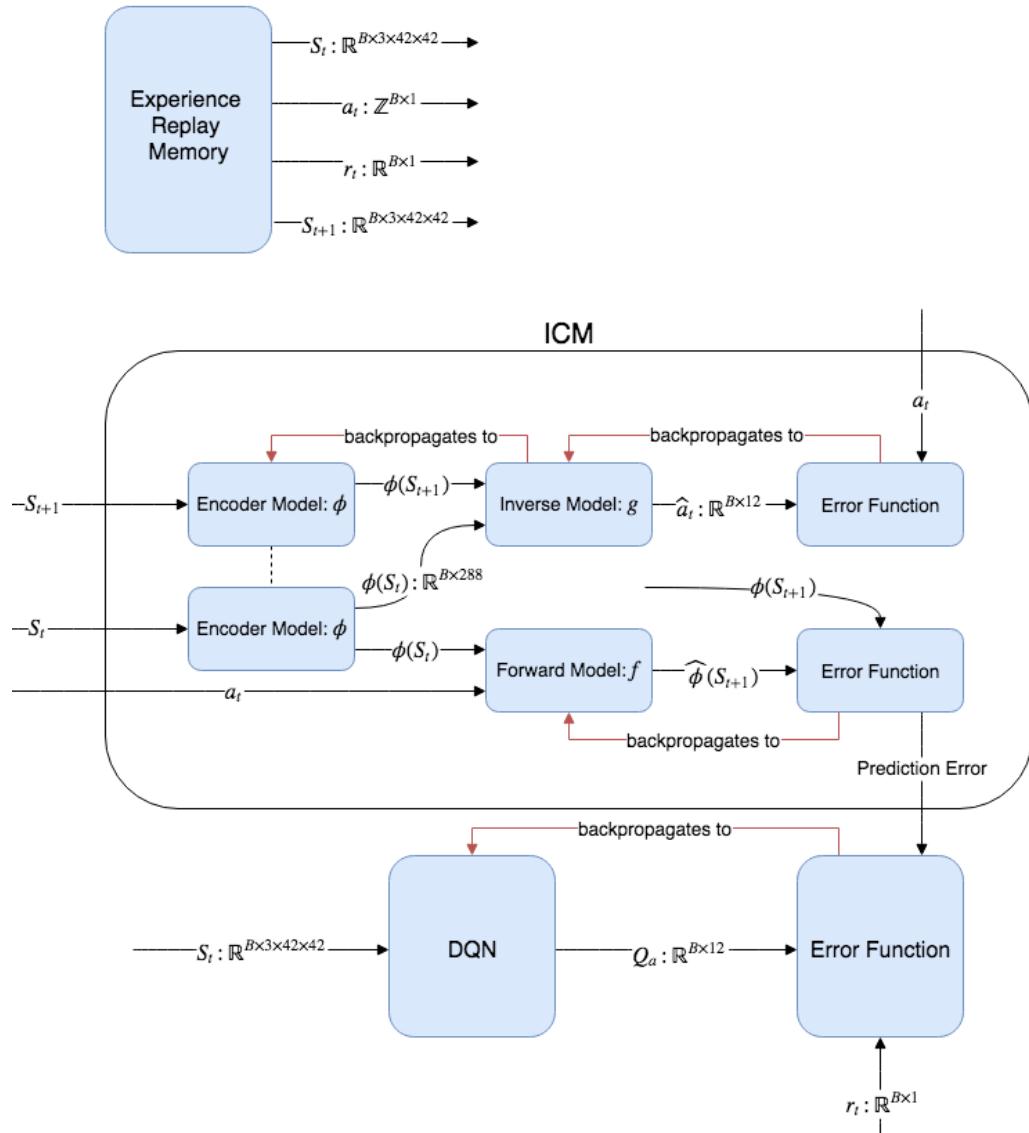


Figure 8.16: A complete view of the overall algorithm including the ICM. First we generate B samples from the experience replay memory and use these for the ICM and DQN. We run the ICM forward to generate a prediction error, which is then provided to the DQN's error function. The DQN then learns to predict action-values that reflect not only extrinsic (environment provided) rewards but also an intrinsic (prediction error-based) reward.

Let's see the code for the components of the ICM.

Listing 8.7: ICM Components

```

class Phi(nn.Module): #A
    def __init__(self):
        super(Phi, self).__init__()
        self.conv1 = nn.Conv2d(3, 32, kernel_size=(3,3), stride=2, padding=1)
        self.conv2 = nn.Conv2d(32, 32, kernel_size=(3,3), stride=2, padding=1)
        self.conv3 = nn.Conv2d(32, 32, kernel_size=(3,3), stride=2, padding=1)
        self.conv4 = nn.Conv2d(32, 32, kernel_size=(3,3), stride=2, padding=1)

    def forward(self,x):
        x = F.normalize(x)
        y = F.elu(self.conv1(x))
        y = F.elu(self.conv2(y))
        y = F.elu(self.conv3(y))
        y = F.elu(self.conv4(y)) #size [1, 32, 3, 3] batch, channels, 3 x 3
        y = y.flatten(start_dim=1) #size N, 288
        return y

class Gnet(nn.Module): #B
    def __init__(self):
        super(Gnet, self).__init__()
        self.linear1 = nn.Linear(576,256)
        self.linear2 = nn.Linear(256,12)

    def forward(self, state1,state2):
        x = torch.cat( (state1, state2) ,dim=1)
        y = F.relu(self.linear1(x))
        y = self.linear2(y)
        y = F.softmax(y,dim=1)
        return y

class Fnet(nn.Module): #C
    def __init__(self):
        super(Fnet, self).__init__()
        self.linear1 = nn.Linear(300,256)
        self.linear2 = nn.Linear(256,288)

    def forward(self,state,action):
        action_ = torch.zeros(action.shape[0],12) #D
        indices = torch.stack( (torch.arange(action.shape[0]), action.squeeze()), dim=0)
        indices = indices.tolist()
        action_[indices] = 1.
        x = torch.cat( (state,action_) ,dim=1)
        y = F.relu(self.linear1(x))
        y = self.linear2(y)
        return y

```

#A Phi is the encoder network

#B Gnet is the inverse model

#C Fnet is the forward model

#D The actions are stored as integers in the replay memory so we convert to a one-hot encoded vector

None of these components have complicated architectures, they're fairly mundane, but together they form a powerful system. We've covered the ICM components, now let's put them together. We're going to define a function that accepts (S_t, a_t, S_{t+1}) , and returns the forward model prediction error and the inverse model error. The forward model error will be used not only to backpropagate and train the forward model but also as the intrinsic reward for the DQN. The inverse model error is only used to backpropagate and train the inverse and encoder models. First we'll show the hyperparameter setup and instantiation of the models.

Listing 8.7: Hyperparameters and Model instantiation

```
params = {
    'batch_size':150,
    'beta':0.2,
    'lambda':0.1,
    'eta': 1.0,
    'gamma':0.2,
    'max_episode_len':100,
    'min_progress':15,
    'action_repeats':6,
    'frames_per_state':3
}

replay = ExperienceReplay(N=1000, batch_size=params['batch_size'])
Qmodel = Qnetwork()
encoder = Phi()
forward_model = Fnet()
inverse_model = Gnet()
forward_loss = nn.MSELoss(reduction='none')
inverse_loss = nn.CrossEntropyLoss(reduction='none')
qloss = nn.MSELoss()
all_model_params = list(Qmodel.parameters()) + list(encoder.parameters()) #A
all_model_params += list(forward_model.parameters()) +
    list(inverse_model.parameters())
opt = optim.Adam(lr=0.001, params=all_model_params)
```

#A We can add the parameters from each model into a single list and pass that into a single optimizer.

Some of the parameters in the `params` dictionary will look familiar, such as `batch_size`, but the others are probably not, we'll go over them, but let's take a look at the overall loss function.

Here's the formula for the overall loss for all 4 models (including the DQN):

$$\text{minimize } [\lambda \cdot Q_{\text{loss}} + (1-\lambda) F_{\text{loss}} + \beta \cdot G_{\text{loss}}]$$

This formula just adds the DQN loss with the forward and inverse model losses each scaled by a coefficient. The DQN loss has a free scaling parameter λ whereas the forward and inverse model losses share a scaling parameter β so that they're inversely related. This is the only loss function we backpropagate through, so at each training step we backpropagate through all 4 models starting from this single loss function.

The `max_episode_len` and `min_progress` parameters are used to set a minimum amount of forward progress Mario must make or we'll reset the environment. Sometimes Mario will get stuck behind an obstacle and will just keep taking the same action forever, so if Mario doesn't move forward enough in a reasonable amount of time we just assume he's stuck and reset the environment.

During training if the policy function says to take action 3 (for example) then we will actually repeat that action 6 times (set according to the `action_repeats` parameter) instead of just once. This helps the DQN learn the value of actions more quickly. During testing (i.e. inference), we only take the action once. The gamma parameter is the same gamma parameter from the DQN chapter. When training the DQN, the target value is not just the current reward r_t but the highest predicted action-value for the next state, so the full target is $r_t + \gamma \cdot \max(Q(S_{t+1}))$. Lastly the `frames_per_state` is set to 3 since each state is the last 3 frames of the game play.

Listing 8.8: The loss function

```
def loss_fn(q_loss, inverse_loss, forward_loss):
    loss_ = (1 - params['beta']) * inverse_loss
    loss_ += params['beta'] * forward_loss
    loss_ = loss_.sum() / loss_.flatten().shape[0]
    loss = loss_ + params['lambda'] * q_loss
    return loss
```

Finally, we get to the actual ICM function.

Listing 8.9: The ICM Prediction Error Calculation

```
def ICM(state1, action, state2, forward_scale=1., inverse_scale=1e4):
    state1_hat = encoder(state1) #A
    state2_hat = encoder(state2)
    state2_hat_pred = forward_model(state1_hat.detach(), action.detach()) #B
    forward_pred_err = forward_scale * forward_loss(state2_hat_pred, \
                                                    state2_hat.detach()).sum(dim=1).unsqueeze(dim=1)
    pred_action = inverse_model(state1_hat, state2_hat) #C
    inverse_pred_err = inverse_scale * inverse_loss(pred_action, \
                                                    action.detach().flatten()).unsqueeze(dim=1)
    return forward_pred_err, inverse_pred_err
```

#A First we encode `state1` and `state2` using the `encoder` model

#B We run the forward model using the encoded states but we make sure to detach them from the graph

#C The inverse model returns a softmax probability distribution over actions

It must be repeated how important is to properly detach nodes from the graph when running the ICM. Recall that PyTorch (and pretty much all other machine learning libraries) builds a computational graph where nodes are individual tensors and connections between nodes are the operations between them. By calling the `.detach()` method we disconnect the tensor from the computational graph and treat it just like raw data; this prevents PyTorch from backpropagating through that node. If we don't detach the `state1_hat` and `state2_hat`

tensors when we run the forward model and its loss then the forward model will backpropagate into the encoder and will corrupt the encoder model.

We've now approached the main training loop. Remember, since we're using experience replay, training only happens when we sample from the replay buffer. We'll set up a function that samples from the replay buffer and computes the individual model errors.

Listing 8.9: Minibatch training using experience replay

```
def minibatch_train(use_extrinsic=True):
    state1_batch, action_batch, reward_batch = replay.get_batch()
    action_batch = action_batch.view(action_batch.shape[0],1) #A
    reward_batch = reward_batch.view(reward_batch.shape[0],1)

    forward_pred_err, inverse_pred_err = ICM(state1_batch, action_batch,
                                              state2_batch) #B
    i_reward = (1. / params['eta']) * forward_pred_err #C
    reward = i_reward.detach() #D
    if use_explicit: #E
        reward += reward_batch
    qvals = Qmodel(state2_batch) #F
    reward += params['gamma'] * torch.max(qvals)
    reward_pred = Qmodel(state1_batch)
    reward_target = reward_pred.clone()
    indices = torch.stack( (torch.arange(action_batch.shape[0]), \
                           action_batch.squeeze()), dim=0)
    indices = indices.tolist()
    reward_target[indices] = reward.squeeze()
    q_loss = 1e5 * qloss(F.normalize(reward_pred),
                          F.normalize(reward_target.detach()))
    return forward_pred_err, inverse_pred_err, q_loss
```

#A We reshape these tensors to add a single dimension to be compatible with the models

#B Run the ICM

#C Scale the forward prediction error using the Eta parameter

#D Start totaling up the reward; make sure to detach the i_reward tensor

#E The use_explicit boolean variable will let us decide whether or not to use explicit rewards in addition to the intrinsic reward

#F We compute the action-values for the next state and use this to add to our target reward term

#G Since the action_batch is a tensor of integers of action indices, we convert this to a tensor of one-hot encoded vectors

Okay, let's tackle the main training loop. We initialize the first state using the `prepare_initial_state(...)` function we defined earlier which just takes the first frame and repeats it 3 times along the channel dimension. We also setup a `deque` instance to which we will append each frame as we observe them. The deque is set to a maxlen of 3 so only the most recent 3 frames are stored. We convert the deque first to a list then to a PyTorch tensor of dimension $1 \times 3 \times 42 \times 42$ before passing to the Q-network.

Listing 8.10: The Training Loop

```
epochs = 5000
env.reset()
```

```

state1 = prepare_initial_state(env.render('rgb_array'))
eps=0.15
losses = []
episode_length = 0
switch_to_eps_greedy = 1000
state_deque = deque(maxlen=params['frames_per_state'])
e_reward = 0.
last_x_pos = env.env.env._x_position #A
for i in range(epochs):
    opt.zero_grad()
    episode_length += 1
    q_val_pred = Qmodel(state1) #B
    if i > switch_to_eps_greedy: #C
        action = int(policy(q_val_pred,eps))
    else:
        action = int(policy(q_val_pred))
    for j in range(params['action_repeats']): #D
        state2, e_reward_, done, info = env.step(action)
        last_x_pos = info['x_pos']
        if done:
            state1 = reset_env()
            break
        e_reward += e_reward_
        state_deque.append(prepare_state(state2))
    state2 = torch.stack(list(state_deque),dim=1) #E
    replay.add_memory(state1, action, e_reward, state2) #F
    e_reward = 0
    if episode_length > params['max_episode_len']: #G
        if (info['x_pos'] - last_x_pos) < params['min_progress']:
            done = True
        else:
            last_x_pos = info['x_pos']
    if done:
        ep_lengths.append(info['x_pos'])
        state1 = reset_env()
        last_x_pos = env.env.env._x_position
        episode_length = 0
    else:
        state1 = state2
    if len(replay.memory) < params['batch_size']:
        continue
    forward_pred_err, inverse_pred_err, q_loss = minibatch_train(use_extrinsic=False)
    #H
    loss = loss_fn(q_loss, forward_pred_err, inverse_pred_err) #I
    loss_list = (q_loss.mean(), forward_pred_err.flatten().mean(), \
                inverse_pred_err.flatten().mean())
    losses.append(loss_list)
    loss.backward()
    opt.step()

```

#A We need to keep track of the last x position in order to reset if no forward progress

#B Run the DQN forward to get action-value predictions

#C After the first 1000 epochs, switch to epsilon-greedy policy

#D Repeat whatever action the policy says 6 times to speed up learning

#E Convert the deque object into a tensor

#F Add the single experience to the replay buffer

#G If Mario is not making sufficient forward progress, restart the game and try again

```
#H Get the errors for one minibatch of data from the replay buffer
#I Compute the overall loss
```

While a bit lengthy, this training loop is pretty simple. All we do is prepare a state, input to the DQN, get action-values (Q-values), input to the policy, get an action to take, and then call the `env.step(action)` method to perform the action. We then get the next state and some other metadata. We add this full experience as a tuple (S_t, a_t, r_t, S_{t+1}) . to the experience replay memory. Most of the action is happening in the minibatch training function we already covered.

That is all the main code you need to build an end-to-end DQN and ICM to train on Super Mario Bros. Let's test it out by training for 5000 epochs, which takes about 30 or so minutes running on a MacBook Air (no GPU). We will train with `use_extrinsic=False` in the minibatch function, so it is learning only from the intrinsic reward. You can plot the individual losses for each of the ICM components and the DQN with the following code. We log-transform the loss data to keep them on a similar scale.

```
>>> losses_ = np.array(losses)
>>> plt.figure(figsize=(8,6))
>>> plt.plot(np.log(losses_[:,0]),label='Q loss')
>>> plt.plot(np.log(losses_[:,1]),label='Forward loss')
>>> plt.plot(np.log(losses_[:,2]),label='Inverse loss')
>>> plt.legend()
>>> plt.show()
```

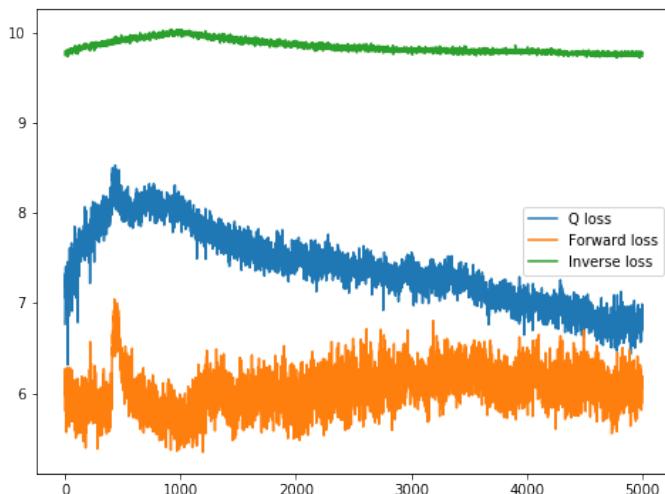


Figure 8.17: These are the losses for the individual components of the ICM and the DQN. The losses do not smoothly decrease like we're used to with a single supervised neural network because the DQN and ICM are trained adversarially.

The DQN loss is clearly trending downward after initially increasing. The forward loss just looks pretty noisy with no clear up or down trend. The inverse model looks sort of flat-lined but if you zoom in, it does seem to very slowly decrease over time. The loss plots look a lot nicer if you set `use_extrinsic=True` and use the extrinsic rewards. But don't be let down by the loss plots. If we test the trained DQN, you will see it does a lot better than the loss plots suggest. This is because the ICM and DQN are behaving like an adversarial dynamical system since the forward model is trying to lower its prediction error but the DQN is trying to maximize the prediction error (by steering the agent toward unpredictable states of the environment).

If you look at the loss plot for a generative adversarial network (GAN), the generator and discriminator loss look somewhat similar to our DQN and forward model loss with `use_extrinsic=False`. The losses do not smoothly decrease like you're used to when you train a single machine learning model.

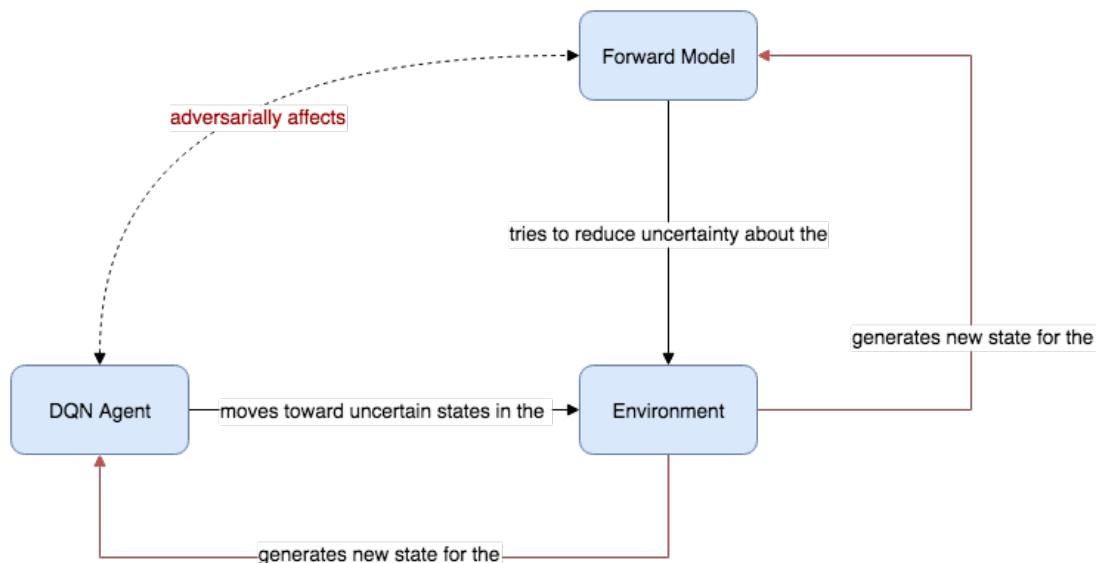


Figure 8.18: The DQN agent and forward model are trying to optimize antagonistic objectives and hence form an adversarial pair.

A better assessment of how well the overall training is going is to track the episode length over time. The episode length should be increasing if the agent is learning to how to progress through the environment more effectively. In our training loop, whenever the episode finished (i.e. the `done` variable becomes True because agent dies or agent doesn't make sufficient forward progress), we save the current `info['x_pos']` to the `ep_lengths` list. We expect to see that the maximum episode lengths will get longer and longer over training time.

```
>>> plt.figure()
```

```
>>> plt.plot(losses_[:,3], label='Episode length')
```

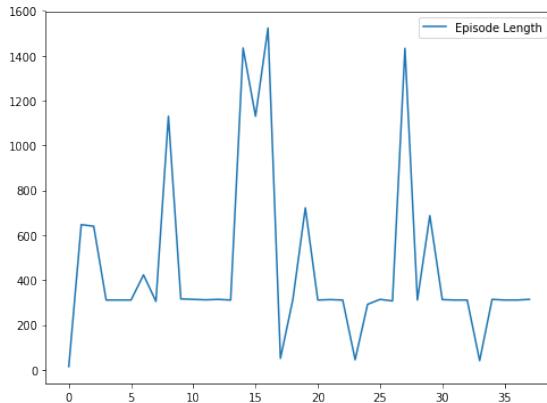


Figure 8.19: Training time is on the x-axis and episode length is on the Y-axis. We see bigger and bigger spikes over training time, which is what we expect.

We see that early on the biggest spike is getting to the 650 mark (i.e. x position in the game), but by the 15th episode the agent is able to get farther than the 1500 x position.

The episode length plot looks promising, but let's actually render a video of our trained agent playing Super Mario Bros. If you're running this off your own computer, the OpenAI Gym provides the render function which will open a new window with live game play. Unfortunately, this won't work if you're using a remote machine or cloud virtual machine. In those cases, the easiest alternative is to just use `plt.imshow(env.render("rgb_array"))` in a loop.

Listing 8.11: Testing the trained agent

```
eps=0.1
done = True
state_deque = deque(maxlen=params['frames_per_state'])
for step in range(5000):
    if done:
        env.reset()
        state1 = prepare_initial_state(env.render('rgb_array'))
        q_val_pred = Qmodel(state1)
        action = int(policy(q_val_pred,eps))
        state2, reward, done, info = env.step(action)
        state2 = prepare_multi_state(state1,state2)
        state1=state2
        env.render()
env.close()
```

There's not much to explain here if you followed the training loop since we're just extracting the part that runs the network forward and takes an action. Notice we still use an epsilon

greedy policy with epsilon set to 0.1. Even during inference the agent needs a little bit of randomness to keep it from getting stuck. One difference to notice is that in test (or inference) mode, we only enact the action once and not 6 times like we did in training. Assuming you get the same results as us, your trained agent should impressively make fairly consistent forward progress and should be able to jump over obstacles. Congratulations!



Figure 8.20: Mario agent trained only from intrinsic reward successfully jumping over a chasm. This demonstrates it has learned basic skills without any explicit rewards to do so. With a random policy the agent would not even be able to move forward let alone learn to jump over obstacles.

If you’re not getting the same results, try changing the hyperparameters, particularly the learning rate, minibatch size and maximum episode length and minimum forward progress. Training for 5000 epochs with intrinsic reward only works but in our experience is sensitive to these hyperparameters.

HOW WILL THIS WORK IN OTHER ENVIRONMENTS? While we trained a DQN agent with an ICM-based reward on a single environment, Super Mario Bros, the paper “Large-Scale Study of Curiosity-Driven Learning” Burda et al 2018 demonstrated how effective intrinsic rewards alone can be. They ran a number of experiments using curiosity-based rewards only across multiple games, finding that a curious agent could progress through 11 levels in Super Mario Bros. and learn to play pong, among others. They used essentially

the same ICM we just built, except they used a more sophisticated agent model called proximal policy optimization (PPO) rather than DQN. An experiment you can try is to replace the encoder network with a random projection. A random projection just means multiplying the input data by a randomly initializing matrix (e.g. a randomly initialized neural network that is fixed and not trained). The Burda et al 2018 paper demonstrated that a random projection works almost as well as the trained encoder.

8.7 Alternative Intrinsic Reward Mechanisms

In this chapter we've described the serious problem faced by RL agents in environments with sparse rewards. We considered the solution as imbuing agents with a sense of curiosity. In this chapter, we implemented an approach from the Pathak et al 2017 paper, one of the most widely cited papers in reinforcement learning research in recent years. We chose to demonstrate this approach not just because it is popular, but because it builds off what we've learned in previous chapters without introducing too many new notions. Curiosity-based learning (which goes by many names) is a very active area of research and there are many alternative approaches, some of which we think are better than the ICM.

Many of the other exciting methods use Bayesian inference and information theory to come up with novel mechanisms to drive curiosity. The prediction error (PE) approach we used in this chapter is just one implementation under a broader PE umbrella. The basic idea, as we now know, is that the agent wants to reduce its PE (or in other words, its uncertainty about the environment) but it must do so by actively seeking out novelty lest it be surprised by something unexpected.

Another umbrella is that of agent *empowerment*. Rather than seeking to minimize prediction error and make the environment more predictable, empowerment strategies optimize the agent to maximize its control over the environment. One paper in this area is "Variational Information Maximisation for Intrinsically Motivated Reinforcement Learning" by Mohamed et al 2015. We can make this informal statement about maximizing control over the environment into a precise mathematical statement (which we will only approximate here).

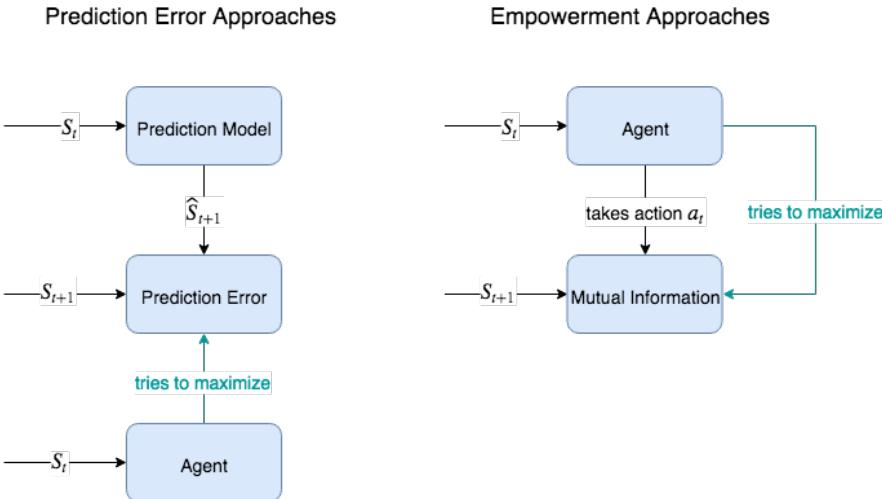


Figure 8.21: The two main approaches for solving the sparse reward problem with curiosity-like methods are prediction error methods like the one we used in this chapter and empowerment methods. Rather than trying to maximize the prediction error between a given state and the next predicted state, in empowerment methods the goal is to maximize the mutual information (MI) between the agent's actions and the next states. If the MI between the agent's action and the next state is high, then that means the agent has a high-level of control (or power) over the resulting next states, i.e. if you know which action the agent took you can predict the next state well. This incentivizes the agent to learn how to maximally control the environment.

The premise relies on the quantity called mutual information. We will not define it mathematically here, but informally, mutual information (MI) measures how much information is shared between two sources of data called random variables (because usually we deal with data that has some amount of randomness or uncertainty). Another less tautological definition is that MI measures how much your uncertainty about one quantity x is reduced given another quantity y .

Information theory was first developed with real world communication problems in mind, where one problem is how to best encode messages across a possibly noisy communication channel so that the received message is the least corrupted. So we have an original message x we want to send across a noisy communication line (for example, using radio waves) and we want to maximize the mutual information between x and the received message y . We do this by developing some way of encoding x , which may be a textual document for example, into a pattern of radio waves that minimizes the probability of the data being corrupted by noise. So once someone else receives the de-coded message y , they can be assured that their received message is very close to the original message.

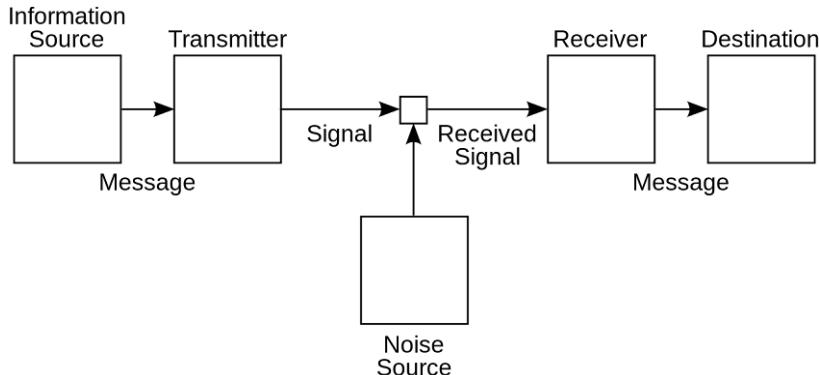


Figure 8.22: Claude Shannon developed communication theory, which was born from the need to encode messages efficiently and robustly across noisy communication channels as depicted here. The goal is to encode the message such that the mutual information between the received message and the sent message is maximal.

In the previous example x and y were both some sort of written message, but x and y need not be the same type of quantities. For example, we can ask what the mutual information is between the 1 year stock price history of a company and its annual revenue, i.e. if I start with a very uncertain estimate about the annual revenue of a company and then I learn the 1 year stock price history, how much is my uncertainty reduced? If it's reduced a lot, then the MI is high. These are different quantities but both using the units of dollars, but that need not be the case either. We could ask what the mutual information is between the daily temperature and the sales of ice cream shops.

In the case of agent empowerment in reinforcement learning, the objective is to maximize the mutual information between an action (or sequence of actions) and the resulting future state(s). Maximizing this objective means that if you know what action the agent took, you will have a high confidence about what the resulting state was, which means the agent has a high degree of control over the environment since it can reliably reach states given its actions. Hence, a maximally empowered agent has the maximal degrees of freedom.

This is different than the prediction error approach because minimizing PE directly encourages exploration, whereas maximizing empowerment may induce exploratory behavior as a means to learn empowering skills, but only indirectly. Consider a young woman, Sarah, who decides to travel the world and explore as much as possible. She is reducing her uncertainty about the world. Compare her to Bill Gates, who by being extraordinarily rich, has a high degree of power. He may not be interested in traveling as much as Sarah, but he can if he wants and no matter where he is at any time he can go where he wants to go.

Both empowerment and curiosity objectives have their use cases. Empowerment-based objectives have been shown to be useful for training agents to acquire complex skills without any extrinsic reward (e.g. robotic tasks or sports games), whereas curiosity-based objectives tend to be more useful for exploration (e.g. games like Super Mario Bros. where the goal is to

progress through levels). In any case, these two metrics are more similar than they are different.

8.8 Summary

- In this chapter we learned about the problem of sparse rewards and covered techniques aimed to solving it.
- We implemented a Deep Q-network agent and paired it with an intrinsic curiosity module.
- The intrinsic curiosity module consists of three independent neural networks: a forward prediction model, inverse model and encoder.
- The encoder encodes high-dimensional states into a low-dimensional vector with high-level features (removes noise and trivial features)
- The forward prediction model predicts the next encoded state and its error provides the curiosity signal
- The inverse model trains the encoder by taking two successive encoded states and predicting the action that was taken
- We learned about the broader subfield of intrinsic motivation in reinforcement learning agents and discussed the empowerment approach as an alternative to the ICM.

9

Multi-Agent Reinforcement Learning

In this chapter we learn

- Why ordinary Q-learning can fail in the multi-agent setting
- How to deal with the “curse of dimensionality” with multiple agents
- How to implement multi-agent Q-learning models that can perceive other agents
- How to scale multi-agent Q-learning by using the mean field approximation
- Use DQNs to control dozens of agents in a multi-agent physics simulation and game

9.1 From one to many agents

So far the reinforcement learning algorithms we have covered: Q-learning, policy gradients, and actor-critic algorithms, were all applied to the case where we are controlling a single agent in an environment. But what about situations where we want to control more than one agent that can interact with each other? The simplest example of this would be a two-player game where each player is implemented as a reinforcement learning agent. But there are other situations in which we may want to model hundreds or thousands of individual agents all interacting with each other, such as a traffic simulation. In this chapter we will learn how to adapt what we’ve learned so far into the multi-agent scenario by implementing an algorithm called *Mean Field Q-learning* (MF-Q), first described in a paper called “Mean Field Multi-Agent Reinforcement Learning” by Yang et al 2018.

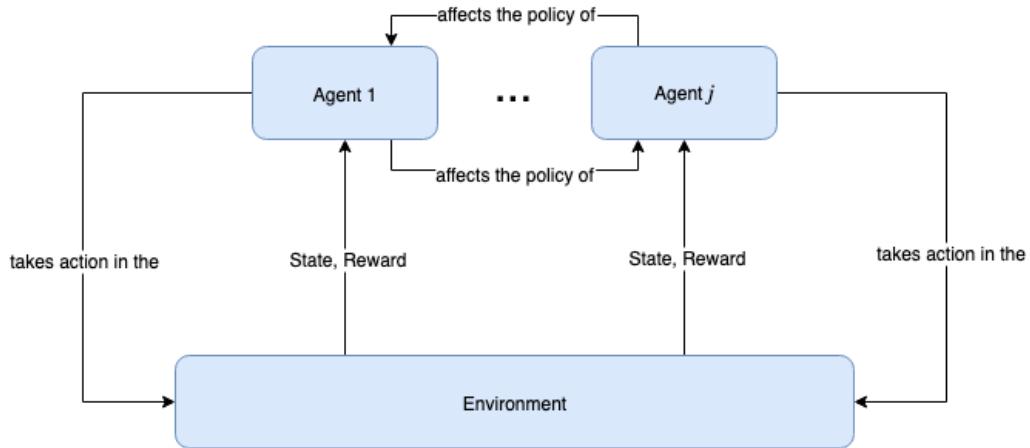


Figure 9.1: In the multi-agent setting, each agent's actions not only affect the evolution of the environment, but also the policies of other agents, leading to highly dynamic agent interactions. The environment will produce a state and reward, which each agent 1 through j use to take actions using their own policies. However, each agent's policy will affect all the other agents' policies.

In the case of games, the environment might contain other agents that we do not control, often called non-player characters (NPCs). For example, in chapter 8 we trained an agent to play Super Mario Bros., which has many NPCs. These NPCs are controlled by some other unseen game logic but can and often do interact with the main player. From the perspective of our Deep Q-network (DQN) agent, for example, these NPCs are nothing more than patterns in the state of the environment that change over time. Our DQN is not directly aware of the actions of the other players. This is not an issue, however, because these NPCs do not learn; they have fixed policies.

Imagine, however, we directly want to control the actions of many interacting agents in some environment using a deep reinforcement learning algorithm. For example, there are games with multiple players grouped into teams and we may want to develop an algorithm that can play a bunch of players on a team against another team. Or we may want to control the actions of hundreds of simulated cars to model traffic patterns. Or maybe we're economists and we want to model the behavior of thousands of agents in a model of an economy. This is a different situation than having NPCs, because unlike NPCs, these other agents all learn and their learning is affected by each other.

The most straightforward way to extend what we know already into the multi-agent setting is to just instantiate multiple DQNs (or some other similar algorithm) for each agent and then each agent just sees the environment as it is and takes actions. If the agents we are trying to control all use the same policy, which is a reasonable assumption in some cases (for example in a multi-player game where each player is identical), then we could even re-use a single DQN to model multiple agents (i.e. a single set of parameters).

This approach is called **independent Q-learning (IL-Q)**, and it works reasonably well but it misses the fact that interactions between agents affect the decision-making of each. With an IL-Q algorithm, each agent is completely unaware of what other agents are doing and how their actions might affect itself. Each agent only gets a state representation of the environment, which includes the current state of each other agent, but it essentially treats the activity of other agents in the environment as noise (since the behavior of other agents is, at most, only partially predictable).

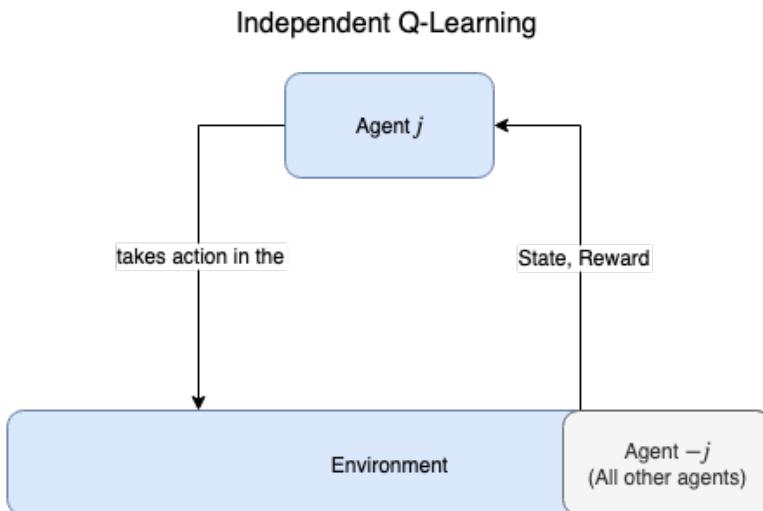


Figure 9.2 In independent Q-learning, each agent does not directly perceive the actions of other agents but rather just pretends they are part of the environment. This is an approximation that loses the convergence guarantees that Q-learning has in the single-agent setting since the other agents make the environment non-stationary.

In the ordinary Q-learning we've done before now where there's only a single agent in the environment, we know the Q-function will converge to the optimal value, and hence we will converge on an optimal policy (it is mathematically guaranteed to converge in the long run). This is because in the single-agent setting, the environment is **stationary**, meaning the distribution of rewards for a given action in a given state is always the same. This stationarity feature is violated in the multi-agent setting since the rewards an individual agent receives will vary not only based on its own actions but of the actions of other agents. This is because all agents are reinforcement learning agents and learn through experience, and thus their policies are constantly changing in response to changes in the environment. If we use IL-Q in this non-stationary environment, we lose the convergence guarantee, and this can impair the performance of independent Q-learning significantly.

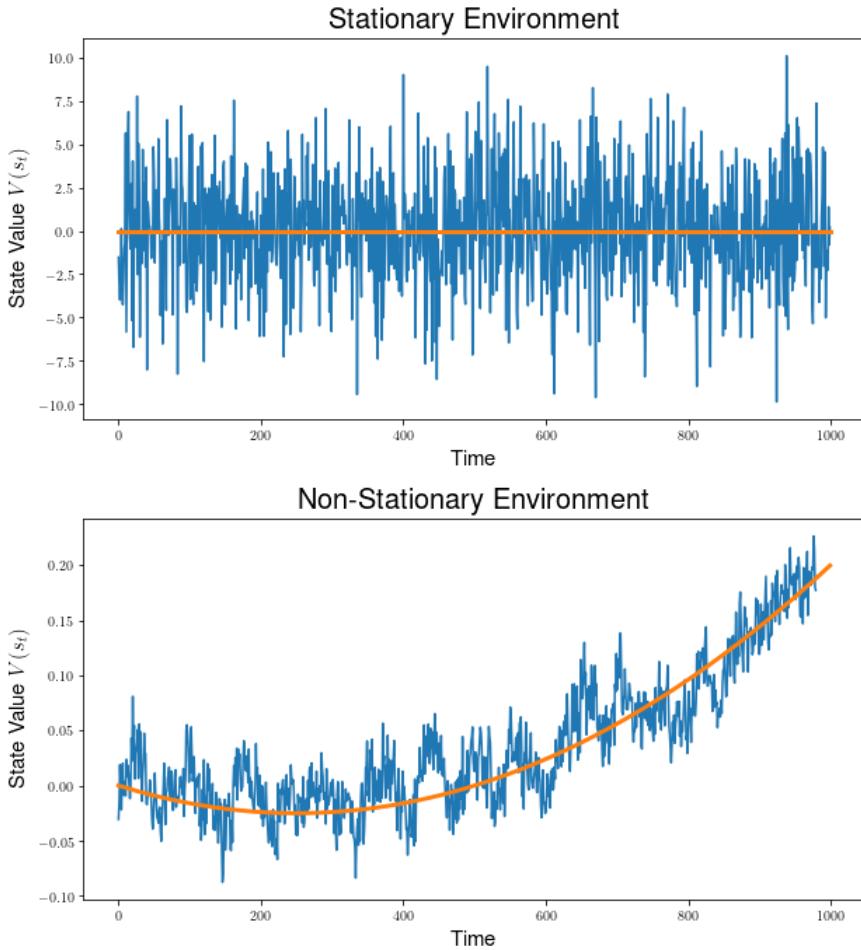


Figure 9.3 In a stationary environment the expected (i.e. average) value over time for a given state will remain constant (stationary). Any particular state transition may have a stochastic component, hence the noisy-looking time series, but the mean of the time series is constant. In a non-stationary environment, the expected value for a given state transition will change over time, which is depicted in this time series as a changing mean or baseline over time. The Q-function is trying to learn the expected value for state-actions and it can only converge if the state-action values are stationary, but in the multi-agent setting, the expected state-action values can change over time due to the evolving policies of other agents.

A normal Q-function is a function $Q(s,a): S \times A \rightarrow R$, a function from a state-action pair to a reward (some real number). We can remedy the problems with IL-Q by making a slightly more sophisticated Q-function that incorporates the knowledge of the actions of other agents, Q_j

$(s, a_j, a_{-j}): S \times A_j \times A_{-j} \rightarrow R$, which is a Q-function for the agent indexed by j that takes a tuple of the state, agent j 's action, and all the other agents actions (denoted $-j$, pronounced "not j ") to the predicted reward for this tuple (again, just a real number). It is known that a Q-function of this sort regains the convergence guarantee that we will eventually learn the optimal value and policy functions, and thus this modified Q-function is able to perform much better.

Unfortunately, this new Q-function is intractable in general (when the number of agents is large) because the joint action-space a_{-j} is extremely large and grows exponentially in the number of agents. Remember how we encode an action? We use a vector with length equal to the number of actions. If we want to encode a single action, we make this a one-hot vector where all elements are 0 except at the position corresponding to the action, which is set to 1. For example, in the Gridworld environment the agent has four actions (up, down, left, right) and so we encode actions as a length 4 vector, where [1,0,0,0] could be encoded as "up" and [0,1,0,0] could be "down" and so forth.

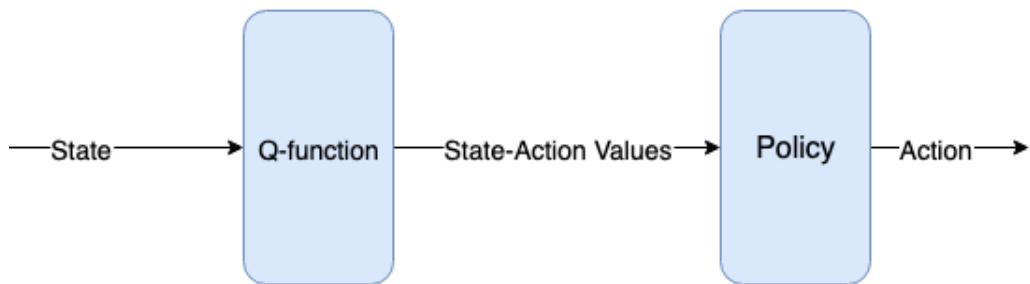


Figure 9.4 The Q-function takes a state and produces state-action values (Q-values), which are then used by the policy function to produce an action. Alternatively, we can directly train a policy function that operates on a state and returns a probability distribution over actions.

Remember, the policy $\pi(s):S \rightarrow \mathcal{A}$ is a function that takes a state and returns an action. If it is a deterministic policy, it will have to return one of these one-hot vectors, or if it is a stochastic policy then it returns a probability distribution over the actions, e.g. [0.25,0.25,0.2,0.3]. The exponential growth is due to the fact that if we want to unambiguously encode a joint-action, for example, the joint-action of two agents with 4 actions each in Gridworld, then we have to use a $4^2=16$ length one-hot vector instead of just a 4 length vector. This is because there are 16 different possible combinations of actions between two agents with 4 actions each (see Figure 9.5), e.g. [Agent 1: Action 1, Agent 2: Action 4], [Agent 1: Action 3, Agent 2: Action 3] and so on.

If we want to model the joint-action of 3 agents, then we have to use a $4^3=64$ length vector. So in general for Gridworld, we have to use a 4^N length vector where N is the number of agents. For any environment, the size of the joint-action vector will be $|\mathcal{A}|^N$ where $|\mathcal{A}|$ refers to the size of the action space (i.e. the number of discrete actions). That is an exponentially growing vector in the number of agents, and this is just impractical and

intractable for any significant number of agents. Exponential growth is always a bad thing since it means your algorithm can't scale.

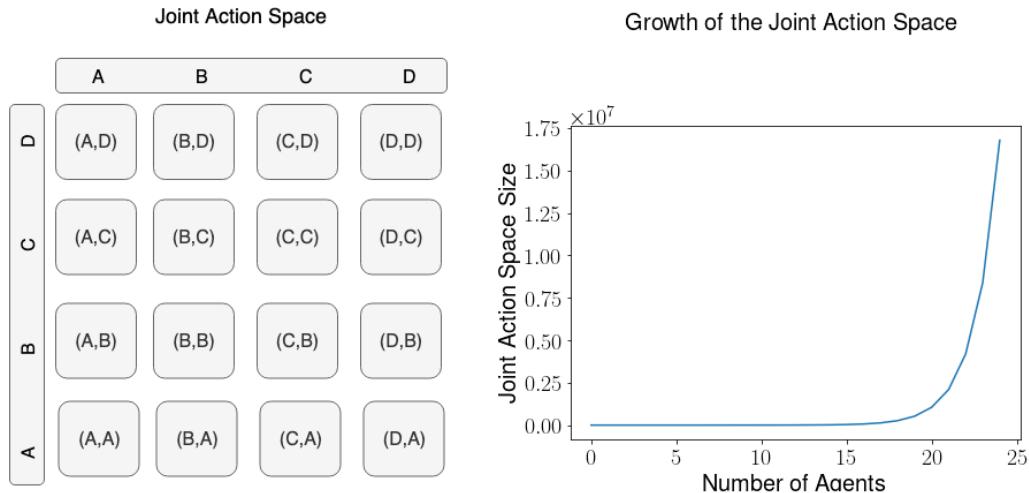


Figure 9.5 If each agent has an action space of size 4 (i.e. it is represented by a 4 element one-hot vector), then the joint-action space of two agents is $4^2=16$, or 4^N where N is the number of agents. This means the growth of the joint-action space is exponential in the number of agents. The figure on the right shows the joint-action space size for agents with individual action spaces of size 2. Even with just 25 agents the joint-action space becomes a 33,554,432 element one-hot vector, which is computationally impractical to work with.

This exponentially large joint-action space is the main new complication that MARL brings, and it is the problem we spend this chapter solving.

9.2 Neighborhood Q-learning

You might be wondering if there is a more efficient and compact way of representing actions and joint-actions that might get around this issue of an impractically large joint-action space, but unfortunately there is no unambiguous way to represent an action using a more compact encoding. Try thinking of how you could communicate, unambiguously, which actions a group of agents took using a single number and you'll realize you can't do it better than with an exponentially growing number.

At this point, MARL doesn't seem practical, but we can make it practical by making some approximations to this idealized joint-action Q-function. One option is to recognize that in most environments, only agents within close proximity to each other will have any significant effect on each other. So we don't necessarily need to model the joint-actions of *all* the agents in the environment, we can approximate this by only modeling the joint-actions of agents within the same **neighborhood**. In a sense, we divide the full joint-action space into a set of

overlapping subspaces and only compute Q-values with these much smaller subspaces. We might call this method **neighborhood Q-learning** or **subspace Q-learning**.

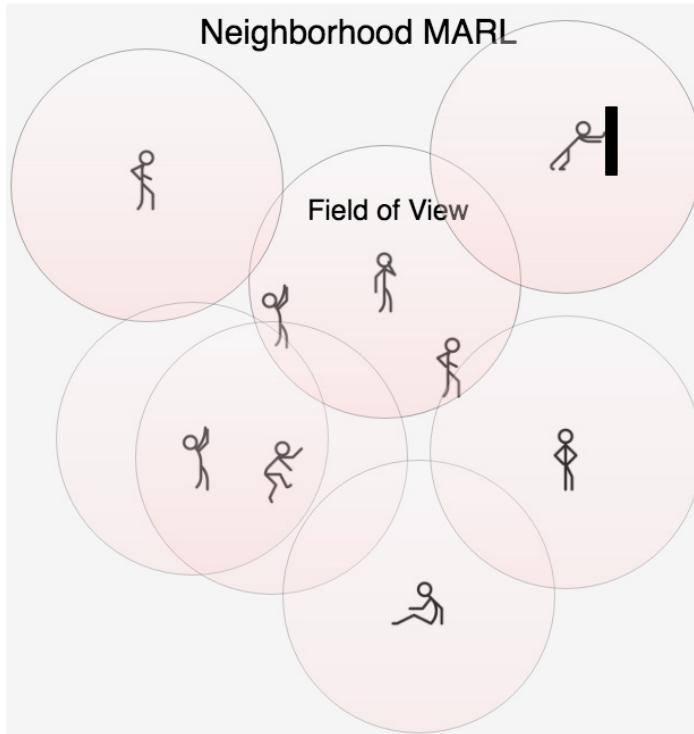


Figure 9.6 In neighborhood MARL, each agent has a field of view (FOV) or neighborhood and it can only see the actions of the other agents within its neighborhood. However, it may still get the full state information about the environment.

By constraining the size of the neighborhood, we stop the exponential growth of the joint-action space to be the fixed size of whatever we set the neighborhood size to be. If we have a multi-agent Gridworld with 4 actions of each agent and 100 agents total, then the full joint-action space is $4^4=100$, which is an intractable size, no computer could possibly compute with (or even store) such a large vector. However, if we use subspaces of the joint-action space and set the size of each subspace (neighborhood) to be fixed at 3 (so the size of each subspace is $4^3=64$), then this is a much bigger vector than with a single agent but definitely something we can compute with. In this case, if we're computing the Q-values for agent 1, then we find the 3 agents closest in distance to agent 1 and build a joint-action one-hot vector of length 64 for these 3 agents and give that to the Q-function. So for each agent of 100 total, we would build these subspace joint-action vectors and use that to compute Q-values for each agent, and then use those Q-values to take actions as usual.

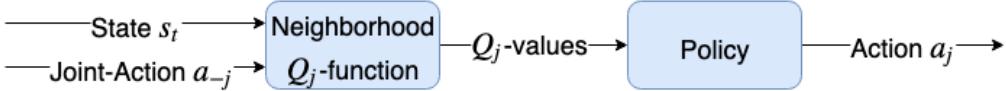


Figure 9.7 The neighborhood Q-function for agent j accepts the current state and the joint-action vector for the other agents within its neighborhood (or field of view), denoted a_{-j} , and produces q-values that get passed to the policy function that chooses the action to take.

Let's write some pseudocode for how this works.

Listing 9.1 Pseudocode for Neighborhood Q-learning, part 1

```

# Initialize actions for all agents

for j in agents: #A
    state = environment.get_state() #B
    neighbors = get_neighbors(j, num=3) #C
    joint_action = get_joint_action(neighbors) #D
    q_values = Q(state, joint_action) #E
    j.action = policy(q_values) #F
    environment.take_action(j.action)
    reward = environment.get_reward()

#A Iterate through all the agents in the environment, stored in a list
#B Retrieve the current environment state
#C This function will find the closest 3 agents to agent j
#D This function will return the joint action of agent j's neighbors
#E Get the q-values for each action of agent j given the state and the joint-action of its neighbors
#F This function will return a discrete action using the q-values
  
```

We need a function that takes the current agent j and finds us its nearest 3 neighbors, and then we need another function that will build the joint-action using these 3 nearest neighbors. At this point, we have another problem: how do we build the joint-action without already knowing the actions of the other agents? In order to compute the Q-values for agent j (and thus take an action), we need to know the actions that agents $-j$ are taking (we use $-j$ to denote the agents that are *not* agent j , but in this case only the nearest neighbors). But in order to figure out the actions of agents $-j$, we would need to compute all of their Q-values, and then it seems like we get into an infinite loop and never get anywhere.

To avoid this problem, when we start we simply initialize all the actions for the agents randomly, and then we can compute the joint-actions using these randomly-initialized actions. But if that's all we did, then using joint-actions wouldn't be much help since they're random, so we re-run this process a few times (that's the `for m in range(M)` part, where M is some small number like 5). The first time we run this, the joint-action will be random, but then all the agents will have taken an action based on their Q-functions, so the second time it will be slightly less random, and if we keep doing this a few more times, the initial randomness will be sufficiently diluted and then we can actually take these actions at the end of this iteration in the real environment.

Listing 9.2 Pseudocode for Neighborhood Q-learning, part 2

```
# Initialize actions for all agents

for m in range(M): #A
    for j in agents:
        state = environment.get_state()
        neighbors = get_neighbors(j, num=3)
        joint_actions = get_joint_action(neighbors)
        q_values = Q(state, joint_actions)
        j.action = policy(q_values)

for j in agents: #B
    environment.take_action(j.action)
    reward = environment.get_reward()
```

#A Iterate through the process of computing joint-actions and q-values a few times to dilute initial randomness
#B Need to loop through agents again to actually take the final actions that were computed in the previous loop

The way we build a joint-action from a set of individual actions is by using the **outer** product operation from linear algebra. The simplest way to express this is to “promote” an ordinary vector to a matrix. For example, we have might a length 4 vector and we promote it to a 4×1 matrix. In PyTorch and Numpy we can do this using the reshape method on a tensor, e.g. `torch.Tensor([1,0,0,0]).reshape(1,4)`. The result we get when multiplying two matrices depends on their dimensions and the order in which we multiply them. If we take a $A:1 \times 4$ matrix and multiply it by another matrix $B:4 \times 1$, then we get a 1×1 result, which is a scalar (a single number). This would be the inner product of two vectors (promoted to matrices) since the largest dimensions are sandwiched in between the two singlet dimensions. The outer product is just the reverse of this, where the two large dimensions are on the outside and the two singlet dimensions are on the inside, resulting in a $4 \times 1 \otimes 1 \times 4 = 4 \times 4$ matrix.

If we have two agents in Gridworld with individual actions [0,0,0,1] (“right”) and [0,0,1,0] (“left”) then their joint-action can be computed by taking the outer product of these vectors. Here’s how we do it in numpy:

```
>>> np.array([[0,0,0,1]]).T @ np.array([[0,1,0,0]])
array([[0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 0, 0, 0],
       [0, 1, 0, 0]])
```

The result is a 4×4 matrix, with a total of 16 elements as we calculated above. The dimension of the result of the outer product between two matrices is $\text{dim}(A) * \text{dim}(B)$ where A and B are vectors and `dim` refers to the size (dimension) of the vector. The outer product is the reason why the joint-action space grows exponentially. Generally, we need our neural network Q-function to operate on inputs that are vectors, so since the outer product gives us a matrix result, we simply flatten it into a vector.

```
>>> z = np.array([[0,0,0,1]]).T @ np.array([[0,1,0,0]])
>>> z.flatten()
```

```
array([0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0])
```

Hopefully, you can appreciate that the neighborhood Q-learning approach is not much more complicated than ordinary Q-learning. We just need to give it an additional input which is the joint-action vector of each agent's nearest neighbors. Let's figure out the details by tackling a real problem.

9.3 The 1-Dimensional Ising Model

In this section we're going to apply MARL to solve a real physics problem that was first described in the early 1920s by physicist Wilhelm Lenz and his student Ernst Ising. First, a brief physics lesson. Physicists were trying to understand the behavior magnetic materials such as iron by mathematical models. A piece of iron that you can hold in your hand is a collection of iron atoms that are grouped together by metallic bonding. An atom is composed of a nucleus of protons (positively charged) and neutrons (no charge) and an outer "shell" of electrons (negatively charged). Electrons, like other elementary particles, have a property called **spin**, which is quantized such that an electron can only have a spin "up" or spin "down" at any time.

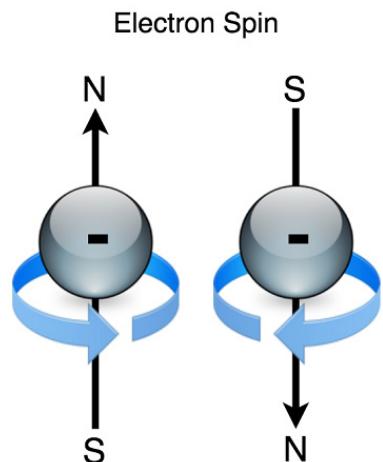


Figure 9.8 Electrons are negatively charged elementary particles that surround the nucleus of every atom. They have a property called spin, and they can either be "spin up" or "spin down." Since they are charged particles they generate a magnetic field, and the direction they spin determines the orientation of the poles (north or south) of the magnetic field.

The spin property can be thought of as the electron rotating either clockwise or counter-clockwise, however, this is not literally true but it suffices for our purposes. When a charged object rotates, it creates a magnetic field, so if you took a rubber balloon, gave it a static charge by rubbing it on the carpet and then spun it around, you would have yourself a balloon

magnet (albeit an extremely weak magnet). Electrons likewise create a magnetic field by virtue of their spin and electric charge, hence electrons really are very tiny magnets, and since all the iron atoms have electrons, the entire piece of iron can become a big magnet if all of its electrons are aligned in the same direction (i.e. all spin up or all spin down).

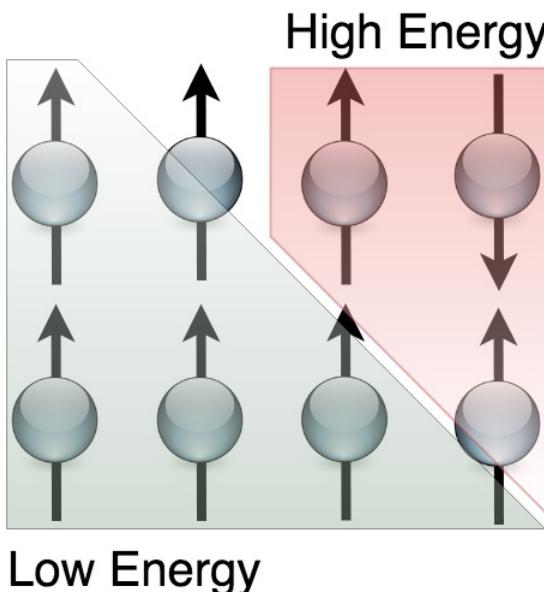


Figure 9.9 When electrons are packed together, they prefer to have their spins aligned in the same direction because it is a lower energy configuration than when their spins are anti-aligned, and all physical systems tend toward lower energy (all else being equal).

Physicists were trying to study how the electrons “decide” to align themselves, and how the temperature of the iron affects this process. If you heat up a magnet, at some point the aligned electrons will start randomly alternating their spins so that the material loses its net magnetic field. Physicists knew that an individual electron creates a magnetic field, and that a tiny magnetic field will affect a nearby electron. If you’ve ever played with two bar magnets, you’ve noticed that they will naturally line up in one direction or repel along the opposite direction. The electrons do the same thing. It makes sense that electrons would also try to align themselves to be the same spin.

There’s one added complexity though. A random piece of iron you pick up is not usually magnetized because the electrons organize into small domains where the electrons in a given domain are all aligned (either spin up or down) but other nearby domains may be in the opposite orientation. While individual electrons have a tendency to align themselves to nearby electrons, at a larger scale these domains will organize such that they are (on average) anti-aligned. This is because as a domain grows larger (i.e. the number of electrons in it that are

all aligned the same grows), the magnetic field grows, and the larger this bulk magnetic field is, it actually creates some internal strain on the material. So at the super local level, electrons minimize their energy by being aligned, but if too many are aligned and the magnetic field becomes too strong, then the overall energy of the system grows, and that causes the electrons to align only into relatively small clusters called domains.

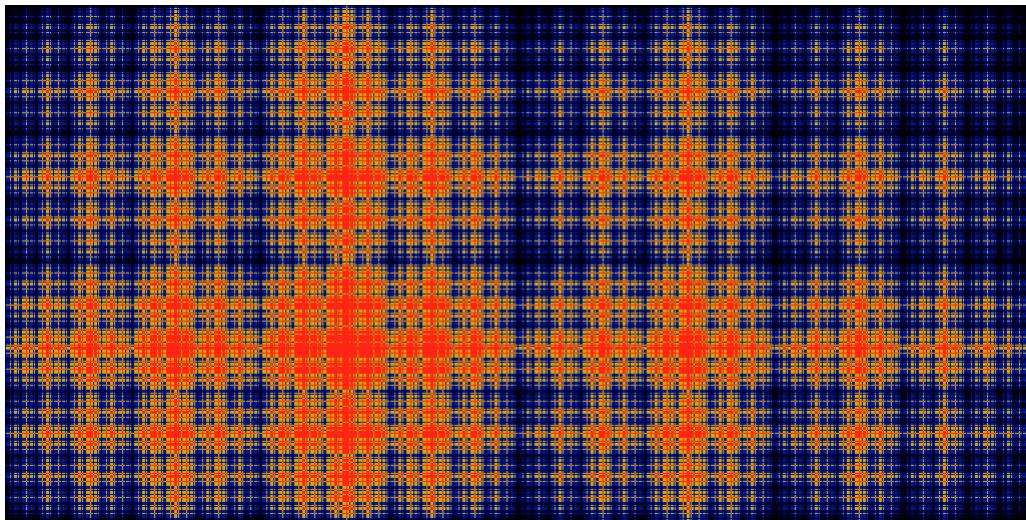


Figure 9.10 This is an image of a high-resolution Ising model where each pixel represents an electron. The lighter pixels are spin up, and black is spin down. You can see the electrons organize into domains where all the electrons within a domain are aligned. This organization reduces the energy of the system.

Presumably the interactions between trillions of electrons in the bulk material result in the complex organization of electrons into domains, however, it is very difficult to model that many interactions. So physicists made a simplifying assumption that a given electron is only affected by its nearest neighbors, which is exactly the same assumption we've made with neighborhood Q-learning.

Remarkably, we can model the behavior of many electrons and observe the large-scale emergent organization by multi-agent reinforcement learning. All we need to do is interpret the energy of an electron as its "reward." If an electron changes its spin to align with its neighbor, we will give it a positive reward, if it decides to anti-align, then we give it a negative reward. When all the electrons are trying to maximize their reward, this is the same as trying to minimize their energy, and we will get the same result the physicists get when they use energy-based models. As we'll see, we can also model the temperature of the system by changing the amount of exploration/exploitation. Remember, exploration involves randomly choosing actions, and a high temperature involves random changes as well. They're quite analogous.

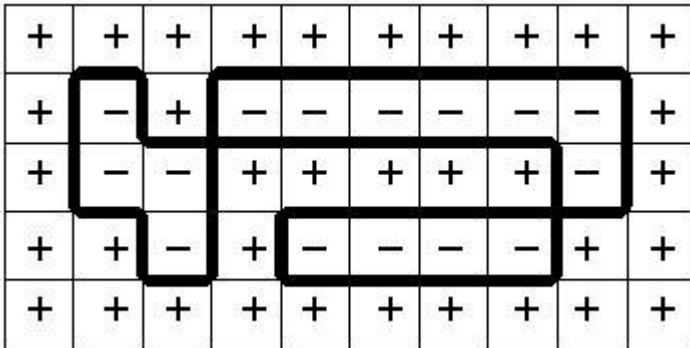


Figure 9.11 This is a depiction of a 2D Ising model of electron spins where + is spin up and - is spin down. There is a domain of electrons that are all spin down (highlighted in black), and these are surrounded by a shell of spin up electrons.

Modeling the behavior of electron spins may seem unimportant, but the same basic modeling technique used for electrons can be used to solve problems in genetics, finance, economics, botany, and sociology among others. It also happens to be one of the simplest ways to test out MARL, so that's our main motivation.

The only thing we need to do to create an Ising model is to create a grid of binary digits where 0 represents spin down and 1 represents spin up. This grid could be of any dimensions. We could have a 1-dimensional grid (a vector), a 2 dimensional grid (a matrix), or some high order tensor. We will first solve the 1D Ising Model since it is so easy that we don't need to use any fancy mechanisms like experience replay or distributed algorithms. We won't even use PyTorch's built-in optimizers, we will write out the gradient descent manually in just a few lines of code.

Listing 9.3 1D Ising Model

```
import numpy as np
import torch
from matplotlib import pyplot as plt

def init_grid(size=(10,)):
    grid = torch.randn(*size)
    grid[grid > 0] = 1
    grid[grid <= 0] = 0
    grid = grid.byte() #A
    return grid

def get_reward(s,a): #B
    r = -1
    for i in s:
        if i == a:
```

```
r += 0.9
r *= 2.
return r
```

#A We convert the floating point numbers into byte object to make it binary.
#B This function takes neighbors in `s` and compares them to agent `a`, if they match the reward is higher

We have created two functions, the first creates a randomly initialized 1-dimensional grid (vector) by first creating a grid of numbers drawn from a standard normal distribution, and then we just set all the negative numbers to be 0 and all the positive numbers to 1, and we will approximately get the same number of 1s and 0s in the grid. We can visualize the grid using matplotlib.

```
>>> grid = init_grid(size=size)
>>> grid
tensor([1, 0, 0, 0, 0, 1, 0, 0, 1, 0, 0, 0, 1, 0, 0, 0, 1, 0, 1, 0, 0],  

      dtype=torch.uint8)

>>> plt.imshow(np.expand_dims(grid,0))
```

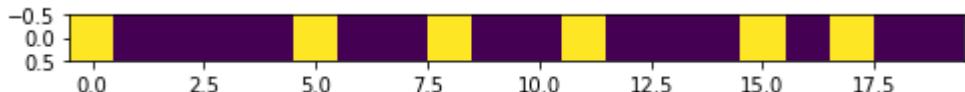


Figure 9.12 This is a 1D Ising Model, representing the electron spins for electrons arranged in a single row.

The 1s are lightly colored and the 0s are dark. We have to use the `np.expand_dims(...)` function to make the vector into a matrix by adding a singlet dimension, since `plt.imshow` only works on matrices or 3-tensors.

The second function we created is our reward function. It accepts a list `s` of binary digits and a single binary digit `a` and then compares how many values in `s` match `a`. If all of the values match, then the reward is maximal, and if none of them match then the reward is negative. The input `s` will be the list of neighbors. In this case, we will use the 2 nearest neighbors, so for a given agent its neighbors will be the agent to its left and right on the grid. If an agent is at the end of the grid, its right neighbor will be the first element in the grid, so we wrap around to the beginning. This makes the grid into a circular grid.

Listing 9.4 The 1D Ising Model

```
def gen_params(N,size): #A
    ret = []
    for i in range(N):
        vec = torch.randn(size) / 10.
        vec.requires_grad = True
        ret.append(vec)
    return ret
```

```
#A This function generates a list of parameter vectors for a neural network
```

Since we will be using a neural network to model the Q-function, we need to generate the parameters for it. In our case, we will use a separate neural network for each agent, although this is unnecessary since each agent has the same policy and thus we could re-use the same neural network. We do this just to show how it works, but for the later examples we will use a shared Q-function for agents with identical policies.

Since the 1D Ising Model is so simple, we will write the neural network manually by specifying all the matrix multiplications rather than using PyTorch's built-in layers. We make a Q-function that accepts a state vector and a parameter vector and in the function body we unpack the parameter vector into multiple matrices that form each layer of the network.

Listing 9.5 The 1D Ising Model

```
def qfunc(s,theta,layers=[(4,20),(20,2)],afn=torch.tanh):
    l1n = layers[0]
    l1s = np.prod(l1n) #A
    theta_1 = theta[0:l1s].reshape(l1n) #B
    l2n = layers[1]
    l2s = np.prod(l2n)
    theta_2 = theta[l1s:l2s+l1s].reshape(l2n)
    bias = torch.ones((1,theta_1.shape[1]))
    l1 = s @ theta_1 + bias #C
    l1 = torch.nn.functional.elu(l1)
    l2 = afn(l1 @ theta_2) #D
    return l2.flatten()
```

#A We take the first tuple in `layers` and multiply those numbers to get the subset of the `theta` vector to use as the first layer.

#B We reshape the `theta` vector subset into a matrix for use as the first layer of the neural network

#C This is the first layer computation. The `s` input is a joint-action vector of dimensions (4,1)

#D We can also input an activation function to use for the last layer; the default is tanh since our reward ranges [-1,1]

This is the Q-function implemented as simple 2-layer neural network. It expects a state vector `s` that is the binary vector of neighbors states and parameter vector `theta`. It also needs the keyword parameter `layers` which is a list of the form $[(s1,s2),(s3,s4)\dots]$ that indicates the shape of the parameter matrix for each layer. As all Q-functions do, this one returns Q-values for each possible action, in this case for down/up (2 actions). For example, it might return the vector $[-1,1]$, indicating the expected reward for changing the spin to down is -1 and the expected reward of changing the spin to up is +1.

The advantage of using a single parameter vector is that it is easy to store all the parameters for multiple neural networks as just a list of vectors, and we just let the neural network unpack the vector into layer matrices. We use the tanh activation function because its output is in the interval $[-1,1]$, and our reward is in the interval $[-2,2]$, so a +2 reward will strongly push the q-value output toward +1. However, we want to be able to re-use this Q-function for our later projects so we actually provide the activation function as an optional keyword parameter, `afn`.

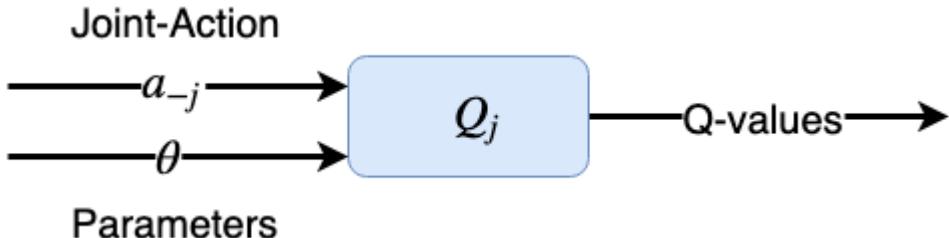


Figure 9.13 The Q-function for agent j accepts a parameter vector and a one-hot encoded joint-action vector for the neighbors of agent j .

Listing 9.6 The 1D Ising Model

```
def get_substate(b): #A
    s = torch.zeros(2)
    if b > 0: #B
        s[1] = 1
    else:
        s[0] = 1
    return s

def joint_state(s): #C
    s1_ = get_substate(s[0]) #D
    s2_ = get_substate(s[1])
    ret = (s1_.reshape(2,1) @ s2_.reshape(1,2)).flatten() #E
    return ret
```

#A This function takes a single binary number and turns it into a one-hot encoded action vector like [0,1]

#B If the input is 0 (down) then action vector is [1,0] otherwise its [0,1]

#C `s` is a vector with 2 elements where s[0] = left neighbor, s[1] = right neighbor

#D Get the action vectors for each element in `s`

#E This creates the joint-action space using the outer-product, then flattens into a vector

These are two auxiliary functions we need to prepare the state information for the Q-function. The `get_substate` function takes a single binary number (0 for spin down and 1 for spin up) and turns it into a one-hot encoded action vector, where 0 becomes [1,0] and 1 becomes [0,1] for an action space of [down, up]. The grid only contains a series of binary digits representing the spin of each agent, but we need to turn those binary digits into action vectors and then take the outer product to get a joint-action vector for the Q-function.

Listing 9.7 The 1D Ising Model

```
plt.figure(figsize=(8,5))
size = (20,) #A
hid_layer = 20 #B
params = gen_params(size[0],4*hid_layer+hid_layer*2) #C
```

```

grid = init_grid(size=size)
grid_ = grid.clone() #D
print(grid)
plt.imshow(np.expand_dims(grid,0))

#A Set the total size of the grid to be a 20 length vector
#B Set the size of the hidden layer. Our Q-function is just a two-layer neural network so there's only one hidden layer
#C This function generates a list of parameter vectors that will parameterize the Q-function
#D We need to make a clone of the grid for reasons that will become clear in the main training loop

```

If you run that code, you should get something like this (yours will look different since it is randomly initialized):

```
tensor([0, 0, 1, 0, 0, 1, 1, 0, 1, 0, 0, 1, 0, 0, 1, 0, 1, 0, 1, 0],  
      dtype=torch.uint8)
```

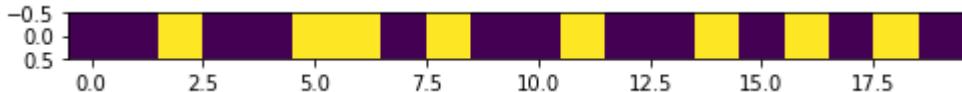


Figure 9.14 A 1D Ising Model of electrons arranged in a single row.

You can notice that the spins are pretty randomly distributed between up (1) and down (0). When we train our Q-function, we expect to get the spins to align themselves in the same direction. They may not *all* align in the same direction, but they should at least cluster into domains that are all aligned. Let's get into the main training loop now that we have all of the necessary functions defined.

Listing 9.8 The 1D Ising Model

```

epochs = 200
lr = 0.001 #A
losses = [[] for i in range(size[0])] #B
for i in range(epochs):
    for j in range(size[0]): #C
        l = j - 1 if j - 1 >= 0 else size[0]-1 #D
        r = j + 1 if j + 1 < size[0] else 0 #E
        state_ = grid[[l,r]] #F
        state = joint_state(state_) #G
        qvals =
            qfunc(state.float().detach(),params[j],layers=[(4,hid_layer),(hid_layer,2)]) #H
            qmax = torch.argmax(qvals,dim=0).detach().item() #H
            action = int(qmax)
            grid_[j] = action #I
            reward = get_reward(state_.detach(),action)
            with torch.no_grad(): #J
                target = qvals.clone()
                target[action] = reward
            loss = torch.sum(torch.pow(qvals - target,2))
            losses[j].append(loss.detach().numpy())
            loss.backward()
            with torch.no_grad(): #K

```

```

    params[j] = params[j] - lr * params[j].grad
    params[j].requires_grad = True
    with torch.no_grad(): #L
        grid.data = grid_.data

#A Learning rate
#B Since we're dealing with multiple agents, each controlled by a separate Q-function, we have to keep track of
    multiple losses
#C Iterate through each agent
#D Get the left neighbor, if at the beginning, loop to end
#E Get the right neighbor, if at the end, loop to beginning
#F The state_ is the two binary digits representing the spins of the left and right neighbors
#G The state_ is a vector of two binary digits representing actions of two agents, turn this into a one-hot joint-action
    vector
#H The policy is to just take the action associated with the highest q-value
#I We only take the action in our temporary copy of the grid, `grid_`, and only once all agents have taken actions do we
    copy them into the make `grid`
#J The target value is the Q-value vector with the q-value associated with the action taken replaced with the reward
    observed
#K Manual gradient descent
#L Copy the contents of the temporary `grid_` into the main `grid` vector

```

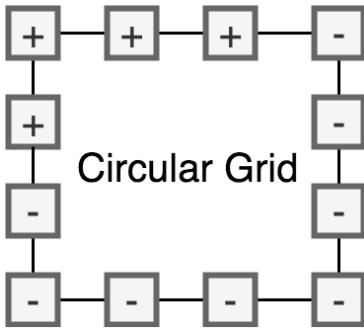


Figure 9.15 While we are representing the 1D Ising model with a single binary vector, it is actually a circular grid because we treat the leftmost electron as being immediately next to the rightmost electron.

In the main training loop, we iterate through all 20 agents (which are representing electrons) and for each one we find its left and right neighbors, get their joint-action vector and use that to compute Q-values for the two possible actions of spin down and spin up. Each agent has its own associated parameter vector that we use to parameterize the Q-function, hence each agent is controlled by a separate Deep Q-network (although it is only a 2 layer neural network, so not really deep). Again, since each agent has the same optimal policy, which is to align the same way as its neighbors, we actually only need to use a single DQN to control them all. We will use this approach in our subsequent projects, but we thought its useful to show how straightforward it is to model each agent separately. In some other environments

where each agent may have differing optimal policies, then you will need to use separate DQNs for each one.

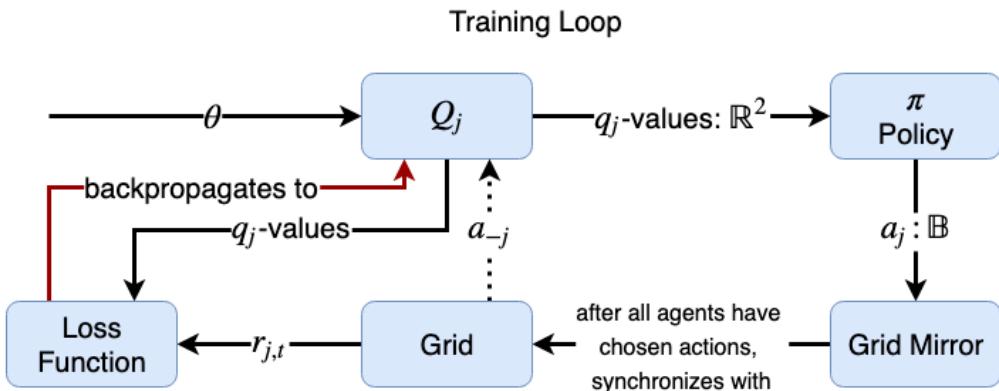


Figure 9.16 This is a string diagram for the main training loop. For each agent j , the corresponding Q-function accepts a parameter vector and the joint-action vector for agent j , denoted a_{-j} . The Q-function outputs a 2-element q-value vector that gets input to the policy function, which chooses an action (a binary digit), which then gets stored in a mirror (clone) of the grid environment. After all agents have chosen actions, the mirrored grid synchronizes with the main grid. The rewards are generated for each agent and passed to the loss function, which computes a loss and backpropagates the loss into the q-function, and ultimately into the parameter vector for updating.

We've simplified this main training function a bit to avoid distractions and it's okay since the problem is so simple. For one, notice that the policy we need is just a greedy policy. The agent takes the action that has the highest Q-value every time, there's no epsilon-greedy where we sometimes take a random action. In general, some sort of exploration strategy is necessary, but this is just such a simple problem that it still works. In the next section, we will solve a 2-dimensional Ising Model on a square grid and in that case we will use a softmax policy where the temperature parameter will model the actual physical temperature of the system of electrons we are trying to model. The other simplification we made is that the target q -value is only set to be r_{t+1} (the reward after taking the action) rather than what it should be, $r_{t+1} + \gamma * V(s_{t+1})$, where the last term is the discount factor gamma times the value of the state after taking the action. The $V(s_{t+1})$ is calculated by just taking the maximum q-value of the subsequent state s_{t+1} . This is the bootstrapping term we learned about in the DQN chapter. We will include this term in the 2D Ising Model later.

If you run the training loop and plot the grid again, you should see something like this:

```
>>> fig,ax = plt.subplots(2,1)
>>> for i in range(size[0]):
...     ax[0].scatter(np.arange(len(losses[i])),losses[i])
...     print(grid,grid.sum())
...     ax[1].imshow(np.expand_dims(grid,0))
```

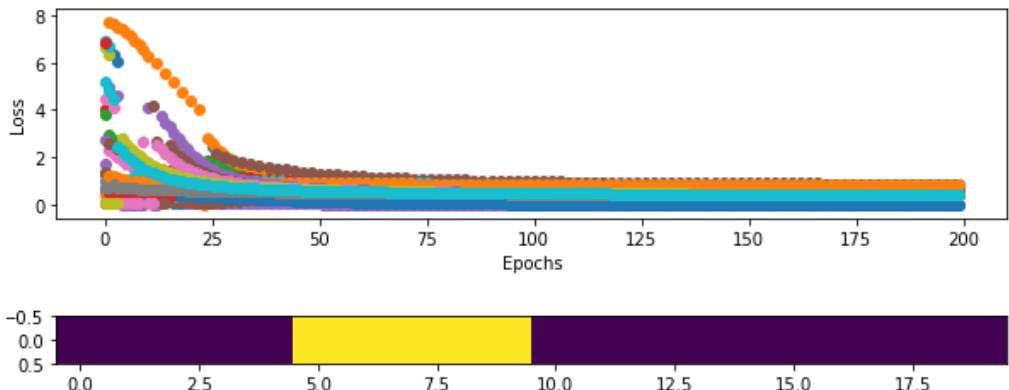


Figure 9.17 Top: Each the losses for each agent over training epochs. You can see they all decrease and are at a minimum after about 30 epochs or so. Bottom: The 1D Ising model after maximizing rewards (minimizing energy). You can see all the electrons are clustered together into domains where they are all oriented the same way.

The first plot is a scatter plot of the losses over each epoch for each agent (each color is a different agent). You can see the losses all fall and plateau around 50 epochs. The bottom plot is our Ising model grid of course, and you can tell it has organized into two domains that are all completely aligned with each other. The lighter part in the middle is a group of agents that are all aligned in the up (1) direction, and the rest are all aligned in the down (0) direction. Much better than the random distribution we started off with, so our MARL algorithm definitely worked in solving this 1D Ising model. Let's add a bit more complexity by moving onto the 2D Ising model. In addition to addressing some of the simplifications we've made, we're also going to introduce a new approach to neighborhood Q-learning called mean field Q-learning.

9.4 Mean Field Q-Learning and the 2D Ising Model

We just saw how a neighborhood Q-learning approach is able to solve the 1D Ising model fairly rapidly. This is because rather than using the full joint-action space that would have been a $2^{20}=1,048,576$ element joint-action vector, which is intractable, we just used each agent's left and right neighbors and that reduced the size down to a $2^2=4$ element joint-action vector, which is very manageable.

In a 2D grid, if we want to do the same thing and just get the joint-action space of an agent's immediate neighbors, then there are 8 neighbors, and thus the joint-action space is a $2^8=256$ element vector. Computing with a 256 element vector is definitely doable, but doing it for say 400 agents in a 20×20 grid is starting to get costly. If we wanted to use a 3D Ising model, then the number of immediate neighbors is 26 and the joint-action space is $2^{26}=67,108,864$ and now we're into intractable territory again.

The point we're trying to make is that the neighborhood approach is much better than using the full joint-action space, but with more complex environments, even the joint-action space of immediate neighbors is too large when the number of neighbors is large. We need to make an even bigger simplifying approximation. Remember, the reason why the neighborhood approach works in the Ising model is because an electron's spin is most affected by the magnetic field of its nearest neighbors. The magnetic field strength decreases proportional to the square of the distance from the field source, so it is definitely reasonable to ignore distant electrons.

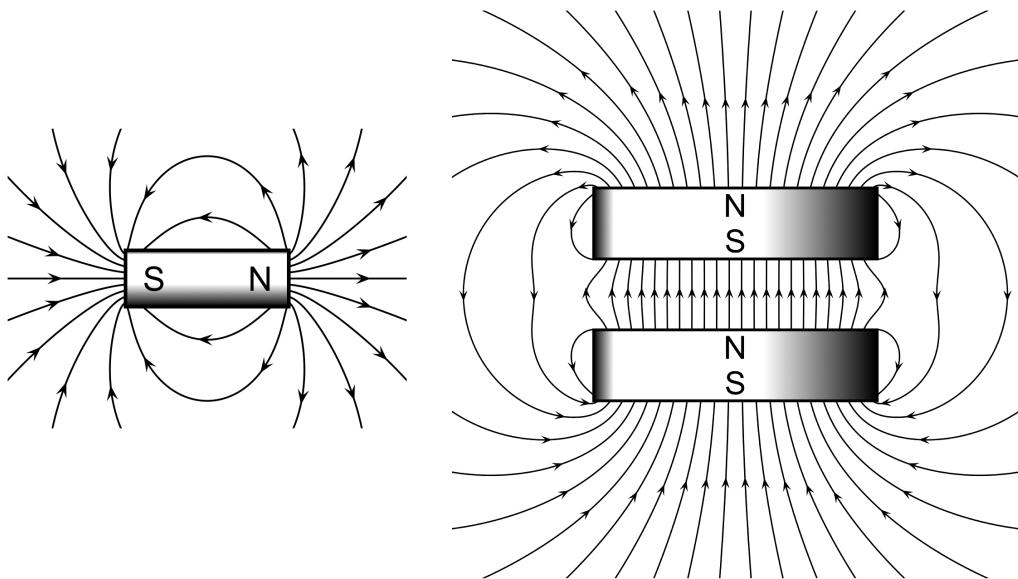


Figure 9.18 Left is a single bar magnetic and its magnetic field lines. Recall a magnet has two magnetic poles, often called North (N) and South (S). Right are two bar magnets put close together and their combined magnetic field is a bit more complicated. When we're modeling how the electron spins behave in a 2D or 3D grid, we care about the overall magnetic field generated by the contributions of all the electrons in a neighborhood; we don't need to know what the magnetic field for each individual electron is.

We can make another approximation by noting that when two magnets are brought together, the resulting field is a kind of sum of these two magnets. We can replace the knowledge of there being two separate magnets with an approximation of there being one magnet and magnetic field that is the sum of the two components. It is not the individual magnetic fields of the nearest neighboring electrons that matter so much as their sum, so rather than giving our Q-function the spin information about each nearest neighboring electron, we can instead just give it the sum of their spins. For example, in the 1D grid, if the left neighbor has an action vector of [1,0] (down) and the right neighbor has an action vector of [0,1] (up) then the sum would be $[1,0] + [0,1] = [1,1]$

Machine learning algorithms perform better when data is normalized within a fixed range like [0,1], partly due to the fact that our activation functions only output data within a limited output range (the codomain) and can be “saturated” by inputs that are too large or too small. For example, the `tanh` function has a codomain (the range of values that it can possibly output) in the interval [-1,+1], so if you give it two really large but non-equal numbers it will output numbers very close to 1, and since computers have limited precision they both might end up rounding to 1 despite being different inputs. If we had normalized these inputs to be within [-1,1] for example, then `tanh` might return 0.5 for one input and 0.6 for the other, a meaningful difference.

So rather than just giving the sum of the individual action vectors to our Q-function, we will give the sum divided by the total value of all the elements, which will normalize the elements in the resulting vector to be between [0,1]. For example, we will compute $[1,0]+[0,1]=[1,1]/2=[0.5,0.5]$. This normalized vector will sum to 1 and each element will be between [0,1], so what does that remind you of? A probability distribution. We will in essence compute a probability distribution over the actions of the nearest neighbors and give that vector to our Q-function.

COMPUTING THE MEAN FIELD ACTION VECTOR

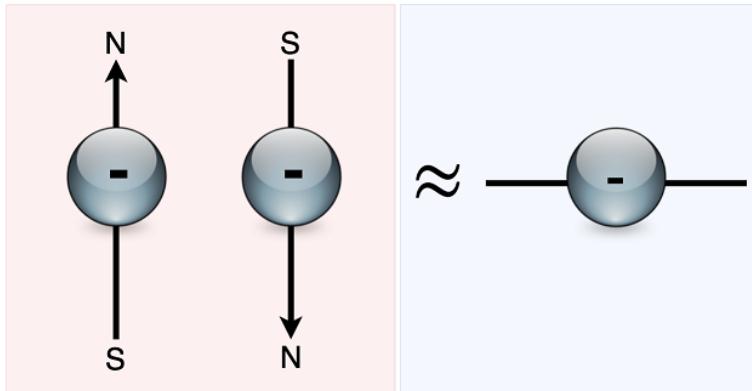
In general, we compute the mean field action vector with the formula:

$$a_{-j} = \frac{1}{N} \sum_{i=0}^N a_i$$

Where a_{-j} is just notation for the mean field of the neighboring agents around agent j , and a_i refers to the action vector for agent i , which is one of agent j 's neighbors. So we sum all the action vectors in the neighborhood of size N for agent j and then divide by the size of the neighborhood to normalize. If the math doesn't suit you, we will see how this works in Python soon.

This approach is called a **mean field approximation**, or in our case, **mean field Q-learning (MF-Q)**. The idea is that we compute a kind of average magnetic field around each electron rather than supplying all the individual magnetic fields of each neighbor. The great thing about this approach is that the mean field vector is only as long as an individual action vector no matter how big our neighborhood size is or how many total agents we have.

Mean Field Approximation



$$[0, 1] \otimes [1, 0] \approx [0.5, 0.5]$$

Figure 9.19 The joint-action for a pair of electron spins is the outer product between their individual action vectors, which is a 4 element one-hot vector. Rather than using this exact joint-action, we can approximate it by taking the average of these two action vectors, resulting in what's called the mean field approximation. For two electrons together with one spin up and the other spin down, the mean field approximation results in reducing this two electron system into a single "virtual" electron with an indeterminate spin of [0.5,0.5].

This means that our mean field vector for each agent will only be a 2 element vector for the 1D Ising model and the 2D Ising model and for higher dimensional Ising models. This means our environment can be arbitrarily complex and high-dimensional and it will still be computationally easy. Let's see how mean field Q-learning (MF-Q) works on the 2D Ising model. The 2D Ising model is exactly the same as the 1D version except now it's a 2D grid (i.e. a matrix). The agent in the top left corner will have its left neighbor be the agent in the top right corner, and its neighbor above will be the agent in the bottom left corner, so the grid is actually a grid wrapped around the surface of a sphere.



Figure 9.20 We represent the 2D Ising model as a 2D square grid (i.e. a matrix), however, we actually design it so that there are no boundaries and the agents that appear on a boundary are actually immediately adjacent to the agents on the opposite side of the grid, thus the 2D grid is really a 2D grid wrapped around the surface of a sphere.

Listing 9.9 Mean Field Q-learning

```
from collections import deque #A
from random import shuffle #B

def softmax_policy(qvals,temp=0.9): #C
    soft = torch.exp(qvals/temp) / torch.sum(torch.exp(qvals/temp)) #D
    action = torch.multinomial(soft,1) #E
    return action

#A We will use the deque data structure as an experience replay storage list since it can be set to have a maximum size.
#B We will use the `shuffle` function to shuffle the experience replay buffer
#C This function will be the policy function that takes in a q-value vector and returns an action, either 0 (down) or 1 (up)
#D This is the softmax function definition
#E The softmax function converts the q-values into a probability distribution over the actions. We use the multinomial function to randomly select an action weighted by the probabilities.
```

The first new function we're going to use for the 2D Ising model is the softmax function. We saw this before in the N-armed bandit chapter when we were introducing the idea of a policy function. A policy function is a function $\pi:s \rightarrow A$, from the space of states to the space of actions, or in other words, you give it a state vector and it returns an action to take. In the policy gradients chapter, we used a neural network as a policy function and directly trained it to output the best actions. In Q-learning, we have this intermediate step of first computing action-values (Q-values) for a given state, and then we use those action-values to decide which action to take. So in Q-learning, the policy function takes in Q-values and returns an action.

SOFTMAX FUNCTION

$$P_t(a) = \frac{\exp(q_t(a)/\tau)}{\sum_{i=1}^n \exp(q_t(i)/\tau)}$$

Where $P_t(a)$ is the probability distribution over actions, $q_t(a)$ is a Q-value vector, and τ is the temperature parameter.

As a reminder, the softmax function takes in a vector with arbitrary numbers and then “normalizes” this vector to be a probability distribution so that all the elements are positive and sum to 1 and each element after the transformation is proportional to the element before the transformation (i.e. if an element was the largest in the vector, it will be assigned the largest probability). The softmax function has one additional input, the temperature parameter, denoted with the Greek symbol tau τ .

If the temperature parameter is large, then it will minimize the difference in probabilities between the elements, and if the temperature is small, then differences in the input will be magnified. For example, the vector `softmax([10,5,90], temp=100)` = [0.2394, 0.2277, 0.5328] and `softmax([10,5,90], temp=0.1)` = [0.0616, 0.0521, 0.8863]. With high temperature, even though the last element 90 is 9 times larger than the second largest element 10, the resulting probability distribution assigns it a probability of 0.53 which is only about twice as big as the second largest probability. When the temperature approaches infinity, then the probability distribution will be uniform (i.e. all probabilities are equal). When the temperature approaches 0, the probability distribution will become a **degenerate distribution** where all the probability mass is at a single point. So by using this as a policy function, with $\tau \rightarrow \infty$ actions will be selected completely randomly and with $\tau \rightarrow 0$ then the policy becomes the argmax function (that we used in the previous section with the 1D Ising model).

The reason this parameter is called “temperature” is because the softmax function is also used in physics to model physical systems like the spins of a system of electrons where the temperature changes the behavior of the system. There’s a lot of cross-pollination between physics and machine learning. In physics it’s called the Boltzmann distribution where it “gives the probability that a system will be in a certain state as a function of that state’s energy and the temperature of the system” (Wikipedia). In some reinforcement learning academic papers you might see the softmax policy under the name Boltzmann policy, but now you know it’s the same thing.

We are using a reinforcement learning algorithm to solve a physics problem, so the temperature parameter of the softmax function actually corresponds to the temperature of the electron system we are modeling. If we set the temperature of the system to be very high, then the electrons will spin randomly and their tendency to align to neighbors will be overcome by the high temperature. If we set the temperature too low then the electrons will be stuck and won’t be able to change much.

Listing 9.10 Mean Field Q-learning

```

def get_coords(grid,j): #A
    x = int(np.floor(j / grid.shape[0])) #B
    y = int(j - x * grid.shape[0]) #C
    return x,y

def get_reward_2d(action,action_mean): #D
    r = (action*(action_mean-action/2)).sum()/action.sum() #E
    return torch.tanh(5 * r) #F

#A This function takes a single index value from the flattened grid and converts it back into [x,y] coordinates
#B Find x coordinate
#C Find y coordinate
#D This is the reward function for the 2D grid
#E The reward is based on how different the action is to the mean field action
#F Scale the reward to be between [-1,+1] using the tanh function

```

It is inconvenient to work with $[x,y]$ coordinates to refer to agents in the 2D grid, so we generally refer to agents using a single index value based on flattening the 2D grid into a vector, but we need to be able to convert this flat index into $[x,y]$ coordinates and that is what the `get_coords` function does. The `get_reward_2d` function is our new reward function for the 2D grid. It computes the difference between an action vector and a mean field vector. For example if the mean field vector is $[0.25, 0.75]$ and the action vector is $[1, 0]$ then the reward should be lower than if the action vector is $[0, 1]$.

```

>>> get_reward_2d(torch.Tensor([1,0]),torch.Tensor([0.25, 0.75]))
tensor(-0.8483)

>>> get_reward_2d(torch.Tensor([0,1]),torch.Tensor([0.25, 0.75]))
tensor(0.8483)

```

Now we need to make the function that will find an agent's nearest neighbors and then computes the mean field vector for these neighbors.

Listing 9.11 Mean Field Q-learning

```

def mean_action(grid,j):
    x,y = get_coords(grid,j) #A
    action_mean = torch.zeros(2) #B
    for i in [-1,0,1]: #C
        for k in [-1,0,1]:
            if i == k == 0:
                continue
            x_,y_ = x + i, y + k
            x_ = x_ if x_ >= 0 else grid.shape[0] - 1
            y_ = y_ if y_ >= 0 else grid.shape[1] - 1
            x_ = x_ if x_ < grid.shape[0] else 0
            y_ = y_ if y_ < grid.shape[1] else 0
            cur_n = grid[x_,y_]
            s = get_substate(cur_n) #D
            action_mean += s
    action_mean /= action_mean.sum() #E
    return action_mean

```

```
#A Convert vectorized index j into grid coordinates [x,y], where [0,0] is top left
#B This will be the action mean vector that we will add to
#C These two for loops allow us to find each of the 8 nearest neighbors of agent `j`
#D Convert each neighbor's binary spin into an action vector
#E Normalize the action vector to be a probability distribution
```

This function accepts an agent index `j` (a single integer, the index based on the flattened grid) and returns that agent's 8 nearest (surrounding) neighbor's mean action on the grid. We find the 8 nearest neighbors by getting the agent's coordinates, for example [5,5] and then we just add every combination of [x,y] where $x,y \in \{0,1\}$. So we'll do [5,5] + [1,0] = [6,5] and [5,5] + [-1,1] = [4,6] etcetera.

These are all the additional functions we need for the 2D case. We'll re-use the `init_grid` function and `gen_params` functions from earlier. Let's initialize the grid and parameters.

```
>>> size = (10,10)
>>> J = np.prod(size)
>>> hid_layer = 10
>>> layers = [(2,hid_layer),(hid_layer,2)]
>>> params = gen_params(1,2*hid_layer+hid_layer*2)
>>> grid = init_grid(size=size)
>>> grid_ = grid.clone()
>>> grid__ = grid_.clone()
>>> plt.imshow(grid)
>>> print(grid.sum())
```

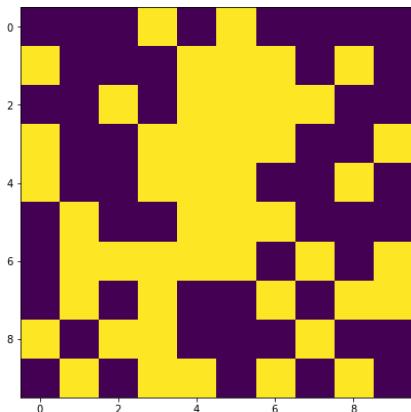


Figure 9.21 This is a randomly initialized 2D Ising model. Each grid square represents an electron. The light-colored grid squares represent electrons oriented with spin “up” and the dark squares are spin “down.”

We're starting with a 10x10 grid to make it run faster, but you should try playing with larger grid sizes. You can see the spins are randomly distributed on the initial grid, so we hope that after we run our MARL algorithm it will look a lot more organized, i.e. we hope to see clusters

of aligned electrons. We've reduced the hidden layer size to 10 to further reduce the computational cost. Notice we're only generating a single parameter vector, and hence we're going to be using a single DQN to control all of the 100 agents since they have the same optimal policy. We're creating 2 copies of the main `grid` for reasons that will be clear once we get to the training loop.

For this example, we are going to be adding some of the complexities we left out in the 1D case since this is a harder problem. We will be using an experience replay mechanism to store experiences and train on minibatches of these experiences. This reduces the variance in the gradients and stabilizes the training. We will also use the proper target q -values: $r_{t+1} + \gamma * V(s_{t+1})$, so we need to calculate q -values twice per iteration, once to decide which action to take and then again to get $V(s_{t+1})$.

Listing 9.11 Mean Field Q-learning

```

epochs = 75
lr = 0.0001
num_iter = 3 #A
losses = [ [] for i in range(size[0])] #B
replay_size = 50 #C
replay = deque(maxlen=replay_size) #D
batch_size = 10 #E
gamma = 0.9 #F
losses = [[] for i in range(J)]

for i in range(epochs):
    act_means = torch.zeros((J,2)) #G
    q_next = torch.zeros(J) #H
    for m in range(num_iter): #I
        for j in range(J): #J
            action_mean = mean_action(grid_,j).detach()
            act_means[j] = action_mean.clone()
            qvals = qfunc(action_mean.detach(),params[0],layers=layers)
            action = softmax_policy(qvals.detach(),temp=0.5)
            grid_[get_coords(grid_,j)] = action
            q_next[j] = torch.max(qvals).detach()
        grid_.data = grid_.data
    grid.data = grid_.data
    actions = torch.stack([get_substate(a.item()) for a in grid.flatten()])
    rewards = torch.stack([get_reward_2d(actions[j],act_means[j]) for j in range(J)])
    exp = (actions,rewards,act_means,q_next) #K
    replay.append(exp)
    shuffle(replay)
    if len(replay) > batch_size: #L
        ids = np.random.randint(low=0,high=len(replay),size=batch_size) #M
        exps = [replay[idx] for idx in ids]
        for j in range(J):
            jacts = torch.stack([ex[0][j] for ex in exps]).detach()
            jrewards = torch.stack([ex[1][j] for ex in exps]).detach()
            jmeans = torch.stack([ex[2][j] for ex in exps]).detach()
            vs = torch.stack([ex[3][j] for ex in exps]).detach()
            qvals = torch.stack([ qfunc(jmeans[h].detach(),params[0],layers=layers) \
                for h in range(batch_size)])
            target = qvals.clone().detach()

```

```

target[:,torch.argmax(jacts,dim=1)] = jrewards + gamma * vs
loss = torch.sum(torch.pow(qvals - target.detach(),2))
losses[j].append(loss.item())
loss.backward()
with torch.no_grad():
    params[0] = params[0] - lr * params[0].grad
params[0].requires_grad = True

```

```

#A `num_iter` controls how many times we iterate to get rid of the initial randomness from the mean field actions
#B Make a list of lists to store the losses for each agent
#C The `replay_size` controls the total number of experiences we store in the experience replay list
#D The experience replay is a deque collection, which is basically a list with a maximum size
#E We set the batch size to 10, so we get a random subset of 10 experiences from the replay and train with that
#F Discount factor
#G This stores the mean field actions for all the agents
#H This stores the q-values for the next state after taking an action
#I Since mean fields are initialized randomly, we need to iterate a few times to dilute the initial randomness
#J Iterate through all agents in the grid
#K Collect an experience and add to the experience replay buffer
#L Once the experience replay buffer has more experiences than our batch size parameter, start training
#M Generate a list of random indices to subset the replay buffer

```

That's a lot of code but it's only a little more complicated than what we had for the 1D Ising model. The first thing to point out is that since the mean fields of each agent depends on its neighbors and the neighbors spins are randomly initialized then all the mean fields will be random to begin with too. To help convergence, we first allow each agent to select an action based on these random mean fields and store the action in the temporary grid copy `grid__` so that the main grid doesn't change until all agents have made a final decision about which action to take. After each agent has made a tentative action in `grid__`, we update the second temporary grid copy `grid_` which is what we're using to calculate the mean fields. So in the next iteration the mean fields will change, and we allow the agents to update their tentative actions. We do this a few times (controlled by the `num_iter` parameter) to allow the actions to stabilize around a near optimal value based on the current version of the Q-function. Then we update the main `grid` and collect all the actions, rewards, mean fields, and `q_next` values ($V(s_{t+1})$) and add it to the experience replay buffer.

Once the replay buffer has more experiences than our batch size parameter, we can begin training on minibatches of experiences in the replay buffer. We generate a list of random index values and then use these to subset some random experiences in the replay buffer. Then we run one step of gradient descent as usual. Let's run the training loop and see what we get.

```

>>> fig,ax = plt.subplots(2,1)
>>> ax[0].plot(np.array(losses).mean(axis=0))
>>> ax[1].imshow(grid)

```

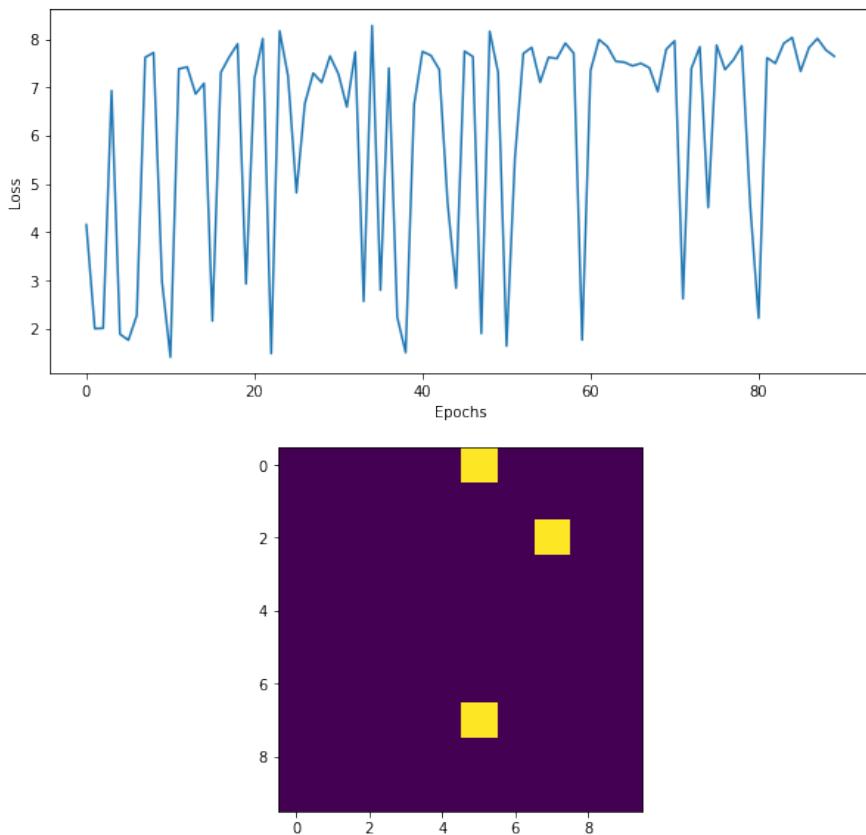


Figure c.: Top: Loss plot for the DQN. The loss doesn't look like it is converging, but we can see that is does indeed learn to minimize the energy of the system (maximize reward) as a whole in the bottom panel.

It worked! All but 3 of the electrons (agents) have their spins aligned in the same direction, which minimizes the energy of the system (and maximizes the reward). The loss plot looks chaotic partly because we're using a single DQN now to model each agent and so the DQN is sort of in a battle against itself when one agent is trying to align to its neighbor but its neighbor is trying to align to another agent so some instability happen.

In the last section we will push our multi-agent reinforcement learning skills to the next level by tackling a harder problem with two teams of agents battling against each other in a game.

9.5 Mixed Cooperative-Competitive Games

If you think of the Ising Model as a multiplayer game then it would be considered a pure cooperative multi-player game since all the agents have the same objective and their reward is maximized when they work together to all align in the same direction. We can imagine a pure competitive game like Chess where when one player is winning then the other player is losing, that is, it is zero-sum. Team based games like a game of basketball or football are called mixed cooperative-competitive games since the agents on the same team need to cooperate in order to maximize their rewards, but when the team as a whole is winning then the other team must be losing so at the team-to-team level it is a competitive game.

In this section we are going to use an open source Gridworld-based game that is specially designed for testing multi-agent reinforcement learning algorithms in cooperative, competitive or mixed cooperative-competitive scenarios. In our case we will setup a mixed cooperative-competitive scenario with two teams of Gridworld agents that can move around in the grid and can also attack other agents on the opposing team. Each agent starts with 1 "health point" (HP) and when being attacked the HP decreases little-by-little until it gets to 0 and then the agent dies and is cleared off the grid. Agents get rewards for attacking and killing agents on the opposing team.

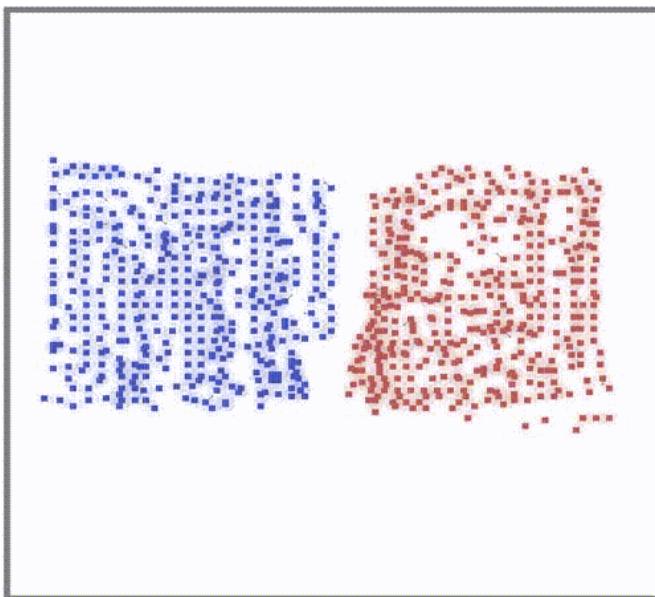


Figure 9.23 Screenshot from the MAgent multi-player Gridworld game with two opposing teams of Gridworld agents. The objective is for each team to kill the other.

Since all the agents on one team shared the same objective and hence optimal policy we can use a single DQN to control all the agents on one team, and a different DQN to control the agents on the other team. It's basically a battle between two DQNs so this is a perfect opportunity to try out different kinds of neural networks and see which is better, but to keep things simple we'll just use the same DQN for each team.

You'll need to go install the MAgent library from <https://github.com/geek-ai/MAgent> by following the instructions on the readme page. From this point we'll assume you have it installed and you can successfully run `import magent` in your Python environment.

Listing 9.12 Creating the MAgent environment

```
import magent
import math
from scipy.spatial.distance import cityblock #A

map_size = 30
env = magent.GridWorld("battle", map_size=map_size) #B
env.set_render_dir("MAgent/build/render") #C

team1, team2 = env.get_handles() #D
```

#A We import the cityblock distance function from scipy to compute distances between agents on the grid

#B Setup the environment in "battle" mode with a 30x30 grid

#C This sets up our ability to view the game after training

#D Initialize the two team objects

MAgent is highly customizable but we will be using the built-in configuration called "battle" to setup a two-team battle scenario. MAgent has an API similar to OpenAI Gym but there are some important differences. First, we have to setup "handles" for each of the two teams. These are objects `team1` and `team2` that have methods and attributes relevant to each team. We generally pass these handles to a method of the environment object `env`. For example, to get a list of the coordinates of each agent on team 1 we use `env.get_pos(team1)`.

We're going to use the same technique to solve this environment as we did for the 2D Ising Model except with 2 DQNs. We'll use a softmax policy and experience replay buffer. Things get a bit complicated because the number of agents changes over training since agents can die and get removed from the grid. With the Ising Model, the state of the environment was the joint-actions, there was no additional state information.

In MAgent we additionally have the positions and health points of agents as state information. So the Q-function will be $Q_j(s_t, a_{-j})$ where a_{-j} is the mean field for the agents within agent j 's field of view (FOV) or neighborhood. By default, each agent has a FOV of the 13×13 grid around itself. Thus each agent will have a state of this binary 13×13 FOV grid that shows a 1 where there are other agents. However, MAgent separates the FOV matrix by teams, so each agent has two 13×13 FOV grids one for its own team and one for the other team hence we will need to combine these into a single state vector by flattening and

concatenating them together. MAgent also provides the health points of the agents in the FOV but for simplicity we will not use these.

We've initialized the environment but we haven't initialized the agents on the grid. We have to decide how many agents and where to place them on the grid for each team.

Listing 9.13 Adding the agents

```
hid_layer = 25
in_size = 359
act_space = 21
layers = [(in_size,hid_layer),(hid_layer,act_space)]
params = gen_params(2,in_size*hid_layer+hid_layer*act_space) #A
map_size = 30
width = height = map_size
n1 = n2 = 16 #B
gap = 1 #C
epochs = 100
replay_size = 70
batch_size = 25

side1 = int(math.sqrt(n1)) * 2
pos1 = []
for x in range(width//2 - gap - side1, width//2 - gap - side1 + side1, 2): #D
    for y in range((height - side1)//2, (height - side1)//2 + side1, 2):
        pos1.append([x, y, 0])

side2 = int(math.sqrt(n2)) * 2
pos2 = []
for x in range(width//2 + gap, width//2 + gap + side2, 2): #E
    for y in range((height - side2)//2, (height - side2)//2 + side2, 2):
        pos2.append([x, y, 0])

env.reset()
env.add_agents(team1, method="custom", pos=pos1) #F
env.add_agents(team2, method="custom", pos=pos2)
```

```
#A Generate two parameter vectors to parameterize two DQNs
#B Set the number of agents for each team to 20
#C Set the initial gap distance between each team's agents
#D Loop to position agents on team 1 on the left side of the grid
#E Loop to position agents on team 2 on the right side of the grid
#F Add the agents to the grid for team 1 using the position lists we just created
```

Here we've just setup our basic parameters as we did before. We're creating a 30x30 grid with 16 agents for each team to keep the computational cost low, but if you have a GPU, feel free to make a bigger grid with more agents. We initialize two parameter vectors, one for each team. Again we're only using a simple two-layer neural network as the DQN. We can now visualize the grid.

```
>>> plt.imshow(env.get_global_minimap(30,30)[::,:,:,].sum(axis=2))
```

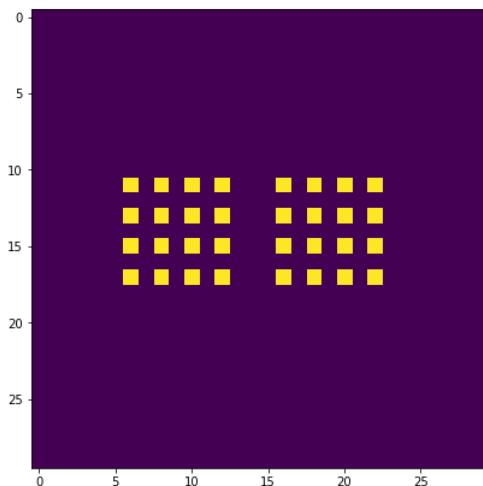


Figure 9.24 The starting positions for two teams of agents in the MAgent environment. The light squares are the individual agents.

Team 2 is on the left and team 1 on the right. All the agents are initialized in a square pattern and the teams are separated by just one grid square. Each agent's action-space is a 21 length vector, depicted here:

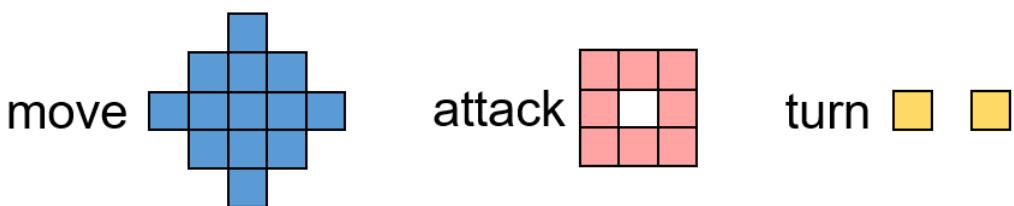


Figure 9.25 This depicts the action-space for agents in the MAgent library. Each agent can move in 13 different directions or attack in 8 directions immediately around it. The turn actions are disabled by default, so the action-space is $13 + 8 = 21$.

Listing 9.14 Finding the neighbors

```
def get_neighbors(j, pos_list, r=6): #A
    neighbors = []
    pos_j = pos_list[j]
    for i, pos in enumerate(pos_list):
        if i == j:
            continue
        dist = cityblock(pos, pos_j)
        if dist < r:
            neighbors.append(i)
    return neighbors
```

```
#A Given [x,y] positions of all agents in `pos_list`, return indices of agents that are within the radius of agent j
```

We need this function to find the neighbors in the FOV of each agent. We can use `env.get_pos(team1)` to get a list of coordinates for each agent on team 1, and then we can pass this into the `get_neighbors` function along with an index `j` to find the neighbors of agent `j`.

```
>>> get_neighbors(5,env.get_pos(team1))
[0, 1, 2, 4, 6, 7, 8, 9, 10, 13]
```

So agent `5` has 10 other agents on team 1 within its 13x13 FOV. We need to create a few other helper functions. The actions that the environment accepts and returns are integers 0 to 20 so we need to be able to convert this to a one-hot action-vector and back to integer form. We also need the function that will get the mean field vector for the neighbors around an agent.

Listing 9.15 Calculating the mean field action

```
def get_onehot(a,l=21): #A
    x = torch.zeros(21)
    x[a] = 1
    return x

def get_scalar(v): #B
    return torch.argmax(v)

def get_mean_field(j,pos_list,act_list,r=7,l=21): #C
    neighbors = get_neighbors(j,pos_list,r=r) #D
    mean_field = torch.zeros(l)
    for k in neighbors:
        act_ = act_list[k]
        act = get_onehot(act_)
        mean_field += act
    tot = mean_field.sum()
    mean_field = mean_field / tot if tot > 0 else mean_field #E
    return mean_field

#A Convert integer representation of action into one-hot vector representation
#B Convert one-hot vector action into integer representation
#C Get's the mean field action of agent `j`, `pos_list` is what is returned by `env.get_pos(team1)`, and `l` is action space dimension
#D This finds all the neighbors of the agents using `pos_list`
#E Need to make sure we don't divide by zero
```

The `get_mean_field` function uses the `get_neighbors` function to get the coordinates of all the agents for agent `j` and then gets their action vectors, adds them and divides by the total. The `get_mean_field` function expects the corresponding action vector `act_list` (a list of integer-based actions) where indices in `pos_list` and `act_list` match to the same agent.

The parameter `r` refers to the radius in grid squares around agent `j` we want to include as neighbors and `l` is the size of the action space which is 21.

Unlike the Ising model examples, we're going to create separate functions to select actions for each agent and to do training since this is a more complex environment and we want to modularize a bit more. After each step in the environment, we get an observation tensor for all the agents simultaneously:

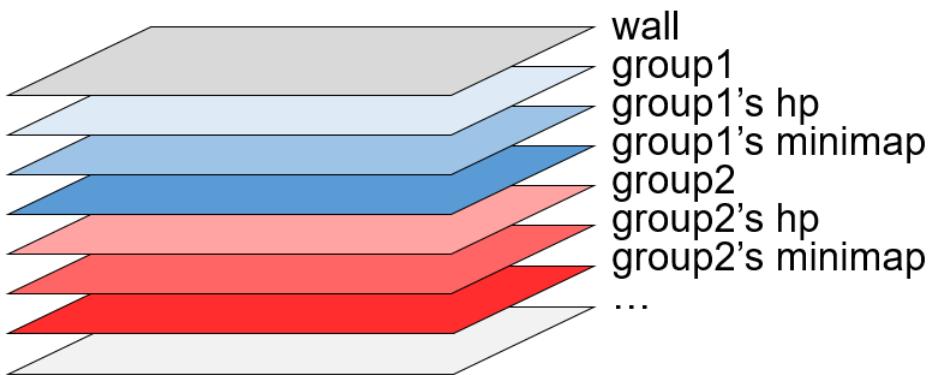


Figure 9.26 This shows the structure of the observation tensor. It is a $N \times 13 \times 13 \times 7$ tensor where N is the number of agents on the team.

The observation returned by `env.get_observation(team1)` is actually a tuple with two tensors. The first tensor is shown in the top portion of the figure above. It is a complex high-order tensor whereas the second tensor in the tuple has some additional information that we will ignore, so from now own when we say observation or state we mean the first tensor.

The observation is an $N \times 13 \times 13 \times 7$ tensor where N is the number of agents, in our case 16. Each 13×13 slice of the tensor for a single agent shows the FOV with the location of the wall (slice 0), team 1 agents (slice 1), team 1 agents' HPs (slice 2) and so forth. We will only be using slices 1 and 4 for the location of the agents on team 1 and team 2 within the FOV. So for a single agent, its observation tensor will be $13 \times 13 \times 2$, and we will flatten this into a vector to get a 338 length state vector. We then concatenate this state vector with the mean field vector that is length 21 to get a $338 + 21 = 359$ length vector that will be given to the Q-function. It would be ideal if we used a two-headed neural network like we did in the curiosity-based learning chapter. That way one head could process the state vector and the other head could process the mean field action vector and then recombine the processed information in a later layer. We did not do that here for simplicity but is a good exercise for you to try.

Listing 9.16 Choosing actions

```
def infer_acts(obs, param, layers, pos_list, acts, act_space=21, num_iter=5, temp=0.5):
```

```

N = acts.shape[0] #A
mean_fields = torch.zeros(N,act_space)
acts_ = acts.clone() #B
qvals = torch.zeros(N,act_space)

for i in range(num_iter): #C
    for j in range(N): #D
        mean_fields[j] = get_mean_field(j, pos_list, acts_)

    for j in range(N): #E
        state = torch.cat((obs[j].flatten(), mean_fields[j]))
        qs = qfunc(state.detach(), param, layers=layers)
        qvals[j,:] = qs[:,]
        acts_[j] = softmax_policy(qs.detach(), temp=temp)
return acts_, mean_fields, qvals

```

#A Get the number of agents

#B Clone the action vector to avoid changing in place

#C Alternate a few times to converge on action

#D Loop through the agents and compute their neighborhood mean field action vectors

#E Use the mean field actions and state to compute Q-values and select actions using a softmax policy

#F Randomly initialize the mean field vectors

This is the function we will use to decide all the actions for each agent after we get an observation. It utilizes a mean field Q-function parameterized by `param` and `layers` to sample actions for all agents using softmax policy.

PARAMETERS FOR THE `INFER_ACTS` FUNCTION

```

`obs` is observation tensor N x 13 x 13 x 2
`mean_fields` is tensor containing all mean field actions for each agent N x
21
`pos_list` is list of positions for each agent returned by `env.get_pos(...)`
`acts` is vector of integer-represented actions of each agent (N,)
`num_iter` is number of times to alternate between action sampling and
policy updates
`temp` is softmax policy temperature to control exploration rate
The function returns a tuple:
    acts_: (N,) vector of integer actions sampled from policy
    mean_fields_: (N,21) tensor of mean field vectors for each agent
    qvals: (N,21) tensor of q values for each action for each agent

```

Lastly, we need the function for training. We will give this function our parameter vector and experience replay buffer and let it do the minibatch stochastic gradient descent.

Listing 9.17 The Training Function

```
def train(batch_size,replay,param,layers,J=64,gamma=0.5,lr=0.001):
```

```

ids = np.random.randint(low=0,high=len(replay),size=batch_size) #A
exps = [replay[idx] for idx in ids] #B
losses = []
jobs = torch.stack([ex[0] for ex in exps]).detach() #C
jacts = torch.stack([ex[1] for ex in exps]).detach() #D
jrewards = torch.stack([ex[2] for ex in exps]).detach() #E
jmeans = torch.stack([ex[3] for ex in exps]).detach() #F
vs = torch.stack([ex[4] for ex in exps]).detach() #G
qs = []
for h in range(batch_size): #H
    state = torch.cat((jobs[h].flatten(),jmeans[h]))
    qs.append(qfunc(state.detach(),param,layers=layers)) #I
qvals = torch.stack(qs)
target = qvals.clone().detach()
target[:,jacts] = jrewards + gamma * torch.max(vs,dim=1)[0] #J
loss = torch.sum(torch.pow(qvals - target.detach(),2))
losses.append(loss.detach().item())
loss.backward()
with torch.no_grad(): #K
    param = param - lr * param.grad
param.requires_grad = True
return np.array(losses).mean()

```

#A Generate a random list of indices to subset the experience replay
#B Subset the experience replay buffer to get a minibatch of data
#C Collect all states from minibatch into single tensor
#D Collect all actions from minibatch into single tensor
#E Collect all rewards from minibatch into single tensor
#F Collect all mean field actions from minibatch into a single tensor
#G Collect all state-values from minibatch into a single tensor
#H Loop through each experience in the minibatch
#I Compute Q-values for each experience in the replay
#J Compute the target Q-values
#K Stochastic gradient descent

This function works pretty much the same way we did experience replay with the 2D Ising Model except the state information is more complicated.

PARAMETERS FOR THE TRAIN FUNCTION

The train function trains a single neural network using stored experiences in an experience replay memory buffer.

Inputs:

```

`batch_size`, int
`replay`, list of tuples (obs_1_small, acts_1,rewards1,act_means1,qnext1)
`param`, vector, neural network parameter vector
`layers`, list, contains shape of neural network layers,
`J`, int, number of agents on this team
`gamma`, float in [0,1], discount factor
`lr`, float, learning rate for SGD

```

Returns

```
`loss` (float)
```

Okay so at this point we've setup the environment, setup the agents for the two teams and defined several functions to ultimately let us train the two DQNs we're using for mean field Q-learning. Now we get into the main loop of game play. Be warned, this is a lot of code but most of it is just boilerplate and isn't critical for understanding the overall algorithm. Let's first setup our preliminary data structures like the replay buffers. We will need separate replay buffers for team 1 and team 2. In fact, we will need separate everything for team 1 and team 2 almost.

Listing 9.18 Initializing the actions

```
N1 = env.get_num(team1) #A
N2 = env.get_num(team2)
step_ct = 0
acts_1 = torch.randint(low=0,high=act_space,size=(N1,)) #B
acts_2 = torch.randint(low=0,high=act_space,size=(N2,))

replay1 = deque(maxlen=replay_size) #C
replay2 = deque(maxlen=replay_size)

qnext1 = torch.zeros(N1) #D
qnext2 = torch.zeros(N2)

act_means1 = init_mean_field(N1,act_space) #E
act_means2 = init_mean_field(N2,act_space)

rewards1 = torch.zeros(N1) #F
rewards2 = torch.zeros(N2)

losses1 = []
losses2 = []
```

```
#A Store the number of agents on each team
#B Initialize the actions for all the agents
#C Create replay buffer use deque data structure
#D Create tensors to store the Q(s') values
#E Initialize the mean fields for each agent
#F Create tensors to store the rewards for each agent
```

We need to keep track of the actions (integers), mean field action vectors, rewards, and next state q-values for each agent so that we can package these into experiences and add them into the experience replay system.

Listing 9.19 Taking a team step and adding to the replay

```
def team_step(team,param,acts,layers):
    obs = env.get_observation(team) #A
    ids = env.get_agent_id(team) #B
    obs_small = torch.from_numpy(obs[0][:,:,:,[1,4]]) #C
    agent_pos = env.get_pos(team) #D
    acts, act_means, qvals = infer_acts(obs_small,\n                                         param,layers,agent_pos,acts) #E
    return acts, act_means, qvals, obs_small, ids
```

```

def add_to_replay(replay,obs_small, acts,rewards,act_means,qnext): #F
    for j in range(rewards.shape[0]): #G
        exp = (obs_small[j], acts[j],rewards[j],act_means[j],qnext[j])
        replay.append(exp)

    return replay

#A Get observation tensor from team 1, which is a 16x13x13x7 tensor
#B Get list of indices for the agents that are still alive
#C Subset the observation tensor to only get the positions of the agents
#D Get the list of coordinates for each agent on team 1
#E Decide which actions to take using the DQN for each agent
#F Add each individual agent's experience separately to the replay buffer
#G Loop through each agent

```

The `team_step` function is the workhouse of the main loop. We use it to collect all the data from the environment and to run the DQN to decide the actions to take. The `add_to_replay` function takes the observation tensor, action tensor, reward tensor, action mean field tensor, and the next state q-value tensor and adds each individual agent experience to the replay buffer separately. The rest of the code is all within a giant `while` loop so we will break it into parts but just remember it's all part of the same loop. Also remember we have all this code together in Jupyter Notebooks on this book's GitHub at <https://github.com/DeepReinforcementLearning/DeepReinforcementLearningInAction/> and it contains all of the code we use to create the visualizations and more comments.

Listing 9.20 Training loop

```

for i in range(epochs):
    done = False
    while not done: #A
        acts_1, act_means1, qvals1, obs_small_1, ids_1 = \
            team_step(team1,params[0],acts_1,layers) #B
        env.set_action(team1, acts_1.detach().numpy().astype(np.int32)) #C

        acts_2, act_means2, qvals2, obs_small_2, ids_2 = \
            team_step(team2,params[0],acts_2,layers)
        env.set_action(team2, acts_2.detach().numpy().astype(np.int32))

        done = env.step() #D

        _, _, qnext1, _, ids_1 = team_step(team1,params[0],acts_1,layers) #E
        _, _, qnext2, _, ids_2 = team_step(team2,params[0],acts_2,layers)

        env.render() #F

        rewards1 = torch.from_numpy(env.get_reward(team1)).float() #G
        rewards2 = torch.from_numpy(env.get_reward(team2)).float()

```

```

#A While game is not over
#B Use the `team_step` method to collect environment data and choose actions for the agents using the DQN
#C Instantiate the chosen actions in the environment

```

```
#D Take a step in the environment which will generate a new observation and rewards
#E Re-run `team_step` to get the q-values for the next state in the environment
#F Render the environment for viewing later
#G Collect the rewards into a tensor for each agent
```

The `while` loop runs as long as the game is not over which happens when all the agents on one team die. Within the `team_step` function, we first get the observation tensor and subset the part we want as we described before, resulting in a $13 \times 13 \times 2$ tensor. We also get `ids_1` which are the indices for the agents that are still alive on team 1. We also need to get the coordinate positions of each agent on each team. Then we use our `infer_acts` function to choose actions for each agent and instantiate them in the environment, and finally take an environment step which will generate new observations and rewards. Let's continue in the `while` loop.

Listing 9.21 Add to replay (still in while loop from Listing 9.21)

```
replay1 = add_to_replay(replay1, obs_small_1,
    acts_1,rewards1,act_means1,qnext1) #A
    replay2 = add_to_replay(replay2, obs_small_2,
    acts_2,rewards2,act_means2,qnext2)
    shuffle(replay1) #B
    shuffle(replay2)

ids_1_ = list(zip(np.arange(ids_1.shape[0]),ids_1)) #C
ids_2_ = list(zip(np.arange(ids_2.shape[0]),ids_2))

env.clear_dead() #D

ids_1_ = env.get_agent_id(team1) #E
ids_2_ = env.get_agent_id(team2)

ids_1_ = [i for (i,j) in ids_1_ if j in ids_1] #F
ids_2_ = [i for (i,j) in ids_2_ if j in ids_2]

acts_1 = acts_1[ids_1_] #G
acts_2 = acts_2[ids_2_]

step_ct += 1
if step_ct > 250:
    break

if len(replay1) > batch_size and len(replay2) > batch_size: #H
    loss1 = train(batch_size,replay1,params[0],layers=layers,J=N1)
    loss2 = train(batch_size,replay2,params[1],layers=layers,J=N1)
    losses1.append(loss1)
    losses2.append(loss2)
```

```
#A Add to experience replay
#B Shuffle the replay buffer
#C We build a zipped list of ids to keep track of which agents died and will be cleared from the grid
#D Clear the dead agents off the grid
#E Now that the dead agents are cleared, get the new list of agent IDs
#F Subset the old list of ids based on which agents are still alive
```

```
#G Subset the action list based on the agents that are still alive
#H If the replay buffers are sufficiently full, start training
```

In this last part of the code all we do is collect all the data into a tuple and append it to the experience replay buffers for training. The one complexity of MAgent is that the number of agents decreases over time as they die, and so we need to do some housekeeping with our arrays to make sure we're keeping the data matched up with the right agents over time.

If you run the training loop even for just a handful of epochs the agents will already start demonstrating some skill in battle since we made the grid very small and only had 16 agents on each team. Go ahead and view the video of the recorded game by following the instructions here: https://github.com/geek-ai/MAgent/blob/master/doc/get_started.md

You should see the agents charge at each other and a few get killed before the video ends. Here's a screenshot toward the end of our video.

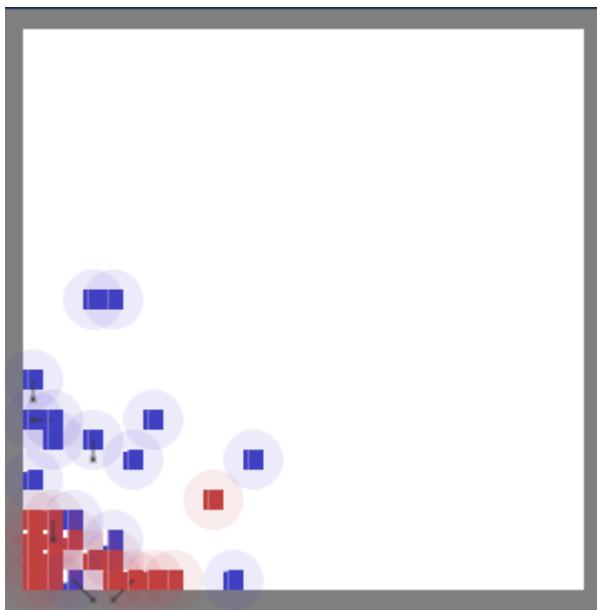


Figure 9.27 Screenshot of the MAgent battle game after training with Mean Field Q-learning. The dark team has forced the light team into the corner and its attacking them.

9.6 Summary

- Ordinary Q-learning does not work well in the multi-agent setting due to the fact that the environment becomes non-stationary from the fact that all the agents are learning new policies
- Non-stationarity of the environment means that the expected value of rewards changes over time

- In order to handle non-stationarity, the Q-function needs to have access to the joint-action space of other agents, however, this joint action-space scales exponentially in the number of agents, which becomes intractable for most practical problems
- Neighborhood Q-learning can mitigate the exponential scaling by only computing over the joint-action space of the immediate neighbors of a given agent, but even this can be too large if the number of neighbors is large
- Mean Field Q-learning (MF-Q) scales linearly in the number of agents because we only compute a mean action rather than a full joint-action space

10

Interpretable Reinforcement Learning: Attention and Relational Models

In this chapter we learn how to:

- Implement a relational reinforcement algorithm using the popular self-attention model
- Visualize attention maps in order to better interpret the reasoning of an RL agent
- Reason about model invariance and equivariance
- Incorporate Double Q-learning to improve stability of training

Hopefully by this point you have come to appreciate just how powerful the combination of deep learning and reinforcement learning is at solving tasks previously thought to be the exclusive domain of humans. Deep learning is a class of powerful learning algorithms that can comprehend and reason through complex patterns and data, and reinforcement learning is the framework we use to solve control problems.

Throughout this book we've focused on using games as a laboratory for experimenting with reinforcement learning algorithms as they allow us to assess the ability of these algorithms in a very controlled setting. When we build an RL agent that learns to play a game well, we are generally satisfied our algorithm is working. Of course, reinforcement learning has many more applications outside of playing games, and in some of these other domains, the raw performance of the algorithm using some metric (e.g. the accuracy percentage on some task) is not useful without knowing *how* the algorithm is making its decision.

For example, machine learning algorithms employed in healthcare decisions need to be explainable since patients have a right to know *why* they are being diagnosed with a particular

disease or why they are being recommended a particular treatment. While conventional deep neural networks can be trained to achieve remarkable feats, it is unclear what process is driving their decision-making.

In this chapter we will introduce a new deep learning architecture that is in the direction of unravelling this problem. Moreover, it not only offers interpretability gains but also performance gains in many cases. This new class of models are called **attention models** because they learn how to *attend to* (or focus on) only the salient aspects of an input. More specifically for our case, we will be developing a **self-attention model**, which is a model that allows each feature within an input to learn to attend to various other features in the input. This form of attention is closely related to the class of neural networks termed **graph neural networks**, which are neural networks explicitly designed to operate on graph structured data.

10.1 Machine Learning Interpretability with Attention and Relational Biases

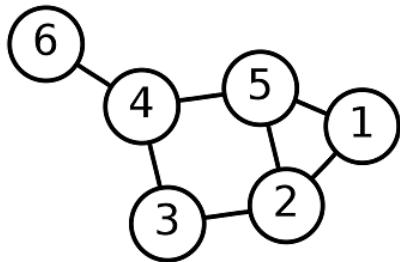


Figure 10.1 A simple graph. Graphs are composed of nodes (the number-labeled circles) and edges (the lines) between nodes that represent relationships between nodes. Some data is naturally represented as this kind of graph structure and traditional neural network architectures are unable to process this kind of data. Graph neural networks (GNNs), on the other hand, can directly operate on graph structured data.

A graph (also called a network) is a data structure that is composed of a set of **nodes** and **edges** (i.e. connections) between nodes. The nodes could represent anything, for example, people in a social network, publications in a publication citation network, cities connected by highways, or even images where each pixel is a node and adjacent pixels are connected by edges. A graph is a very generic structure for representing data with relational structure, which is almost all the data we see in practice. While convolutional neural networks are designed to process grid-like data such as images and recurrent neural networks are well-poised for sequential data, graph neural networks are more generic in that they can handle any data that can be represented as a graph. Graph neural networks have opened up a whole new set of possibilities for machine learning and are an active area of research.

Self-attention models (SAM) can actually be used to construct graph neural networks, but our goal is not to operate on explicitly graph-structured data, we will instead be working with image data as usual, however, we will use our self-attention model to essentially learn a graph

representation of the features within the image. In a sense, we hope the SAM will convert a raw image into a graph structure, and that the graph structure it constructs will be somewhat interpretable. If we train a SAM on a bunch of images of people playing basketball, we might hope it learns to associate the people with the ball, and the ball with the basket. That is, we want it to learn that the ball is a node, the basket is a node, the players are nodes, and to learn the appropriate edges between the nodes. Such a representation would give us much more insight into the mechanics of our machine learning model than a conventional convolutional neural network or the like.

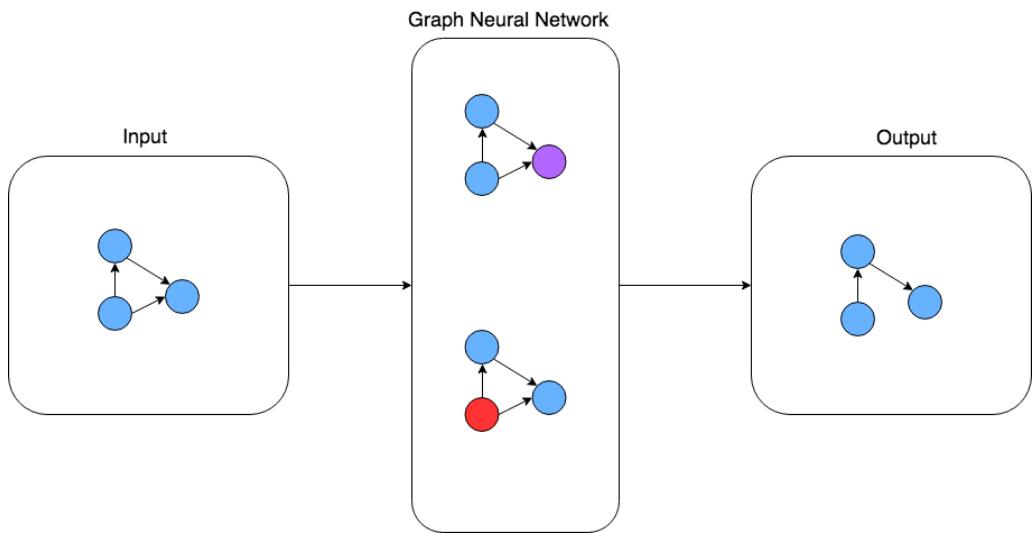


Figure 10.2 A graph neural network can directly operate on a graph, compute over the nodes and edges and return an updated graph. In this example, the graph neural network learns to remove the edge connecting the bottom two nodes.

Different neural network architectures such as convolutional, recurrent or attention have different **inductive biases** that can improve learning when those biases are accurate. Inductive reasoning is when you observe some data and infer some more general pattern or rule from it. Deductive reasoning is what we do in mathematics when we start with some premises and by following some logical rules assumed to be true, we can make a conclusion with certainty. For example, the syllogism “All planets are round. Earth is a planet. Therefore, the Earth is round” is a form of deductive reasoning. There is no uncertainty about the conclusion if we assume the premises to be true.

Inductive reasoning, on the other hand, can only lead to probabilistic conclusions. Inductive reasoning is what you do when you play a game like Chess. You cannot deduce what the other play is going to do, you have to rely on the available evidence and make an inference. Biases are essentially your prior expectations before you have even seen any data.

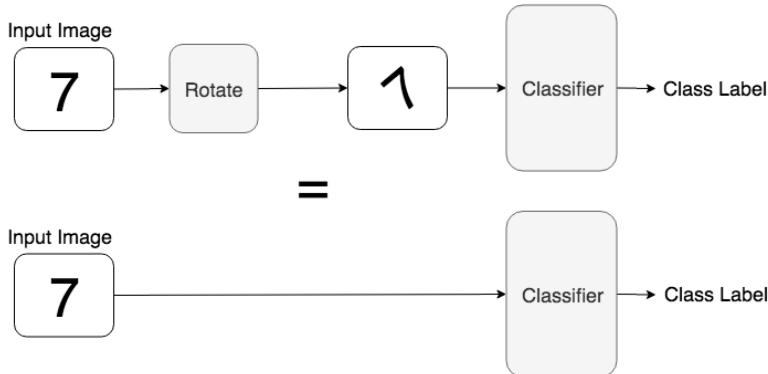
If you always expected your Chess opponent, no matter who it was, to make a particular opening move, that would be a strong (inductive) bias.

Biases are often talked about in the pejorative sense, but in machine learning, architectural biases are actually essential. It is in fact the inductive bias of compositionality (i.e. that complex data can be decomposed into simpler and simpler components in a hierarchical fashion) that makes deep learning so powerful in the first place. If we know our data are images in a grid-like structure, then we can make our models biased toward learning local features as convolutional neural networks do. If we know our data is relational, then a neural network with a relational inductive bias is going to improve performance.

10.1.1 Invariance and Equivariance

Biases are the prior knowledge we have about the structure of the data we wish to learn, which makes learning much faster. But there's more to it than just biases. With a convolutional neural network (CNN), the bias is toward learning local features, but CNNs also have the property of translation **invariance**. A function is said to be invariant to a particular transformation of its input when such a transformation does not change the output. For example, the addition function is invariant to the order of its inputs, i.e. $add(x,y)=add(y,x)$ whereas the subtraction operator does not share this order invariance (this particular invariant property has its own special name called commutativity). In general, a function $f(x)$ is invariant with respect to some transformation $g(x)$ to its input x when $f(g(x))=f(x)$. CNNs are functions in which a translation (movement up, down, left, right) of an object in an image will not impact the behavior of the CNN classifier, it is invariant to translation.

Invariance



Equivariance

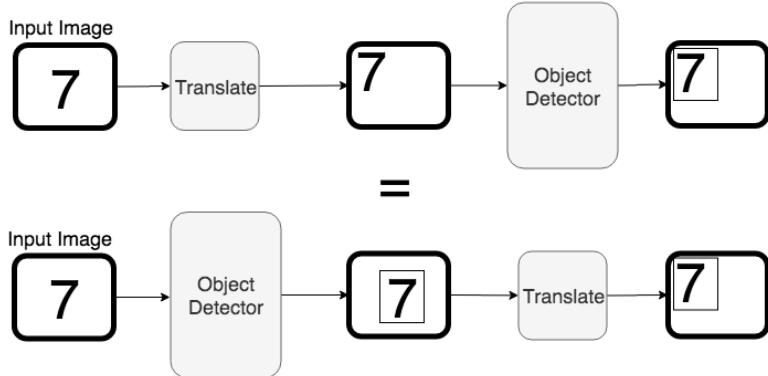


Figure 10.2 Invariance: Rotational invariance is a property of the function such that a rotation transformation of the input does not change the output of the function. **Equivariance:** Translational equivariance for a function is when applying the translation to the input results in the same output as when you just apply the translation after the function is already performed on the unaltered input.

If we use a CNN to detect the location of an object in an image, it is no longer invariant to translation but rather **equivariant**. Equivariance is when $f(g(x)) = g(f(x))$, for some transformation function g . This equation says that if we take an image with a face in the center, and then apply a translation so the face is now in the top left corner and then run it through a CNN face detector, the result is the same as if we had just run through the original centered image and then translated the output to the top left corner. The distinction is subtle and often times these two terms are used interchangeably since they are related.

Ideally, we want our neural network architectures to be invariant to many kinds of transformations our input data might suffer. In the case of images, we generally want our

machine learning model to be invariant to translations, rotations, smooth deformations (e.g. stretching or squeezing) and to noise. CNNs are only invariant/equivariant to translations but are not necessarily robust against rotations or smooth deformations.

In order to get the kind of invariance we want, we need a relational model, i.e. a model that is capable of identifying objects and relating them to one another. If we have an image of a cup on top of a table and we train a CNN to identify the cup, it will perform well. But if we were to rotate the image 90 degrees, it would likely fail because it is not rotation invariant and our training data did not include rotated images. However, a (purely) relational model should, in principle, have no problem with this because it can learn to do relational reasoning. It can learn that “cups are on tables” and this relational description does not depend on a particular viewing angle. Hence, machine learning models with relational reasoning abilities can model powerful and generic relations between objects. Attention models are one way of achieving this and the topic of this chapter.

10.2 Relational Reasoning with Attention

There are many possible ways of implementing a relational model. We know what we want, a model that can learn how objects in an input datum are related to one another. We also want the model to learn higher-level features over such objects just like a CNN does. We also want to maintain the composability of ordinary deep learning models in which we can stack together multiple e.g. CNN layers to learn more and more abstract features. And perhaps most important of all, we need this to be computationally efficient so we can train this relational model on large amounts of data.

A generic model called self-attention achieves all of these desiderata, albeit it is less scalable than the other models we've seen so far. Self-attention, as the name suggests, involves an attention mechanism in which the model can learn to attend to a subset of the input data. But before we get to self-attention, let's first talk about ordinary attention.

10.2.1 Attention Models

As with a number of advances in machine learning, attention models are loosely inspired from thinking about human and animal forms of attention. With human vision, we cannot see or focus on the entire field of view in front of us, our eyes make saccadic (rapid, jerky) movements to scan across the field of view, and we can consciously decide to focus on a particularly salient area within our view. This allows us to only focus on processing the relevant aspects of a scene, which is an efficient use of resources. Moreover, when we're engaged in thought and reasoning, we can only attend to a few things at once. We also naturally tend to employ relational reasoning when we say things like “he is older than her” or “the door closed behind me.” We are relating the properties or behavior of certain objects in the world to others. Indeed, words in human language in general only convey meaning when related to other words. In many cases, there is no absolute frame of reference, we can only describe things as they relate to other things that we know.

Absolute (non-relational) attention models are designed to function like our eyes in that they try to learn how to extract only the relevant parts of input data for efficiency and interpretability (since you can see what the model is learning to attend to in making a decision), whereas the self-attention model we will build here is a way of introducing relational reasoning into the model; the goal is not necessarily to distill the data.

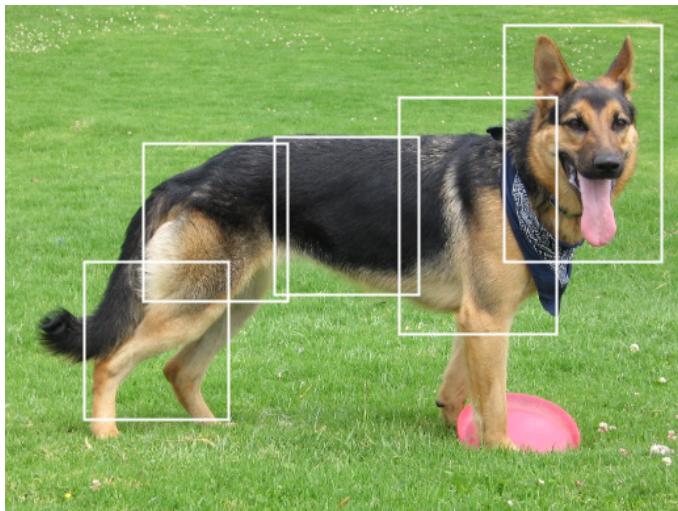


Figure 10.4 An example of hard attention where a function might simply look at sub-regions of an image and only process those one at a time. This can significantly reduce the computational burden since the dimensionality of each segment is much smaller than the whole image.

The simplest form of absolute attention for an image classifier would be to build a model that actively crops the image, i.e. it selects sub-regions from the image and only processes those. The model would have to learn what to focus on, but this would tell us what parts of the image it is using to make its classification. This is actually difficult to implement because cropping is non-differentiable. In order to crop a 28x28 pixel image, we would need our model to produce integer-valued coordinates that form the rectangular sub-region to subset, but integer-valued functions are non-continuous and thus non-differentiable, meaning we can't apply gradient descent-based training algorithms.

We could train such a model using a genetic algorithm as we learned in Chapter 6, or we could also use reinforcement learning. In the reinforcement learning case the model would produce an integer set of coordinates, crop the image based on those coordinates, process the subregion and make a classification decision. If it classifies correctly, it would get a positive reward, and a negative reward for an incorrect classification. In this way, we could employ the REINFORCE algorithm we learned earlier to train the model to perform an otherwise non-differentiable function. This procedure is described in the paper "Recurrent Models of Visual

Attention" by Mnih and others published in 2014. This form of attention is termed "hard" attention because it is non-differentiable.

There is also "soft" attention, which is a differentiable form of attention that simply applies a filter to minimize or maintain certain pixels in the image by multiplying each pixel in the image by a soft attention value between 0 and 1. The attention model can then learn to set certain pixels to 0 or maintain certain relevant pixels. Since the attention values are real numbers and not integers, this form of attention is differentiable, but it loses the efficiency of a hard attention model since it still needs to process the entire image rather than just a portion of it.



Figure 10.5 An example of soft-attention where a model would learn which pixels to keep and which pixels to ignore (i.e. set to 0). Unlike the hard-attention model, the soft-attention model needs to process the entire image at once, which can be computationally demanding.

In a self-attention model (SAM), the process is quite different and more complicated. Remember, the output of a SAM is essentially a graph, except that each node is constrained to only be connected with a few other nodes (hence the attention aspect).

10.2.2 Relational Reasoning

Before we get into the details of self-attention, let's first sketch out how a general relational reasoning module ought to work. Any machine learning model is typically fed some raw data in the form of a vector or higher-order tensor, or perhaps a sequence of such tensors as in language models. Let's actually use an example from language modeling, or natural language processing (NLP) as it is a bit easier to grasp than processing raw images. Let's consider the task of translating a simple sentence from English into Chinese.

English	Chinese
I ate food.	我吃饭了.

Each word w_i in English is encoded as a fixed-length one-hot vector, $w_i \in \mathbb{B}^n$ with dimensionality n . The dimensionality determines the maximal vocabulary size, e.g. if $n=10$ then the model can only handle a vocabulary of 10 words total, so usually it is much larger, e.g. $n \approx 40000$. Likewise, each word in Chinese is encoded as a fixed-length vector as well. We want to build a translation model that can translate each word of English into Chinese. The first approaches were based on recurrent neural networks, which are inherently sequential models as they are capable of storing data from each input. A recurrent neural network, at a high level, is a function that maintains an internal state that is updated with each input that it sees.

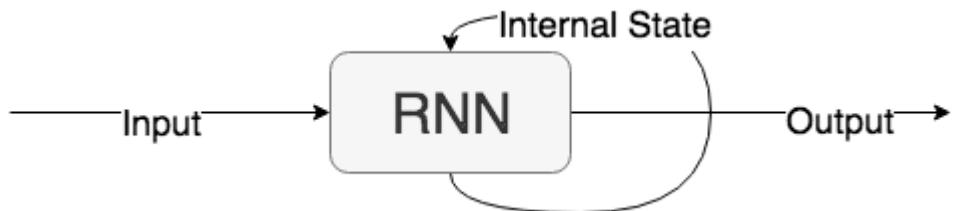


Figure 10.6 A recurrent neural network (RNN) is capable of maintaining an internal state that is updated with each new input it receives. This allows RNNs to model sequential data such as time series or language.

Most RNN models work by first having an encoder model that consumes a single English word at a time, and once done, would give its internal state vector to a different decoder RNN that would output individual Chinese words one at a time until done. The problem with RNNs is that they are not easily parallelized because you must maintain an internal state, which depends on the sequence length. So when sequence lengths vary across inputs and outputs, you have to synchronize all the sequences until they're all done processing.

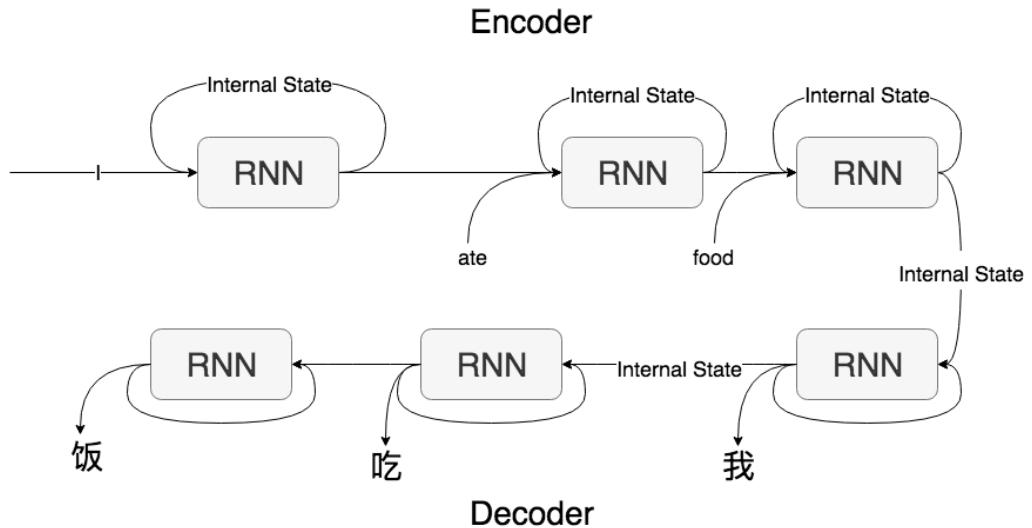


Figure 10.7 Schematic of an RNN language model. Two separate RNNs are used, an encoder and decoder. The encoder takes an input sentence word-by-word and once complete, sends its internal state to the decoder RNN, which produces each word in the target sentence until it halts.

While many thought that language models needed recurrence to work well given the natural sequential nature of language, researchers found that a relatively simple attention model with no recurrence at all could perform even better and is trivially parallelizable making it easier to train faster and with more data. These are the so-called Transformer models, which rely on self-attention. We will not get into their details but sketch out the basic mechanism here.

The idea is that the Chinese word c_i can be translated as a function of the weighted combination of a context of English words e_i . The context is simply a fixed-length collection of words that are in proximity to a given English word. So for the sentence "My dog Max chased a squirrel up the tree and barked at it" with a context of 3 words, the context for the word "squirrel" would be the sub-sentence "Maxed chased a squirrel up the tree" (e.g. we include the 3 words on either side of the target word).

For the above English phrase "I ate food" we would use all three words. Let's say we want to produce the first translated Chinese word for this sentence. The first Chinese word would be produced by taking a weighted sum of all the English words in the sentence, i.e. $c_i = f(\sum a_i \cdot e_i)$, where a_i is the (attention) weight, some number between 0 and 1, such that $\sum a_i = 1$. The function f would be some neural network, such as a simple feedforward neural network. So the function as a whole would need to learn the neural network weights in f as well as the attention weights a_i . The attention weights would be produced by some other neural network function.

After successful training, we can inspect these attention weights and see which English words are attended to when translating into a given Chinese word. For example, when

producing the Chinese word 我, the English word “I” would have a high attention weight associated with it, whereas the other words would be mostly ignored.

This general procedure is called Kernel regression. To take an even simpler example, let’s say we have a dataset that looks like this:

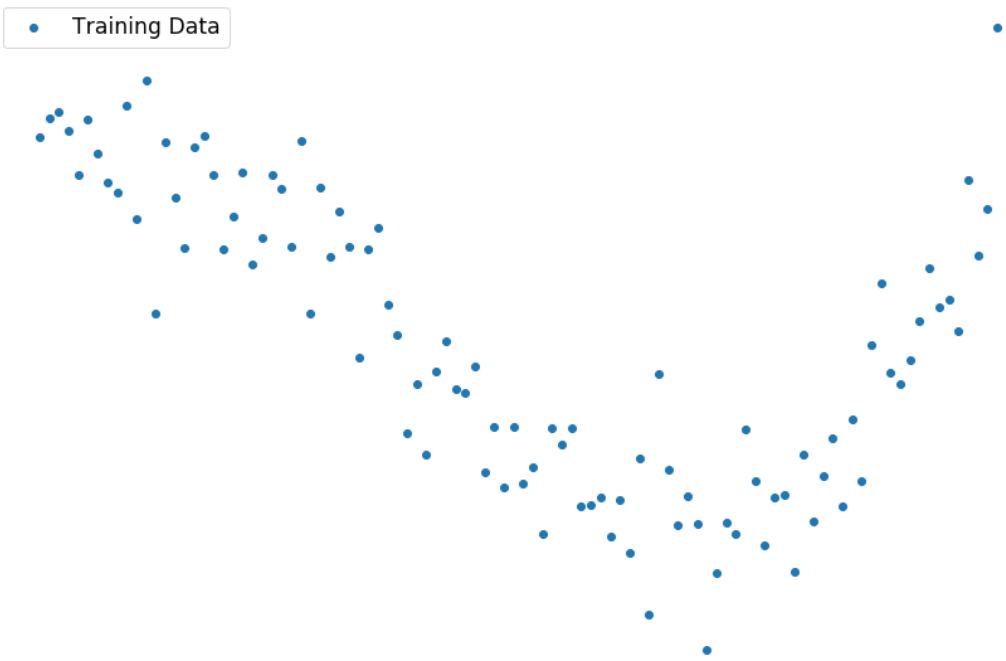


Figure 10.8 Scatter plot of a non-linear dataset on which we might want to train a regression algorithm.

And we want to make a machine learning model that can take an unseen x and predict an appropriate y , given this training data. There are two broad classes of how to do this: nonparametric and parametric methods. Neural networks are parametric models because they have a fixed set of adjustable parameters. A simple polynomial function like $f(x)=ax^3+bx^2+c$ is a parametric model because we have 3 parameters (a,b,c) that we can train to fit this function to some data. A non-parametric model is a model that either has no trainable parameters or has the ability to dynamically adjust the number of parameters it has based on the training data. Kernel regression is an example of a non-parametric model for prediction, and the simplest version of kernel regression is to simply find the nearest x_i points in the training data X to some new input x and then return the corresponding $y \in Y$ in the training data that is the average.

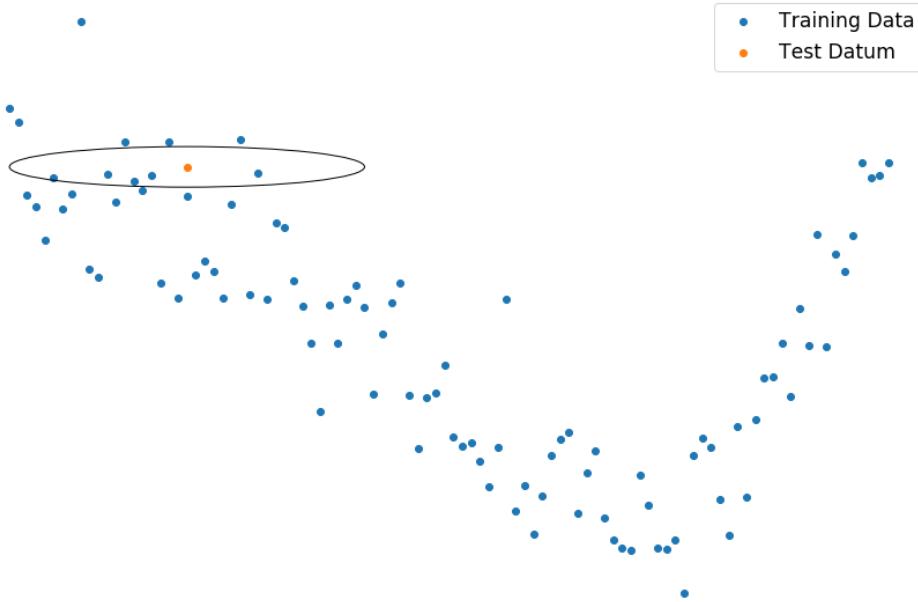


Figure 10.9 One way to perform non-parametric kernel regression to predict the y component of a new x datum is to simply find the most similar (i.e. closest) x 's in the training data and then take the average of their respective y components.

In this case, however, we have to choose how many points qualify as being the nearest neighbor to the input x and it is also problematic since all of these nearest neighbors contribute equally to the outcome. Ideally, we could weight (or attend to) all the points in the dataset according to how similar they are to the input, and then take the weighted sum of their corresponding y_i to make a prediction. We'd need some function $f:X \rightarrow A$, a function that takes an input $x \in X$ and returns a set of attention weights $a \in A$ that we can use to perform this weighted sum. This procedure is essentially exactly what we're doing in attention models, except that the difficulty lies in deciding how to efficiently compute the attention weights.

In general, a self-attention model seeks to take a collection of objects and learn how each of those objects is related to the other objects via attention weights. In graph theory, a graph is a data structure $G = (N, E)$, i.e. a collection of nodes N and edges (connections or relations) between nodes E . The collection N might be just a set of node labels such as $\{0, 1, 2, 3, \dots\}$ or each node might contain data, and thus each node might be represented by some feature vector. In this case, we can store our collection of nodes as a matrix $N: \mathbb{R}^{n \times f}$ where f is the feature dimension, such that each row is a feature vector for that node.

The collection of edges E can be represented by an **adjacency matrix** $E: \mathbb{R}^{n \times n}$ where each row and column are nodes, such that a particular value in (row 2, column 3) represents the strength of the relationship between node 2 and node 3. This is the very basic setup for a

graph, but graphs could get more complicated where even the edges have feature vectors associated with them, but we will not attempt that here.

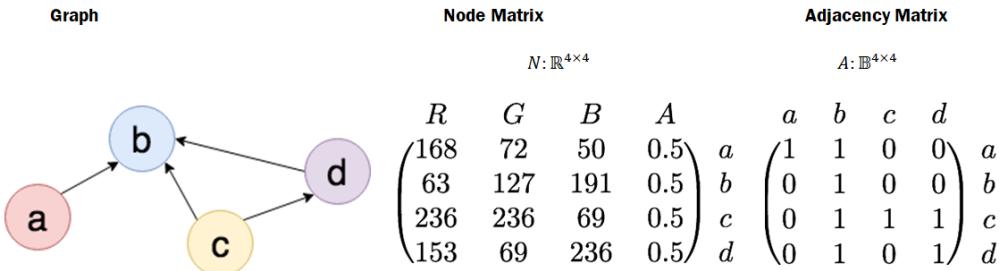


Figure 10.10: A graph structure on the left can be represented quantitatively with a node feature matrix that encodes the individual node features and an adjacency matrix that encodes the edges (i.e. connections, arrows) between nodes. A 1 in the 'a' row in the 'b' column indicates that node 'a' has an edge from 'a' to 'b'. The node features could be something like an RGBA value if the nodes represented pixels.

A self-attention model works by starting with a set of nodes $N: \mathbb{R}^{n \times f}$ and then computes the attention weights between all pairs of nodes, in effect, it creates an edge matrix $E: \mathbb{R}^{n \times n}$. After creating the edge matrix, it will update the node features such that each node sort of gets blended together with the other nodes that it attends to. In a sense, each node sends a message to the other nodes to which it most strongly attends, and when nodes receive messages from other nodes they update themselves. We call this one step process a relational module, after which we get an updated node matrix $\hat{N}: \mathbb{R}^{n \times f}$ that we can pass on to another relational module that will do the same thing. By inspecting the edge matrix, we can see which nodes are attending to which other nodes, and it gives us an idea of the reasoning of the neural network.

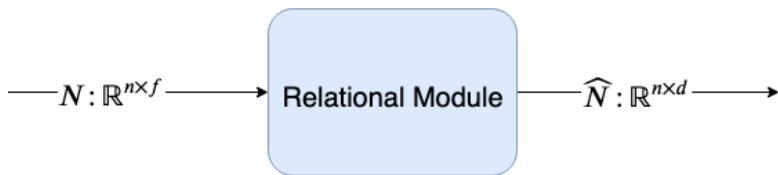
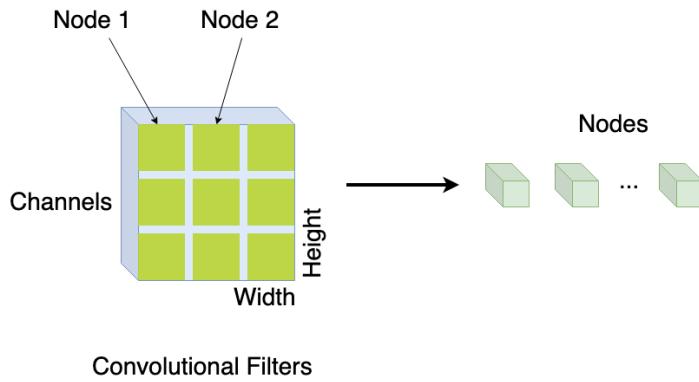


Figure 10.11 A relational module, at the highest level, processes a node matrix $N: \mathbb{R}^{n \times f}$ and outputs a new, updated node matrix $\hat{N}: \mathbb{R}^{n \times d}$ where the dimensionality of the node feature may be different.

In the language model, each word from one language is attending to all the words in context of the other language. In this book we've mostly dealt with machine learning models that operate on visual data, e.g. pixels from a video frame. In this case, the data is not naturally structured as a collection of objects or nodes that we can directly pass into a relational module. We need a way of turning a bunch of pixels into a set of objects. One way to do it

would be to simply call each individual pixel an object. To make things more computationally efficient, and to be able to coarse-grain the image into more meaningful objects, we can first pass the raw image through a few convolutional layers that will return a tensor with dimensions (C,H,W) for channels, height and width, respectively. In this way, we can make the objects along the channel dimension, i.e. each object is a vector of dimension C and there will be $N=H*W$ number of objects.



Convolutional Filters

Figure 10.12 A convolutional layer returns a series of convolutional “filters” stored in a 3-tensor with shape Channels (i.e. number of filters) by Height by Width. We can turn this into a set of nodes by taking slices along the channel dimension where each node is then a channel-length vector for a total of Height times Width number of nodes. We package these into a new matrix of dimension $N \times C$ where N is the number of nodes and C is the channel dimension.

After a raw image has been processed through a few trained CNN layers, we would expect that each position in the feature maps correspond to particular salient features in the underlying image. For example, we hope the CNNs might learn to detect objects in the image that we can then use to pass into our relational module to process relations between objects. Each convolutional filter learns a particular feature for each spatial position, so taking all these learned features for a particular (x,y) grid position in an image yields single vector for that position that encodes all the learned features. We can do this for all the grid positions to collect a set of putative objects in the image, which we can represent as nodes in a graph, except that we do not know the connectivity between the nodes yet, which is what our relational reasoning module will attempt to do.

10.2.3 Self-Attention Models

There are many possible ways to build a relational reasoning module, but as we’ve discussed, we will implement one based on a self-attention mechanism. We have described the idea at a high level, but it is time we got into the details of implementation. The model we build is

based off the one described in the paper "Deep reinforcement learning with relational inductive biases" by Zambaldi et al 2019 from DeepMind.

We already discussed the basic framework of a node matrix $N: \mathbb{R}^{n \times f}$ and an edge matrix $E: \mathbb{R}^{n \times n}$, and we discussed the need to process a raw image into a node matrix. Just like with kernel regression, we need some way of computing the distance (or inversely the similarity) between two nodes. There is no single option for this, but one common approach is to simply take the **inner product** (also called **dot product**) between the two node's feature vectors as their similarity.

The dot product between two equal-length vectors is computed by multiplying corresponding elements in each vector and then summing the result. For example, the inner product between vectors $a = (1, -2, 3)$ and $b = (-1, 5, -2)$ is denoted $\langle a, b \rangle$ and is calculated as $\langle a, b \rangle = \sum a_i b_i$, i.e. in this case $1 \cdot -1 + -2 \cdot 5 + 3 \cdot -2 = -1 - 10 - 6 = -17$. You can tell that the sign of each element in a and b are opposite, so the resulting inner product is a negative number indicating strong disagreement between the vectors. In contrast, if $a = (1, -2, 3)$, $b = (2, -3, 2)$ then $\langle a, b \rangle = 14$, which is a big positive number since the two vectors are more similar element-by-element. Hence the dot product gives us an easy way to compute the similarity between a pair of vectors (e.g. nodes in our node matrix). This approach leads to what is called (scaled) dot product attention; the scaled part will come into play later.

Once we have our initial set of nodes in the node matrix N , we will project this matrix into 3 separate new node matrices that are referred to as **keys, queries, and values**. With the kernel regression example, the query is the new x for which we want to predict the corresponding y , which is the value. The query is x , the y is the value. In order to find the value, we must location the nearest x_i in the training data, which are the keys. We measure the similarity between the query and the keys, find the keys that are most similar to the query, and then return the average value for those set of keys. This is exactly what we will do in self-attention, except that the queries, keys, and values will all come from the same origin. We multiply the original node matrix by 3 separate projection matrices in order to produce a query matrix, a key matrix and a value matrix. The projection matrices will be learned during training just like any other parameters in the model. During training the projection matrices will learn how to produce queries, keys and values that will lead to optimal attention weights.

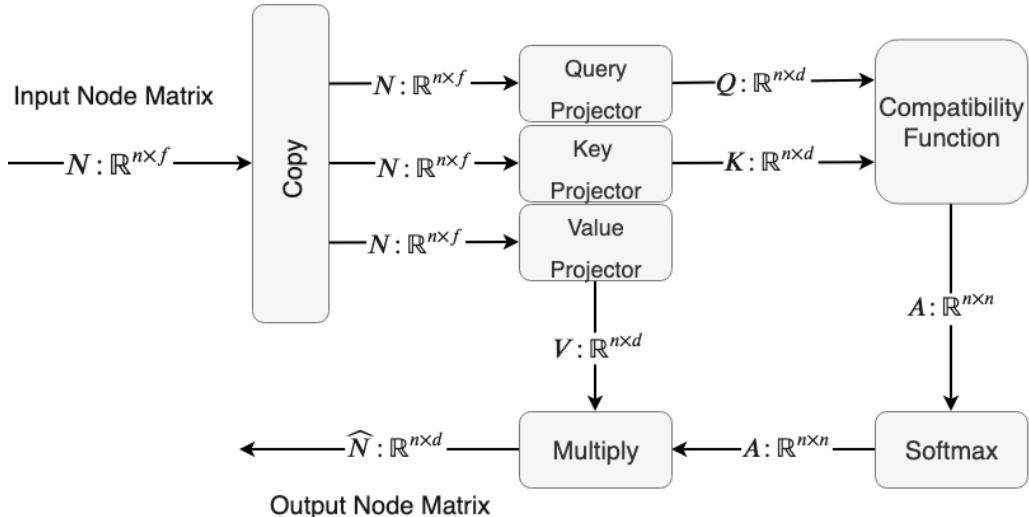


Figure 10.13 Relational module. The input to a relational module is a node matrix $N: \mathbb{R}^{n \times f}$ with n nodes each with an f -dimensional feature vector. The relational module then copies this matrix for a total of 3 copies, and projects each one into a new matrix via a simple linear layer without an activation function, creating separate Query, Key and Value matrices. The Query and Key matrices are input to a compatibility function, which is any function that computes how compatible (similar in some way) each node is to each other node, resulting in a set of unnormalized attention weights $A: \mathbb{R}^{n \times n}$. This matrix is then normalized via the softmax function across the rows, such that each row's values will sum to 1. The Value matrix and normalized attention matrix are then multiplied $\hat{N} = AV$. The output of the relational module is then usually passed through one or more linear layers (not depicted).

Let's take a single pair of nodes to make this concrete. Say we have a node (which is a feature vector) $a: \mathbb{R}^{10}$ and another node $b: \mathbb{R}^{10}$. To calculate the self-attention of these two nodes, we first will project these nodes into a new space by multiplying by some projection matrices, i.e. $a_Q = a^T Q, a_K = a^T K, a_V = a^T V$, where the superscript T indicates transposition, such that the node vector is now a column-vector, e.g. $a^T: \mathbb{R}^{1 \times 10}$ and the corresponding matrix is $Q: \mathbb{R}^{10 \times d}$, such that $a_Q = a^T Q: \mathbb{R}^d$. So now we have three new versions of a that may be of some different dimensionality from the input, e.g. $a_Q, a_K, a_V: \mathbb{R}^d$. We do the same for the node b . We can calculate how related a is to itself first by multiplying (via the inner product) its query and key together. Remember, we compute all pairwise interactions between nodes include self-interactions, and unsurprisingly objects are likely to be related to themselves, but not necessarily since the corresponding queries and keys (after projection) may be different.

When we multiply the query and key together, we get an unnormalized attention weight, i.e. $w_{a,a} = \langle a_Q, a_K \rangle$. We get the unnormalized attention weight between a and b by taking the dot product between the query and the key, which is a single scalar value. We then do the same for the pairwise interaction between a and b and b and a and b and b , thus we get a total of 4 attention weights. These could be arbitrarily small or large numbers, so we

normalize all the attention weights using the softmax function, which as you may recall, takes a bunch of numbers (or a vector) and normalizes all the values to be in the interval [0,1] and force them to sum to 1 so that it forms a proper discrete probability distribution. This constrains the attention mechanism so that it only has a limited amount of “energy” that it can use to attend to various other objects. This way we force the attention mechanism to only attend to what is absolutely necessary for the task. Without this normalization, the model could easily just attend to everything and it would remain un-interpretable.

Once we have the normalized attention weights, we then multiply these by the corresponding value matrix to focus on only certain salient parts of the value matrix, and this will give us a new and updated node matrix. We can efficiently combine all these steps into an efficient matrix multiplication:

$$\hat{N} = \text{softmax}(QK^T)V$$

Where $Q: \mathbb{R}^{n \times f}$, $K^T: \mathbb{R}^{f \times n}$, $V: \mathbb{R}^{n \times f}$, where n is the number of nodes and f is the dimension of the node feature vector. You can see the result of QK^T will be a $n \times n$ dimensional matrix, which is an adjacency matrix as we described earlier. Each row and column represent a node. If the value in row 0 and column 1 is high, then we know that node 0 attends strongly to node 1. The normalized attention (i.e. adjacency) weight matrix $A = \text{softmax}(QK^T): \mathbb{R}^{n \times n}$ tells us all the pairwise interactions between nodes. We then multiply this by the value matrix, which will update each nodes feature vector according to its interactions with other nodes, such that the final result is an updated node matrix $\hat{N}: \mathbb{R}^{n \times f}$. We can then pass this updated node matrix through a linear layer to do additional learning over the node features and apply a non-linearity to be able to model more complex features. We call this whole procedure a relational module or relational block. We can stack these relational modules sequentially to learn higher order and more complex relations.

In most cases, the final output of our neural network model needs to be a small vector, e.g. for Q-values as in DQN. After we’ve processed the input through 1 or more relational modules, we can reduce the matrix down to a vector by either doing a MaxPool operation or an AvgPool operation. For a node matrix $\hat{N}: \mathbb{R}^{n \times f}$ either of these pooling operations applied over the n -dimension would result in a f -dimensional vector. The MaxPool just takes the maximum value along the n -dimension. We can then run this pooled vector through one or more linear layers before returning the final result as our Q-values.

10.3 Implementing Self-Attention for MNIST

Before we delve into the difficulties of reinforcement learning, let’s try building a simple self-attention network to classify MNIST digits. The famous MNIST dataset is 60,000 hand-drawn images of digits, where each image is 28x28 pixels in grayscale. The images are labeled according to the digit that is depicted. The goal is to train a machine learning model to accurately classify the digits. This dataset is very easy to learn even with a simple one-layer neural network (a linear model). A multi-layer CNN can achieve in the 99% accuracy range.

While easy, it is a great dataset to use as a “sanity check” just to make sure your algorithm can learn anything at all. We will first test out our self-attention model on MNIST, but we ultimately plan to use it as our Deep Q-network in game playing, so the only difference between a DQN and an image classifier is that the dimensionality of the inputs and outputs will be different, but everything in between can remain the same.

10.3.1 Transformed MNIST

Before we build the model itself, we need to prepare the data and create some functions to preprocess the data so that it is in the right form for our model. For one, the raw MNIST images are grayscale pixel arrays with values from 0-255, so we need to normalize those values to be between 0 and 1 otherwise the gradients during training will be too variable and training will be unstable. Because MNIST is so easy, we can also strain our model a bit more by adding noise and perturbing the images randomly (e.g. random translations and rotations). This also allows us to assess translational and rotational invariance.

Listing 10.1 Preprocessing Functions

```
import numpy as np
from matplotlib import pyplot as plt
import torch
from torch import nn
import torchvision as TV

mnist_data = TV.datasets.MNIST("MNIST/", train=True, transform=None,\n                                target_transform=None, download=True) #A
mnist_test = TV.datasets.MNIST("MNIST/", train=False, transform=None,\n                                target_transform=None, download=True) #B

def add_spots(x,m=20,std=5,val=1): #C
    mask = torch.zeros(x.shape)
    N = int(m + std * np.abs(np.random.randn()))
    ids = np.random.randint(np.prod(x.shape),size=N)
    mask.view(-1)[ids] = val
    return torch.clamp(x + mask,0,1)

def prepare_images(xt,maxtrans=6,rot=5,noise=10): #D
    out = torch.zeros(xt.shape)
    for i in range(xt.shape[0]):
        img = xt[i].unsqueeze(dim=0)
        img = TV.transforms.functional.to_pil_image(img)
        rand_rot = np.random.randint(-1*rot,rot,1) if rot > 0 else 0
        xtrans,ytrans = np.random.randint(-maxtrans,maxtrans,2)
        img = TV.transforms.functional.affine(img, rand_rot, (xtrans,ytrans),1,0)
        img = TV.transforms.functional.to_tensor(img).squeeze()
        if noise > 0:
            img = add_spots(img,m=noise)
        maxval = img.view(-1).max()
        if maxval > 0:
            img = img.float() / maxval
        else:
            img = img.float()
```

```

    out[i] = img
return out

```

```

#A Download and load the MNIST training data
#B Download and load the MNIST testing data for validation
#C Function to add random spots onto the image
#D Function to preprocess the images and including random transformations of rotation and translation

```

The `add_spots` function takes an image and adds random noise to it. This function is used by the `prepare_images` function which normalizes the image pixels between 0 and 1 and performs random minor transformations such as adding noise, translating (shifting) the image and rotating the image. Here's an example of the original and perturbed MNIST digit.

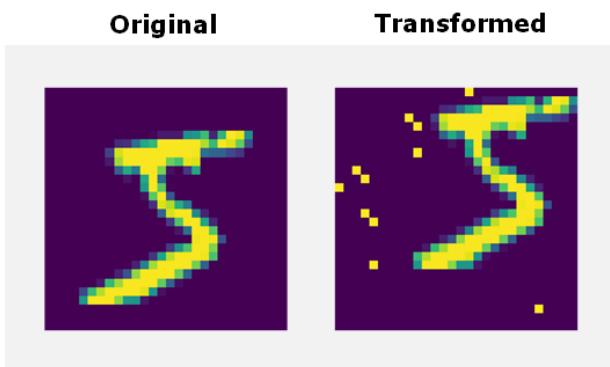


Figure 10.14 Left: Original MNIST digit for the number “5” Right: Transformed version that is translated to the top right and with random noise sprinkled in.

You can see the image is translated up and to the right and has random dots sprinkled in. This makes the learning task more difficult because our model must learn translational, noise, and rotational invariant features in order to successfully classify. The `prepare_images` function has parameters that let you tune how much the image will be perturbed so you can control the difficulty of the problem.

10.3.2 The Relational Module

Now we can dive into the relational neural network itself. Until now, all of the projects in this book were designed to be compelling enough to illustrate an important concept but simple enough to be able to run on a modern laptop without needing a GPU. The computational demands of the self-attention module are significantly greater than any of the other models we have built so far in the book, so while you can still try running this model on your laptop, it will be significantly faster if you have a CUDA-enabled GPU. If you don't have a GPU, you can easily launch a cloud-based Jupyter Notebook using Amazon SageMaker, Google Cloud or

Google Colab (which is free as of this writing). For clarity, the code we reproduce here will not include the necessary (but very minor) modifications necessary to run on the GPU. Please refer to this book's GitHub at <https://github.com/DeepReinforcementLearning/DeepReinforcementLearningInAction> to see how to enable the code to run on the GPU or consult the PyTorch documentation at <https://pytorch.org/docs/stable/notes/cuda.html>

Listing 10.2 Relational Module

```
class RelationalModule(torch.nn.Module):
    def __init__(self):
        super(RelationalModule, self).__init__()
        self.ch_in = 1
        self.conv1_ch = 16 #A
        self.conv2_ch = 20
        self.conv3_ch = 24
        self.conv4_ch = 30
        self.H = 28 #B
        self.W = 28
        self.node_size = 36 #C
        self.lin_hid = 100
        self.out_dim = 10
        self.sp_coord_dim = 2
        self.N = int(16**2) #D

        self.conv1 = nn.Conv2d(self.ch_in, self.conv1_ch, kernel_size=(4,4))
        self.conv2 = nn.Conv2d(self.conv1_ch, self.conv2_ch, kernel_size=(4,4))
        self.conv3 = nn.Conv2d(self.conv2_ch, self.conv3_ch, kernel_size=(4,4))
        self.conv4 = nn.Conv2d(self.conv3_ch, self.conv4_ch, kernel_size=(4,4))

        self.proj_shape = (self.conv4_ch+self.sp_coord_dim, self.node_size) #E
        self.k_proj = nn.Linear(*self.proj_shape)
        self.q_proj = nn.Linear(*self.proj_shape)
        self.v_proj = nn.Linear(*self.proj_shape)

        self.norm_shape = (self.N, self.node_size)
        self.k_norm = nn.LayerNorm(self.norm_shape, elementwise_affine=True) #F
        self.q_norm = nn.LayerNorm(self.norm_shape, elementwise_affine=True)
        self.v_norm = nn.LayerNorm(self.norm_shape, elementwise_affine=True)

        self.linear1 = nn.Linear(self.node_size, self.node_size)
        self.norm1 = nn.LayerNorm([self.N, self.node_size], elementwise_affine=False)
        self.linear2 = nn.Linear(self.node_size, self.out_dim)
```

#A Define the number of channels for each convolutional layer

#B self.H and self.W are the height and width of the input image, respectively

#C The dimension of the nodes after passing through the relational module

#D The number of objects or nodes, which is just the number of pixels after passing through the convolutions

#E The dimensionality of each node vector is the number of channels in the last convolution plus 2 spatial dimensions

#F Layer normalization improves learning stability

The basic setup of our model is an initial block of 4 convolutional layers that we use to preprocess the raw pixel data into higher level features. Our ideal relational model would be

completely invariant to rotations and smooth deformations, and by including these convolutional layers that are only translation-invariant, our whole model now is less robust to rotations and deformations. However, the CNN layers are more computationally efficient than relational modules, so doing some pre-processing with CNNs usually works out well in practice.

After the CNN layers, we have 3 linear projection layers that project a set of nodes into a higher-dimensional feature space. We also have some LayerNorm layers (discussed in more detail below) and lastly just a couple linear layers at the end. Overall, it's not a complicated architecture, but the details are in the forward pass of the model.

Listing 10.3 (continued from 10.2): The Forward Pass

```
def forward(self,x):
    N, Cin, H, W = x.shape
    x = self.conv1(x)
    x = torch.relu(x)
    x = self.conv2(x)
    x = x.squeeze()
    x = torch.relu(x)
    x = self.conv3(x)
    x = torch.relu(x)
    x = self.conv4(x)
    x = torch.relu(x)

    _,_,cH,cW = x.shape
    xcoords = torch.arange(cH).repeat(cW,1).float() / cW #G
    ycoords = torch.arange(cH).repeat(cW,1).transpose(1,0).float() / cH
    spatial_coords = torch.stack([xcoords,ycoords],dim=0)
    spatial_coords = spatial_coords.unsqueeze(dim=0)
    spatial_coords = spatial_coords.repeat(N,1,1,1)
    x = torch.cat([x,spatial_coords],dim=1)
    x = x.permute(0,2,3,1)
    x = x.flatten(1,2)

    K = self.k_proj(x) #H
    K = self.k_norm(K)

    Q = self.q_proj(x)
    Q = self.q_norm(Q)

    V = self.v_proj(x)
    V = self.v_norm(V)
    A = torch.einsum('bfe,bge->bfg',Q,K) #I
    A = A / np.sqrt(self.node_size)
    A = torch.nn.functional.softmax(A,dim=2)
    with torch.no_grad():
        self.att_map = A.clone()
    E = torch.einsum('bfc,bcd->bfd',A,V) #J
    E = self.linear1(E)
    E = torch.relu(E)
    E = self.norm1(E)
    E = E.max(dim=1)[0]
    y = self.linear2(E)
    y = torch.nn.functional.log_softmax(y,dim=1)
```

```

    return y

#G Append the (x,y) coordinates of each node to its feature vector and normalize to within the interval [0, 1]
#H Project the input node matrix into key, query, and value matrices
#I Batch matrix multiply the query and key matrices
#J Batch matrix multiply the attention weight matrix and the value matrix

```

Let's see how this forward pass corresponds to the schematic in Figure 10.12. There are a few novelties used in this code that have not come up elsewhere in the book and that you may be unaware of. One is the use of the `LayerNorm` layer in PyTorch, which unsurprisingly stands for layer normalization.

`LayerNorm` is one form of neural network normalization, another popular one is called Batch Normalization (or just `BatchNorm`). The problem with unnormalized neural networks is that the magnitude of the inputs to each layer in the neural network can vary dramatically and the range of values that the inputs can take can change from batch to batch. This increases the variability of the gradients during training and leads to instability, which can significantly slow training. Normalization seeks to keep all inputs at each major step of computation to be bounded within a relatively fixed, narrow range (i.e. with some constant mean and variance). This keeps gradients more stable and can make training much faster. As we have been discussing, self-attention (and the broader class of relational or graph) models are capable of feats that ordinary feedforward models struggle with due to their inductive bias of data being relational. Unfortunately, because the model involves a softmax in the middle, this can make training unstable and difficult as the softmax restricts outputs within a very narrow range that can become saturated if the input is too big or small. Thus it is critical to include normalization layers to reduce these problems, and in our experiments `LayerNorm` improves training performance substantially, as expected.

10.3.3 Tensor Contractions and Einstein Notation

The other novelty in this code is the use of the function `torch.einsum`. Einsum is short for "Einstein summation" (or also called just Einstein notation) and was introduced by Albert Einstein as a new notation for representing certain kinds of operations with tensors. While we could have written the same code without Einsum, it is much simpler with it, and we encourage its use when it offers improved code readability. To understand it, we must recall that tensors (in the machine learning sense, which are just multi-dimensional arrays) may have 0 or more dimensions that are accessed by corresponding indices. Recall that a scalar (single number) is a 0-tensor, a vector is a 1-tensor, a matrix is a 2-tensor, and so on. The number corresponds to how many indices each tensor has. A vector has 1 index because each element in a vector can be addressed and accessed by a single non-negative integer index value. A matrix element is accessed by two indices, its row and column position. This generalizes to arbitrary dimensions.

If you've made it this far, you're familiar with operations like the inner (dot) product between two vectors and matrix multiplication (either multiplying a matrix with a vector or another matrix). The generalization of these operations to arbitrary order tensors (e.g. the

“multiplication” of two 3-tensors) is called a **tensor contraction**. Einstein notation makes it easy to represent and compute any arbitrary tensor contraction, and with self-attention, we’re attempting to contract two 3-tensors (and later two 4-tensors) so it becomes necessary to use Einsum or we would have to reshape the 3-tensor into a matrix, do a normal matrix multiplication, and then reshape it back into a 3-tensor (which makes it much less readable than just using Einsum).

This is the general formula for a tensor contraction of two matrices:

EINSTEIN SUMMATION AND TENSOR CONTRACTION

$$C_{i,k} = \sum_j A_{i,j} B_{j,k}$$

The output on the left $C_{i,k}$ is the resulting matrix from multiplying matrices $A:i\times j$ and $B:j\times k$ (where i,j,k are the dimensions) such that dimension j for each matrix is the same size (as we know is required to do matrix multiplication). What this tells us is that element $C_{0,0}$, for example, is equal to $\sum A_{0,j} B_{j,0}$ for all j . The first element in the output matrix C is computed by taking each element in the first row of A , multiplying it by each element in the first column of B , and then summing these all together. We can figure out each element of C by this process of summing over a particular **shared index** between two tensors. This summation over a shared index is the process of tensor contraction, since we start with e.g. two input tensors with two indices each (for a total of 4 indices) and the output has 2 indices because 2 of the 4 get contracted away. If we did a tensor contraction over two 3-tensors, then the result would be a 4-tensor.

TENSOR CONTRACTION: EXAMPLE

Let’s tackle a concrete example of a tensor contraction; we’ll be showing how to contract two matrices (which, in this case would be just an ordinary matrix multiplication) using Einstein notation.

$$A = \begin{bmatrix} 1 & -2 & 4 \\ -5 & 9 & 3 \end{bmatrix} \quad B = \begin{bmatrix} -3 & -3 \\ 5 & 9 \\ 0 & 7 \end{bmatrix}$$

Matrix A is a 2×3 matrix and matrix B is a 3×2 . We now want to label the dimensions of these matrices using arbitrary characters. For example we label matrix $A:i\times j$ with dimensions (indices) i and j and matrix $B:j\times k$ with indices j and k . We could have labeled the indices using any characters, but we want to contract over the shared dimensions of $A=j=B=3$ so we label them with the same character.

$$C = \begin{bmatrix} x_{0,0} & x_{0,1} \\ x_{1,0} & x_{1,1} \end{bmatrix}$$

This C matrix represents the output. Our goal is to figure out the values of each x value, which are labeled by their indexed positions. Using the formula from above, we can figure out $x_{0,0}$ by finding row 0 of matrix A and column 0 of matrix B , i.e. $A_{0,j} = [1, -2, 4]$ and $B_{j,0} = [-3, 5, 0]^T$. Now we loop over the j index, multiplying each element of $A_{0,j}$ with $B_{j,0}$ and then summing them altogether to get a single number, which will be $x_{0,0}$. In this case, $x_{0,0} = \sum A_{0,j} \cdot B_{j,0} = (1 \cdot -3) + (-2 \cdot 5) + (4 \cdot 0) = -3 - 10 = -13$. That was the calculation just for one element in the output matrix, element $C_{0,0}$. But we do this same process for all elements in C and finally we get all the values. Of course we never do this by hand, but this is what is happening under the hood when we do a tensor contraction and this process generalizes to tensors of higher order than just matrices.

Most of the time we see Einstein notation written without the summation symbol, where it is assumed we sum over the shared index. That is, rather than explicitly writing $C_{i,k} = \sum A_{i,j} \cdot B_{j,k}$, we often just write $C_{i,k} = A_{i,j} B_{j,k}$ and omit the summation.

Einstein notation can also easily represent a batch matrix multiplication in which we have two collections of matrices and we want to multiply the first two matrices together, the second two together, etc. until we get a new collection of multiplied matrices.

EINSUM: BATCH MATRIX MULTIPLICATION

$$C_{b,i,k} = \sum_j A_{b,i,j} B_{b,j,k}$$

Where the b dimension is the batch dimension and we just contract over the shared j dimension. We will use Einsum notation to do batch matrix multiplication, but we can also use it to contract over multiple indices at once when using higher-order tensors than matrices.

In the code above we used `A = torch.einsum('bfe,bge->bfg', Q, K)` to compute a batched matrix multiply of the Q and K matrices. Einsum accepts a string that contains the instructions for which indices to contract over and then the tensors that will be contracted. The string '`bfe,bge->bfg`' associated with tensors Q and K , means that Q is a tensor with 3 dimensions labeled '`bfe`' and K is a tensor with 3 dimensions labeled '`bge`' and that we want to contract these tensors to get an output tensor with 3 dimensions labeled '`bfg`'. We can only contract over dimensions that are the same size and are labeled the same, so in this case we contract over the '`e`' dimension, which is the node feature dimension, leaving us with two copies of the node dimension, which is why the output is of dimension $b \times n \times n$. When using Einsum, we can label the dimensions of each tensor with any alphabetic characters, but we must make sure that dimension we wish to contract over is labeled with the same character for both tensors.

After the batch matrix multiplication to get the unnormalized adjacency matrix, we then did `A = A / np.sqrt(self.node_size)` to re-scale the matrix to reduce excessively large values to improve training performance; this is why we earlier referred to this as *scaled* dot product attention.

In order to get the Q, K, and V matrices, as we discussed earlier, we took the output of the last convolutional layer which is a tensor of dimensions batch x channels x height x width, and we collapse the height and width dimensions into a single dimension of (height x width = n) for the number of nodes, since each pixel position will become a potential node or object in the node matrix. Thus we get an initial node matrix of $N:b \times c \times n$ that we reshape into $N:b \times n \times c$.

By collapsing the spatial dimensions into a single dimension, the spatial arrangement of the nodes is scrambled and thus the network would struggle to discover that certain nodes (which were originally nearby pixels) are related spatially. That is why we add two extra channel dimensions that encode the (x, y) position of each node before it was collapsed. We normalize the positions to be in the interval $[0, 1]$, since normalization almost always helps with performance.

Adding these absolute spatial coordinates to the end of each node's feature vector helps maintain the spatial information, but it is not ideal since these coordinates are in reference to an external coordinate system, which means we're dampening some of the invariance to spatial transformations that a relational module should have in theory. A more robust approach is to encode *relative* positions with respect to other nodes, which would maintain spatial invariance. However, this approach is more complicated and we can still achieve good performance and interpretability with the absolute encoding.

We then pass this initial node matrix through 3 different linear layers to project it into three different matrices with a potentially different channel dimension (which we call node-feature dimension from this point).

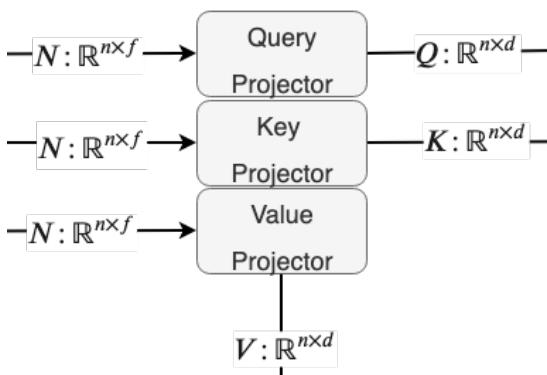


Figure 10.15 The projection step in self-attention. The input nodes are projected into a (usually) higher-dimensional feature space by simple matrix multiplication.

Once we multiply the query and key matrices, we get an unnormalized attention weight matrix $A:b \times n \times n$ where b = batch and n = number of nodes. We then normalize it by applying the softmax across the rows (dimension 1, counting from 0) such that each row sums to 1. This forces each node to only pay attention to a small number of other nodes, or spread its attention very thinly across many nodes.

Then we multiply the attention matrix by the value matrix to get an updated node matrix, such that each node is now a weighted combination of all the other nodes. So if node 0 pays strong attention to nodes 5 and 9 but ignores the others, once we multiply the attention matrix with the value matrix, node 0 will be updated to be a weighted combination of nodes 5 and 9 (and itself because in general nodes pay some attention to themselves). This general operation is termed **message passing** because each node sends a message (i.e. its own feature vector) to the nodes to which it is connected.

Once we have our updated node matrix, we can reduce it down to a single vector by either averaging or max-pooling over the node dimension, to get a single d -dimensional vector that should summarize the graph as a whole, and we can pass that through a few ordinary linear layers before getting our final output, which is just a vector of Q-values. Thus we are building a relational Deep-Q-network or Rel-DQN.

10.3.4 Training the Relational Module

You might have noticed the last function call in the code is actually a `log_softmax`, which is not something we would use for Q-learning. But before we get to Q-learning we want to test our relational module on classifying MNIST digits and compare it to a conventional non-relational convolutional neural network. Given that our relational module has the ability to model long-distance relationships in a way that a simple convolutional neural network cannot, we would expect our relational module to perform better in the face of strong transformations. Let's see how it does.

Listing 10.4 MNIST Training Loop

```
agent = RelationalModule() #A
epochs = 1000
batch_size=300
lr = 1e-3
opt = torch.optim.Adam(params=agent.parameters(), lr=lr)
lossfn = nn.NLLLoss()
for i in range(epochs):
    opt.zero_grad()
    batch_ids = np.random.randint(0, 60000, size=batch_size) #B
    xt = mnist_data.train_data[batch_ids].detach()
    xt = prepare_images(xt, rot=30).unsqueeze(dim=1) #C
    yt = mnist_data.train_labels[batch_ids].detach()
    pred = agent(xt)
    pred_labels = torch.argmax(pred, dim=1) #D
    acc_ = 100.0 * (pred_labels == yt).sum() / batch_size #E
    correct = torch.zeros(batch_size, 10)
    rows = torch.arange(batch_size).long()
    correct[[rows, yt.detach().long()]] = 1.
```

```
loss = lossfn(pred,yt)
loss.backward()
opt.step()
```

```
#A Create an instance of our relational module
#B Randomly select a subset of the MNIST images
#C Perturb the images in the batch using the prepare_images function we created, using max rotation of 30 degrees
#D The predicted image class is the output vector's argmax
#E Calculate prediction accuracy within the batch
```

This is a pretty straightforward training loop to train our MNIST classifier. We omitted the code necessary to store the losses for later visualization but the unabridged code can be found at this book's GitHub repository. We told the `prepare_images` function to randomly rotate the images by up to 30 degrees in either direction, which is a significant amount. Here's how the relational module performed after 1,000 epochs (which is not long enough to reach maximum accuracy):

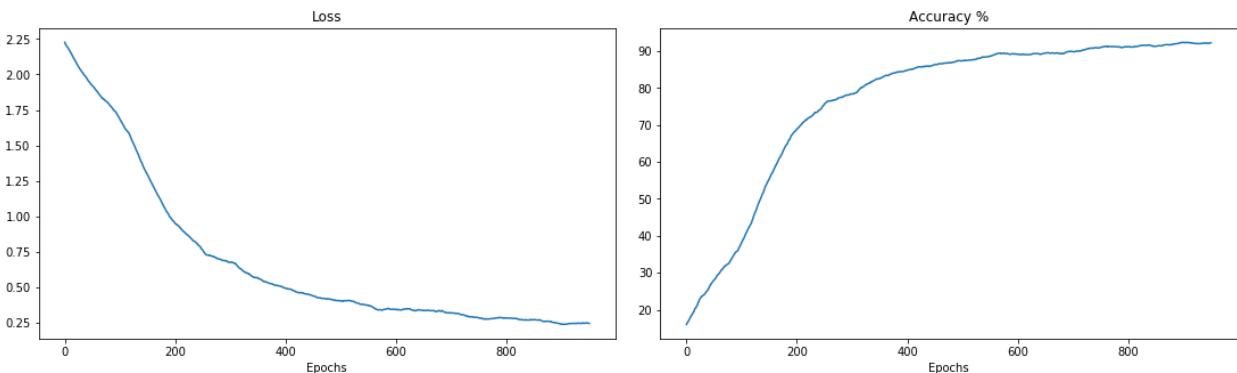


Figure 10.16 The loss and accuracy over training epochs for the relational module on classifying MNIST digits.

The plots look good, but this is just performance on the training data. To really know how well it performs, we need to run the model on the test data, which is a held-out set of data that the model has never seen before. We'll run it on 500 examples from the test data to calculate its test-time accuracy.

Listing 10.5 MNIST Test Accuracy

```
def test_acc(model,batch_size=500):
    acc = 0.
    batch_ids = np.random.randint(0,10000,size=batch_size)
    xt = mnist_test.test_data[batch_ids].detach()
    xt = prepare_images(xt,maxtrans=6,rot=30,noisy=10).unsqueeze(dim=1)
    yt = mnist_test.test_labels[batch_ids].detach()
    preds = model(xt)
```

```

pred_ind = torch.argmax(preds.detach(), dim=1)
acc = (pred_ind == yt).sum().float() / batch_size
return acc, xt, yt

acc2, xt2, yt2 = test_acc(agent)
print(acc2)
>>> 0.9460

```

We get nearly 95% accuracy at test time with the relational module after just 1,000 epochs. Again, 1,000 epochs with a batch size of 300 is not enough to reach maximal accuracy. Maximal accuracy with any decent neural network on (unperturbed) MNIST should be around the 98-99% mark. But we're not going for maximum accuracy, we're just making sure it works and that it performs better than a convolutional neural network with a similar number of parameters. We use the following simple CNN as a baseline which has 88,252 trainable parameters compared to the relational module's 85,228. The CNN actually has about 3,000 more parameters than our relational module, so it has a bit of an advantage.

Listing 10.6 Convolutional Neural Network Baseline for MNIST

```

class CNN(torch.nn.Module):
    def __init__(self):
        super(CNN, self).__init__()
        self.conv1 = nn.Conv2d(1, 10, kernel_size=(4, 4)) #A
        self.conv2 = nn.Conv2d(10, 16, kernel_size=(4, 4))
        self.conv3 = nn.Conv2d(16, 24, kernel_size=(4, 4))
        self.conv4 = nn.Conv2d(24, 32, kernel_size=(4, 4))
        self.maxpool1 = nn.MaxPool2d(kernel_size=(2, 2)) #B
        self.conv5 = nn.Conv2d(32, 64, kernel_size=(4, 4))
        self.lin1 = nn.Linear(256, 128)
        self.out = nn.Linear(128, 10) #C
    def forward(self, x):
        x = self.conv1(x)
        x = nn.functional.relu(x)
        x = self.conv2(x)
        x = nn.functional.relu(x)
        x = self.maxpool1(x)
        x = self.conv3(x)
        x = nn.functional.relu(x)
        x = self.conv4(x)
        x = nn.functional.relu(x)
        x = self.conv5(x)
        x = nn.functional.relu(x)
        x = x.flatten(start_dim=1)
        x = self.lin1(x)
        x = nn.functional.relu(x)
        x = self.out(x)
        x = nn.functional.log_softmax(x, dim=1) #D
        return x

```

#A The architecture consists of 5 convolutional layers total

#B After the first 4 convolutional layers we MaxPool to reduce the dimensionality

#C The last layer is a linear layer after we flatten the output from the CNN

```
#D Lastly, we apply the log_softmax function to classify the digits probabilistically
```

Instantiate this CNN and swap it in for the relational module in the previous training loop and see how it compares. We get a test accuracy of only 87.80% with this CNN, demonstrating that our relational module is outperforming a CNN architecture, controlling for the number of parameters. Moreover, if you crank up the transformation level (e.g. add more noise, rotate even more), the relational module will maintain a higher accuracy than the CNN. As we noted earlier, our particular implementation of the relational module is not practically invariant to rotations and deformation because, in part, we've added the absolute coordinate positions, so it's not all relational, but it has the ability to compute long-distance relations between features in the image as opposed to a CNN that can just compute local features.

We wanted to demonstrate relational modules not merely because they might get better accuracy on some dataset, but because they are more interpretable than traditional neural network models. We can inspect the learned relationships in the attention weight matrix to see which parts of the input the relational module is using in order to classify images or predict Q-values.

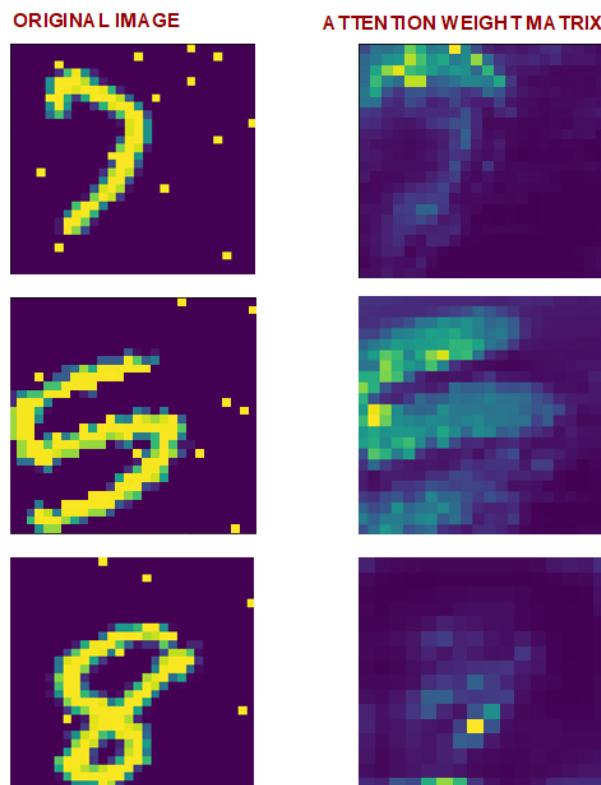


Figure 10.17 Left column: Original input MNIST images (after transformation). Right column: Corresponding

self-attention weights showing where the model is paying most attention.

We visualize this attention map by just reshaping the attention map into a square image:

```
>>> plt.imshow(agent.att_map[0].max(dim=0)[0].view(16,16))
```

The attention weight matrix is a $Batch \times n \times n$ where n is the number of nodes, which is $16^2=256$ in our example, since after the convolutional layers the spatial extent is reduced from the original 28×28 . Notice in the top 2 examples that attention maps highlight the contour of the digit but with more intensity at certain parts. If you look through a number of these attention maps you'll notice that the model tends to pay most attention to the inflection and crossover points of the digit. If you look at the example of the digit 8, it can successfully classify this image as the number 8 just by paying attention to the center of the 8 and the bottom part. You can also notice that in none of the examples is attention given to the added spots of noise in the input; attention is only given to the real digit part of the image, demonstrating that the model is learning to separate the signal from the noise to a large degree.

10.4 Multi-Head Attention and Relational DQN

We've demonstrated our relational model performs well on a simple task of classifying MNIST digits and furthermore that by visualizing the learned attention maps we can get a sense of what data the model is using to make its decisions. If for example the trained model keeps mis-classifying a particular image, we can inspect its attention map and see if perhaps it is getting distracted by some noise.

One problem with the self-attention mechanism we've employed so far is that it severely constrains the amount of data that can be transmitted due to the softmax. If the input had hundreds or thousands of nodes, the model would only be able to put attention weight on a very small subset of those, and it may not be enough. We want to be able to bias the model toward learning relationships, which the softmax helps promote, but we don't want to necessarily limit the amount of data that can pass through the self-attention layer.

In effect, we need a way to increase the bandwidth of the self-attention layer without fundamentally altering its behavior. To address this issue, we allow our model to have multiple attention "heads," meaning that the model learns multiple attention maps that operate independently and then are later combined. One attention head might focus on a particular region or features of the input whereas another head would focus elsewhere. This way we can increase the bandwidth through the attention layer but yet we can still keep the interpretability and relational learning intact. In fact, multi-head attention can improve interpretability because within each attention head, each node can more strongly focus on a smaller subset of other nodes rather than having to spread its attention more thinly. Thus, multi-head attention can give us a better idea of which nodes are strongly related.

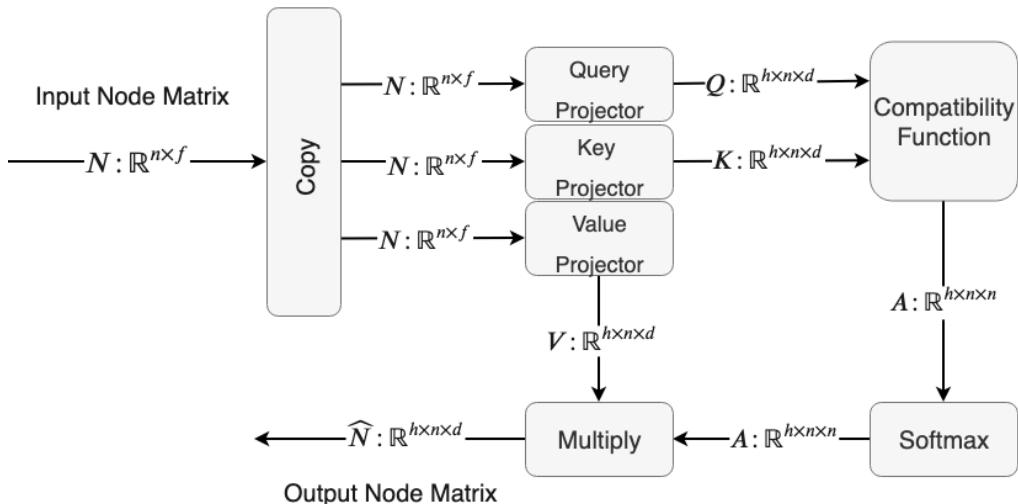


Figure 10.18 Multi-head dot product attention (MHDPA). Rather than a single attention matrix, we can have multiple attention matrices called “heads” that can independently attend to different aspects of an input. The only difference is adding a new head dimension to the Query, Key and Value tensors.

With multi-head attention, the utility of Einsum becomes even more obvious as we will be operating on 4-tensors of dimension *Batch* × *Head* × *Number of nodes* × *Features*. Multi-head attention will not be particularly useful for MNIST because the input space is already small and sparse enough that a single attention head has enough bandwidth and interpretability. Hence, this is a good time to introduce our reinforcement learning task for this chapter. Because the relational module is the most computationally expensive model we’ve implemented in this book so far, we want to use a simple environment that still demonstrates the power of relational reasoning and interpretability in reinforcement learning.

We will be coming full circle in a way and returning to a Gridworld environment that we first encountered all the way back in Chapter 3. But the Gridworld environment we will be using in this chapter is much more sophisticated. We’ll be using the library MiniGrid found at <<https://github.com/maximecb/gym-minigrid>>, which is implemented as an OpenAI Gym environment. It includes a wide variety of different kinds of Gridworld environments of varying complexity and difficulty. Some of these Gridworld environments are so difficult (largely due to sparse rewards) that only the most cutting-edge reinforcement learning algorithms are capable of making headway. Install the package using pip:

```
>>> pip3 install gym-minigrid
```

We will be using a somewhat difficult environment in which the Gridworld agent must navigate to a key, pick it up, use it to open a door, and then navigate to a goalpost in order to receive a positive reward. This is a lot of steps before it ever sees a reward, and thus we encounter the sparse reward problem. This would actually be a great opportunity to employ curiosity-based

learning, but we will restrict ourselves to the smallest version of the grid so that even a random agent would eventually find the goal and we can successfully train without curiosity. For the larger grid variants of this environment, curiosity or related approaches would be almost necessary.

There are a few other complexities to the MiniGrid set of environments. One is that they are partially observable environments, meaning the agent cannot see the whole grid but only a small region immediately surrounding it. Another is that the agent does not simply move left, right, up, down but has an orientation. The agent can only move forward, turn left, turn right, so it is always oriented in a particular direction and must turn around before moving backward, for example. The agent's partial view of the environment is egocentric, meaning the agent sees the grid as if it were facing it. When the agent changes direction without moving position, its view changes.

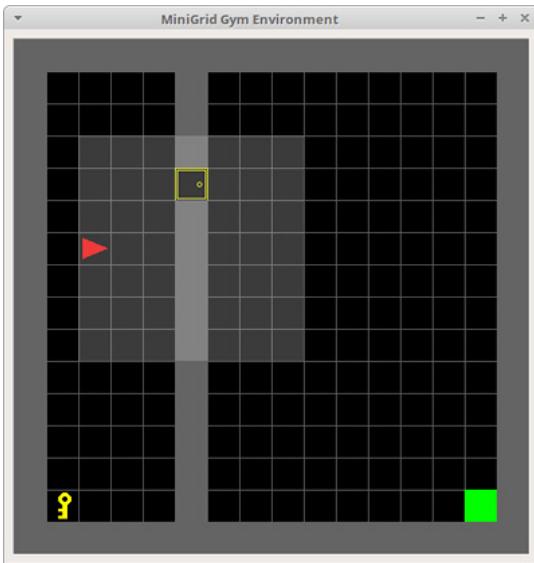


Figure 10.19 The MiniGrid-DoorKey environment. In this environment the agent (triangle) must first navigate to the key, pick it up, navigate to the door (the hollow square), open it, and then navigate to the solid square. Each game initializes the objects on the grid randomly and the agent only has a partial view of the grid indicated by the highlighted region around it.

The state we receive from the environment is a $7 \times 7 \times 3$ tensor, so the agent only sees a 7×7 sub-region of the grid in front of it and the last (channel) dimension of the state encodes which object (if any) is present at that position. The other advantage to using this Gridworld environment for trying our relational agent is that game is naturally represented by a set of objects (or nodes) and so each “pixel” position in the grid really is an actual object, unlike in the MNIST example. This means we can see exactly which other objects the agent is paying

attention to. We might hope it learns to pay most attention to the key, door and the goal square, and that the key is related to the door. If this turns out to be the case, then it suggests it is learning not too differently than how a human would learn how to relate the objects on the grid.

Overall we will re-purpose the relational module we made earlier to be a relational DQN, so we really only need to change the output to be a normal activation function rather than the `log_softmax` we use for classification. But first, let's get back to implementing multi-head attention. As operating on higher-order tensors gets more complicated, we will use the help of a package called **Einops** that extends the capabilities of PyTorch's built-in `Einsum` function. You can install it using pip.

```
>>> pip install einops
>>> from einops import rearrange
```

There are only 2 important functions in this package (`rearrange` and `reduce`) and we will only use one, the `rearrange` function. `Rearrange` basically lets us reshape the dimensions of a higher-order tensor more easily and readably than the built-in PyTorch functions and it has a syntax similar to `Einsum`. For example, we can re-order the dimensions of a tensor like this:

```
>>> x = torch.randn(5,7,7,3)
>>> rearrange(x, "batch h w c -> batch c h w").shape
torch.Size([5, 3, 7, 7])
```

Or if we had collapsed the spatial dimensions “h” and “w” into a single dimension “N” for nodes, we can undo this:

```
>>> x = torch.randn(5,49,3)
>>> rearrange(x, "batch (h w) c -> batch h w c", h=7).shape
torch.Size([5, 7, 7, 3])
```

In this case we tell it that the input has 3 dimensions but the 2nd dimension is secretly two dimensions ($h \cdot w$) that were collapsed and we want to extract them out into separate dimensions again. We only need to tell it the size of h or w and it can infer the size of the other dimension.

The main change for multi-head attention is that when we project the initial node matrix $N: \mathbb{R}^{bxnxn}$ into key, query and value matrices, we add an extra head dimension, i.e. $Q, K, V: \mathbb{R}^{bxhxnxn}$ where b is the batch dimension, and h is the head dimension. We will set the number of heads to be 3 for this example so $h=3$, $n=7 \cdot 7 = 49$, $d=64$, where n is the number of nodes (which is just the total number of grid positions in view), and d is the dimensionality of the node feature vectors, which is just something we choose empirically to be 64, but smaller or larger values might work just as well.

We will need to do a tensor contraction between the query and key tensors to get an attention tensor $A: \mathbb{R}^{bxhxnxn}$, pass it through a softmax, and then contract this with the value tensor, and collapse the head dimension with the last n dimension, contract the last (collapsed) dimension with a linear layer to get our updated node tensor $N: \mathbb{R}^{bxnxn}$, which we could then pass through another self-attention layer or collapse all the nodes into a single

vector and pass through some linear layers to the final output. We stick with a single-attention layer for all examples.

First we'll go over some specific lines in the code that are different and then the full model is reproduced later. In order to use PyTorch's built-in linear layer module (which is just a matrix multiplication plus a bias vector), we will create a linear layer where the last dimension size is expanded by the number of attention heads.

```
>>> self.proj_shape = (self.conv4_ch+self.sp_coord_dim, self.n_heads * self.node_size)
>>> self.k_proj = nn.Linear(*self.proj_shape)
>>> self.q_proj = nn.Linear(*self.proj_shape)
>>> self.v_proj = nn.Linear(*self.proj_shape)
```

We make 3 separate ordinary linear layers just as we did before for the single-head attention model, but this time we expand the last dimension by multiplying it by the number of attention heads. The input to these projection layers is a batch of initial node matrices $N: \mathbb{R}^{b \times n \times c}$, and the c dimension is equal to the output channel dimension of the last convolutional layer plus the two spatial coordinates that we append. The linear layer thus contracts over the channel dimension to give us query, key and value matrices $Q, K, V: \mathbb{R}^{b \times n \times (h \cdot d)}$, so we will use the Einops function `rearrange` to expand out the last dimension into head and d dimensions.

```
>>> K = rearrange(self.k_proj(x), "b n (head d) -> b head n d", head=self.n_heads)
```

We extract out the separate head and d dimension and simultaneously re-order the dimensions so that the head dimension comes after the batch dimension. Without Einops this would be more code and not nearly as readable. For this example, we will also abandon the dot (inner) product as the compatibility function (recall, this is the function that determines the similarity between the query and keys) and instead use something called additive attention. The dot product attention would still work fine, but we wanted to illustrate that it is not the only kind of compatibility function and the additive function is actually a bit more stable and expressive.

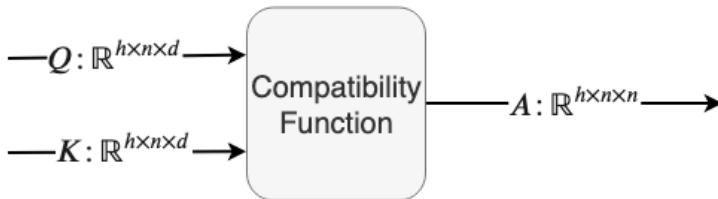


Figure 10.20 The compatibility function computes the similarity between each key and query vector resulting in an adjacency matrix.

With dot product attention, we compute the compatibility (i.e. similarity) between each query and key by simply taking the dot product between each vector. When the two vectors are similar element-wise, the dot product will yield a large positive value, and when they are

dissimilar, it may yield a value near zero or a big negative value. This means the output of the (dot product) compatibility function is unbounded in both directions, meaning we can get arbitrarily large or small values. This can be problematic when we then pass this through the softmax function, which can easily saturate. By saturate we mean that when a particular value in an input vector is dramatically larger than other values in the vector, the softmax may assign all its probability mass to that single value, setting all the others to zero or vice versa. This can make our gradients too large or too small for particular values and de-stabilize training.

Additive attention can solve this problem at the expense of introducing additional parameters. Instead of simply multiplying the Q and K tensors together, we instead pass them both through independent linear layers, add them together, and then apply an activation function, followed by another linear layer. This allows for a more complex interaction between Q and K without as much risk of causing numerical instability, since addition will not exaggerate numerical differences like multiplication does.

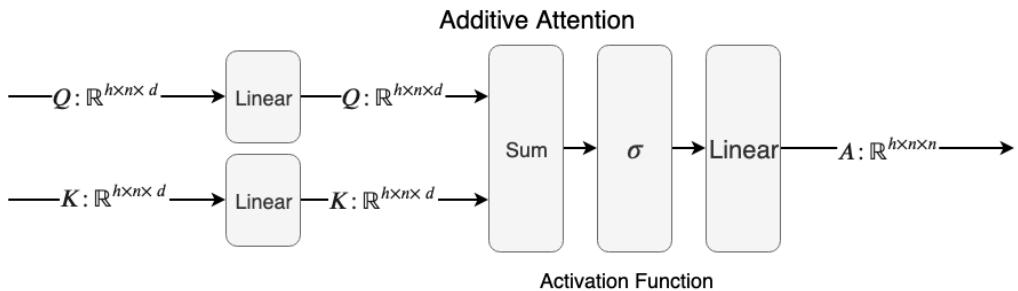


Figure 10.21 Additive attention is an alternative to dot product attention that can be more stable. Instead of multiplying the Queries and Keys together, we first pass them independently through linear layers and then add them together, apply a non-linear function and then pass through another linear layer to change the dimensionality.

First we need to add three new linear layers for the additive attention.

```
>>> self.k_lin = nn.Linear(self.node_size, self.N)
>>> self.q_lin = nn.Linear(self.node_size, self.N)
>>> self.a_lin = nn.Linear(self.N, self.N)
```

Then in the forward method:

```
>>> A = torch.nn.functional.elu(self.q_lin(Q) + self.k_lin(K))
>>> A = self.a_lin(A)
>>> A = torch.nn.functional.softmax(A, dim=3)
```

As you can see, we pass Q through a linear layer and K through its own linear layer, we add them together and then apply a non-linear activation function. Then we pass this result through another linear layer and lastly apply the softmax across the node rows. Now we do

the same as before and contract this tensor with the V tensor along the last n dimension to get a tensor with dimensions $b \times h \times n \times d$.

```
>>> E = torch.einsum('bhfc,bhcd->bhfd',A,V)
```

What we want at the end of the self-attention module is an updated node matrix with dimensions $b \times n \times d$, so we will concatenate or collapse the head dimension and d dimension, and then pass this through a linear layer to reduce the dimensionality back down to size d .

```
>>> E = rearrange(E, 'b head n d -> b n (head d)')
>>> E = self.linear1(E)
>>> E = torch.relu(E)
>>> E = self.norm1(E)
```

The final shape of this is now $b \times n \times d$, exactly what we want. Since we're only going to use a single self-attention module, we want to reduce this 3-tensor into a 2-tensor of just a batch of vectors, so we will maxpool over the n dimension, and then pass the result through a final linear layer, which represents the Q-values.

```
>>> E = E.max(dim=1)[0]
>>> y = self.linear2(E)
>>> y = torch.nn.functional.elu(y)
```

And that's it. We just went through all the core lines of code, but now let's see it all together and test it out.

Listing 10.7 The Full Model

```
class MultiHeadRelationalModule(torch.nn.Module):
    def __init__(self):
        super(MultiHeadRelationalModule, self).__init__()
        self.conv1_ch = 16
        self.conv2_ch = 20
        self.conv3_ch = 24
        self.conv4_ch = 30
        self.H = 28
        self.W = 28
        self.node_size = 64
        self.lin_hid = 100
        self.out_dim = 5
        self.ch_in = 3
        self.sp_coord_dim = 2
        self.N = int(7**2)
        self.n_heads = 3

        self.conv1 = nn.Conv2d(self.ch_in, self.conv1_ch, kernel_size=(1,1), padding=0)
    #A
        self.conv2 =
        nn.Conv2d(self.conv1_ch, self.conv2_ch, kernel_size=(1,1), padding=0)
        self.proj_shape = (self.conv2_ch+self.sp_coord_dim, self.n_heads *
        self.node_size)
        self.k_proj = nn.Linear(*self.proj_shape)
        self.q_proj = nn.Linear(*self.proj_shape)
        self.v_proj = nn.Linear(*self.proj_shape)
```

```

self.k_lin = nn.Linear(self.node_size, self.N) #B
self.q_lin = nn.Linear(self.node_size, self.N)
self.a_lin = nn.Linear(self.N, self.N)

self.node_shape = (self.n_heads, self.N, self.node_size)
self.k_norm = nn.LayerNorm(self.node_shape, elementwise_affine=True)
self.q_norm = nn.LayerNorm(self.node_shape, elementwise_affine=True)
self.v_norm = nn.LayerNorm(self.node_shape, elementwise_affine=True)

self.linear1 = nn.Linear(self.n_heads * self.node_size, self.node_size)
self.norm1 = nn.LayerNorm([self.N, self.node_size], elementwise_affine=False)
self.linear2 = nn.Linear(self.node_size, self.out_dim)

def forward(self, x):
    N, Cin, H, W = x.shape
    x = self.conv1(x)
    x = torch.relu(x)
    x = self.conv2(x)
    x = torch.relu(x)
    with torch.no_grad():
        self.conv_map = x.clone() #C
    _, cH, cW = x.shape
    xcoords = torch.arange(cW).repeat(cH, 1).float() / cW
    ycoords = torch.arange(cH).repeat(cW, 1).transpose(1, 0).float() / cH
    spatial_coords = torch.stack([xcoords, ycoords], dim=0)
    spatial_coords = spatial_coords.unsqueeze(dim=0)
    spatial_coords = spatial_coords.repeat(N, 1, 1, 1)
    x = torch.cat([x, spatial_coords], dim=1)
    x = x.permute(0, 2, 3, 1)
    x = x.flatten(1, 2)

    K = rearrange(self.k_proj(x), "b n (head d) -> b head n d",
                  head=self.n_heads)
    K = self.k_norm(K)

    Q = rearrange(self.q_proj(x), "b n (head d) -> b head n d",
                  head=self.n_heads)
    Q = self.q_norm(Q)

    V = rearrange(self.v_proj(x), "b n (head d) -> b head n d",
                  head=self.n_heads)
    V = self.v_norm(V)
    A = torch.nn.functional.elu(self.q_lin(Q) + self.k_lin(K)) #D
    A = self.a_lin(A)
    A = torch.nn.functional.softmax(A, dim=3)
    with torch.no_grad():
        self.att_map = A.clone() #E
    E = torch.einsum('bhfc,bhcd->bhfd', A, V) #F
    E = rearrange(E, 'b head n d -> b n (head d)')
    E = self.linear1(E)
    E = torch.relu(E)
    E = self.norm1(E)
    E = E.max(dim=1)[0]
    y = self.linear2(E)
    y = torch.nn.functional.elu(y)
    return y

```

```
#A We use 1x1 convolutions to preserve the spatial organization of the objects in the grid
#B Setup linear layers for additive attention
#C Save a copy of the post-convolved input for later visualization
#D Additive attention
#E Save a copy of the attention weights for later visualization
```

10.5 Double Q-learning

Now let's get to training it. Because this Gridworld environment has sparse rewards, we need to make our training process as smooth as possible, especially since we're not using curiosity-based learning. Remember back in Chapter 3 when we introduced Q-learning and a target network to stabilize training? If not, the idea was that in ordinary Q-learning, we compute the target Q-value by this equation:

$$Q_{new} = r_t + \gamma \cdot \max(Q(s_{t+1}))$$

The problem with this is that every time we update our DQN according to this equation so that its predictions get closer to this target, the $Q(s_{t+1})$ is changed, which means the next time we go to update our Q-function, the target Q_{new} is going to be different even for the same state. This is problematic because as we train the DQN its predictions are chasing a moving target, leading to very unstable training and poor performance. In order to stabilize training, we create a duplicate Q-function called the target function that we can denote Q' and we use the value $Q'(s_{t+1})$ to plug into the equation and update the main Q-function. We only train (and hence backpropagate into) the main Q-function, but we copy the parameters from the main Q-function to the target Q-function Q' every 100 (or some other arbitrary number of) epochs. This greatly stabilizes training because the main Q-function is no longer chasing a constantly moving target, but a relatively fixed target.

But that's not all that's wrong with that simple update equation. Because it involves the max function, i.e. we select the maximum predicted Q-value for the next state, it leads our agent to over-estimate Q-values for actions, which can especially impact training early on. If the DQN takes action 1 and learns an erroneously high Q-value for action 1, then that means action 1 is going to get selected more often in subsequent epochs, further causing it to be over-estimated, which again leads to training instability and poor performance.

In order to mitigate this problem and get more accurate estimates for Q-values, we will implement Double Q-learning, which solves the problem by disentangling action-value estimation from action selection as we will see. A Double Deep Q-Network (DDQN) involves a simple modification to normal Q-learning with a target network. As usual, we use the main Q-network to select actions using an epsilon-greedy policy. But when it comes time to compute Q_{new} , we will first find the argmax of Q (the main Q-network), let's say $a = \text{argmax}(Q(s_{t+1})) = 2$, so action 2 is associated with the highest action-value in the next state given the main Q-function. We then use this to index into the target network Q' to get the action-value we will use in the update equation.

$$a = \text{argmax}(Q(s_{t+1}))$$

$$x = Q'(s_{t+1})[a]$$

$$Q_{new} = r_t + \gamma \cdot x$$

We're still using the Q-value from the target network Q' , but we don't choose the highest Q-value from Q' , we choose the Q-value in Q' based on the action associated with the highest Q-value in the main Q-function. In code:

```
>>> state_batch, action_batch, reward_batch, state2_batch, done_batch =
    get_minibatch(replay, batch_size)
>>> q_pred = Gwagent(state_batch)
>>> astar = torch.argmax(q_pred, dim=1)
>>> qs = Tnet(state2_batch).gather(dim=1, index=astar.unsqueeze(dim=1)).squeeze()
>>> targets = get_qtarget_ddqn(qs.detach(), reward_batch.detach(), gamma, done_batch)
```

The `get_qtarget_ddqn` function just computes $Q_{new} = r_t + \gamma \cdot x$.

```
>>> def get_qtarget_ddqn(qvals, r, df, done):
>>>     targets = r + (1 - done) * df * qvals
>>>     return targets
```

We provide `done`, which is a Boolean, because if the episode of the game is done, there is no next state on which to compute $Q(s_{t+1})$, therefore we just train on r_t and set the rest of the equation to 0. And that's all there is to double Q-learning; just another simple way to improve training stability and performance.

10.6 Training and Attention Visualization

We have most of the pieces now, but we need a few other helper functions before training.

Listing 10.8 Preprocessing Functions

```
import gym
from gym_minigrid.minigrid import *
from gym_minigrid.wrappers import FullyObsWrapper, ImgObsWrapper
from skimage.transform import resize

def prepare_state(x): #A
    ns = torch.from_numpy(x).float().permute(2,0,1).unsqueeze(dim=0)#
    maxv = ns.flatten().max()
    ns = ns / maxv
    return ns

def get_minibatch(replay, size): #B
    batch_ids = np.random.randint(0, len(replay), size)
    batch = [replay[x] for x in batch_ids] #list of tuples
    state_batch = torch.cat([s for (s,a,r,s2,d) in batch],)
    action_batch = torch.Tensor([a for (s,a,r,s2,d) in batch]).long()
    reward_batch = torch.Tensor([r for (s,a,r,s2,d) in batch])
    state2_batch = torch.cat([s2 for (s,a,r,s2,d) in batch],dim=0)
    done_batch = torch.Tensor([d for (s,a,r,s2,d) in batch])
    return state_batch,action_batch,reward_batch,state2_batch, done_batch
```

```

def get_qtarget_ddqn(qvals,r,df,done): #C
    targets = r + (1-done) * df * qvals
    return targets

#A Normalizes the state tensor and converts to PyTorch tensor
#B Gets a random minibatch from the experience replay memory
#C Calculates the target Q-value

```

These functions just prepare the state observation tensor, produce a minibatch and calculate the target Q-value as we discussed earlier.

Listing 10.9 Preprocessing

```

def lossfn(pred,targets,actions): #A
    loss = torch.mean(torch.pow(\n
        targets.detach() - \n
            pred.gather(dim=1,index=actions.unsqueeze(dim=1)).squeeze()\n
            ,2),dim=0)
    return loss

def update_replay(replay,exp,replay_size): #B
    r = exp[2]
    N = 1
    if r > 0:
        N = 50
    for i in range(N):
        replay.append(exp)
    return replay

action_map = { #C
    0:0,
    1:1,
    2:2,
    3:3,
    4:5,
}

#A Loss function
#B Adds new experiences to the experience replay memory; if the reward is positive we add 50 copies of the memory
#C We map the action outputs of the DQN to a subset of actions in the environment

```

The `update_replay` function adds new memories to the experience replay if it is not yet full, and if it is full, it will replace random memories with new ones. If the memory resulted in a positive reward, then we add 50 copies of that memory since positive reward memories are rare and we want to enrich the experience replay with these more important memories. All the MiniGrid environments have 7 actions but in the environment we will use in this chapter we only need to use 5 of the 7 actions, so we use a dictionary to translate from the output of DQN which will produce actions 0-4 to the appropriate actions in the environment which are {0,1,2,3,5}.

ACTIONS

```
[<Actions.left: 0>,
 <Actions.right: 1>,
 <Actions.forward: 2>,
 <Actions.pickup: 3>,
 <Actions.drop: 4>,
 <Actions.toggle: 5>,
 <Actions.done: 6>]
```

Listing 10.10 The Main Training Loop

```
from collections import deque
env = ImgObsWrapper(gym.make('MiniGrid-DoorKey-5x5-v0')) #A
state = prepare_state(env.reset())
GWagent = MultiHeadRelationalModule() #B
Tnet = MultiHeadRelationalModule() #C
maxsteps = 400 #D
env.max_steps = maxsteps
env.env.max_steps = maxsteps

epochs = 50000
replay_size = 9000
batch_size = 50
lr = 0.0005
gamma = 0.99
replay = deque(maxlen=replay_size) #E
opt = torch.optim.Adam(params=GWagent.parameters(), lr=lr)
eps = 0.5
update_freq = 100
for i in range(epochs):
    pred = GWagent(state)
    action = int(torch.argmax(pred).detach().numpy())
    if np.random.rand() < eps: #F
        action = int(torch.randint(0,5,size=(1,)).squeeze())
    action_d = action_map[action]
    state2, reward, done, info = env.step(action_d)
    reward = -0.01 if reward == 0 else reward #G
    state2 = prepare_state(state2)
    exp = (state,action,reward,state2,done)

    replay = update_replay(replay,exp,replay_size)
    if done:
        state = prepare_state(env.reset())
    else:
        state = state2
    if len(replay) > batch_size:

        opt.zero_grad()

        state_batch,action_batch,reward_batch,state2_batch,done_batch =
        get_minibatch(replay,batch_size)

        q_pred = GWagent(state_batch).cpu()
        astar = torch.argmax(q_pred,dim=1)
        qs = Tnet(state2_batch).gather(dim=1,index=astar.unsqueeze(dim=1)).squeeze()

        targets =
```

```

get_qtarget_ddqn(qs.detach(), reward_batch.detach(), gamma, done_batch)

loss = lossfn(q_pred, targets.detach(), action_batch)
loss.backward()
torch.nn.utils.clip_grad_norm_(GWagent.parameters(), max_norm=1.0) #H
opt.step()

if i % update_freq == 0: #I
    Tnet.load_state_dict(GWagent.state_dict())

```

#A Setup environment
#B Create main relational DQN
#C Create target DQN
#D Set the maximum steps before game will end
#E Create the experience replay memory
#F Use an epsilon-greedy policy for action selection
#G Re-scale the reward to be slightly negative on non-terminal states
#H Clip the gradients to prevent overly large gradients
#I Synchronize the main DQN with the target DQN every 100 steps

It will learn how to play fairly well after about 10,000 epochs but may take up to 50,000 epochs before it reaches maximum accuracy. Here is the log-loss plot we get and we also plot the average episode length. As the agent learns to play, it should be able to solve the games in fewer and fewer steps.

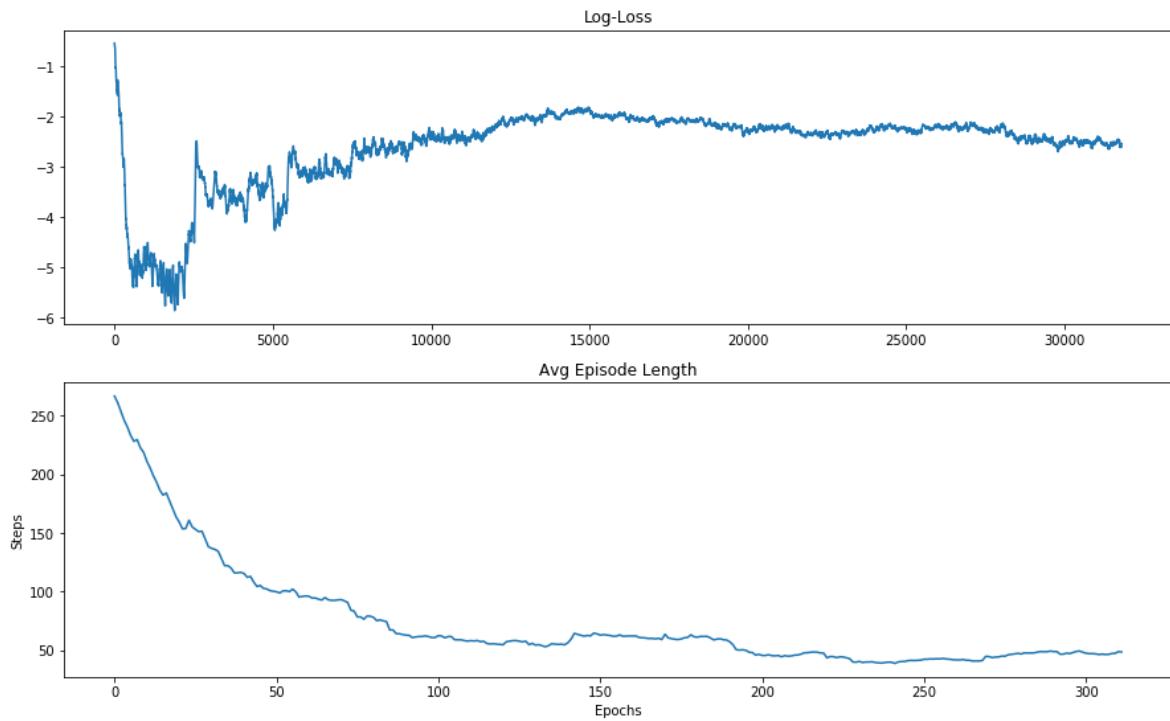


Figure 10.22 Top: Log-loss plot during training. The loss drops quickly in the beginning, increases a bit and then very slowly begins decreasing again. Bottom: Average episode length. This gives us a better idea of the performance of the agent since we can clearly see it is solving the episodes in a shorter number of steps during training.

If you test the trained algorithm it should be able to solve $\geq 94\%$ of the episodes within the maximum step limit. We even recorded video frames during training and the agent clearly knows what it is doing when you watch it in real-time. We have omitted a lot of this accessory code to keep the text clear; please see the GitHub repository for the complete code.

Maximum Entropy Learning. Notice we are using an epsilon-greedy policy with epsilon set to 0.5, hence the agent is taking random actions 50% of the time. We tested using a number of different epsilon levels but found 0.5 to be about the best. If you train the agent with epsilon values ranging from a low of 0.01, to 0.1, to 0.2, all the way to a high of say 0.95, you will notice the training performance follows an inverted-U curve, where too low of an epsilon leads to poor learning due to lack of exploration, and too high of an epsilon leads to poor learning due to lack of exploitation. So how can the agent perform so well even though it is acting randomly half the time? By setting the epsilon to be as high as it can until it degrades performance, we are utilizing an approximation to the principle of maximum entropy, or maximum entropy learning.

We can think of the entropy of an agent's policy as the amount of randomness it exhibits, and it turns out that maximizing entropy up until it starts to be counter-productive actually leads to better performance and generalization. If an agent can successfully achieve a goal even in the face of taking a high proportion of random agents, it must have a very robust policy that is insensitive to random transformations and thus it will be able to handle more difficult environments.

Curriculum Learning. We trained this agent only on the 5x5 version of this Gridworld environment so that it would have a small chance of randomly achieving the goal and receiving a reward. There are also bigger environments including a 16x16 environment, which would make randomly winning extremely unlikely. An alternative to curiosity learning (or in addition to) is to use a process called curriculum learning, which is when we train an agent on an easy variant of a problem, then re-train on a slightly harder variant, and keep re-training on harder and harder versions of the problem until it can successfully achieve the ultimate task that would have been too hard to start with. We could attempt to solve the 16x16 grid without curiosity by first training to maximum accuracy on the 5x5 grid, then re-train on the 6x6 grid, then the 8x8 grid and finally the 16x16 grid.

Visualizing Attention Weights. We know we can successfully train a relational DQN on this somewhat difficult Gridworld task, but we could have used a much less fancy DQN to do the same thing. What we also care about is visualizing the attention weights to see what exactly it has learned to focus on in playing the game. Some of the results are surprising, and some are what we would expect.

In order to visualize the attention weights, we had our model save a copy of the attention weights each time it is run forward and we can access it by calling `GWagent.att_map`, which returns a $batch \times head \times height \times width$ tensor. All we need to do is run the model forward on some state, select an attention head and select a node to visualize and then reshape the tensor into a 7×7 grid and plot it using `plt.imshow`.

```
>>> state_ = env.reset()
>>> state = prepare_state(state_)
>>> GWagent(state)
>>> plt.imshow(env.render('rgb_array'))
>>> plt.imshow(state[0].permute(1,2,0).detach().numpy())
>>> head, node = 2, 26
>>> plt.imshow(GWagent.att_map[0][head][node].view(7,7))
```

We decided to look at the attention weights for the key node, the door node, and the agent node to see which objects are related to each other. We found the node in the attention weights that corresponds to the corresponding node in the grid by counting the grid cells since both the attention weights and the original state are a 7×7 grid.

Here are the original full view of the grid in a random initial state and the corresponding prepared state:

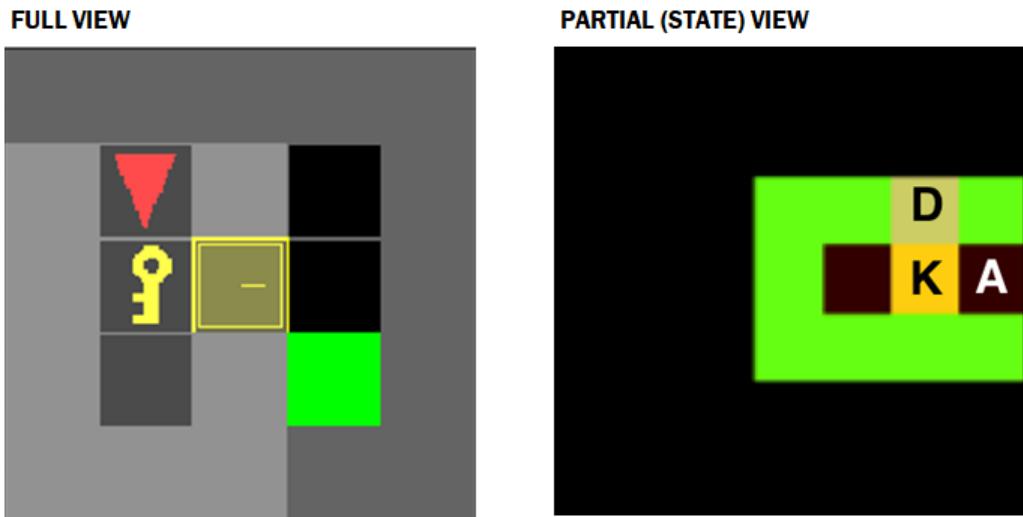


Figure 10.23 Left: The full observation of the environment. Right: The corresponding partial state view that the agent has access to.

The partial view is a little confusing at first because it is an egocentric view, so we annotated it with the positions of the agent (A), key (K) and the door (D). Because the agent's partial view is always 7×7 and the size of the full grid is only 5×5 , the partial view always includes some empty space. Now let's visualize the corresponding attention weights for this state.

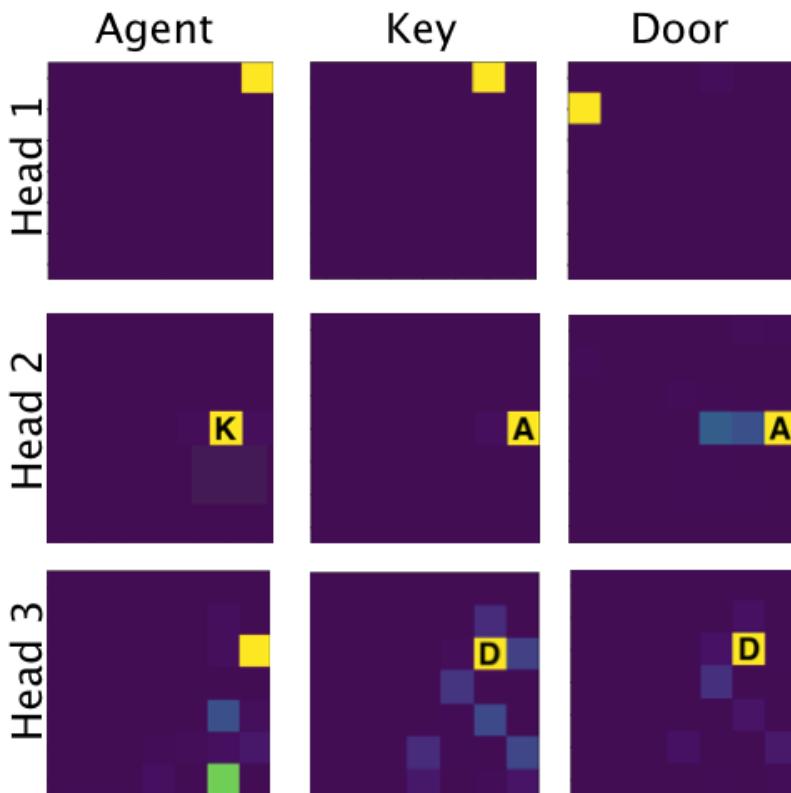


Figure 10.24 Each row corresponds to an attention head, e.g. row 1 corresponds to attention head 1. Left column: The self-attention weights for the agent, which shows the objects to which the agent is paying most attention. Middle column: The self-attention weights for the key, which shows the objects to which the key is paying most attention. Right column: The self-attention weights for the door.

Each column is labeled as a particular node's attention weights (i.e. the nodes to which it is paying attention), restricting ourselves to just the agent, key and door nodes out of a total of $7 \times 7 = 49$ nodes. Each row is an attention head, from head 1 to head 3, top to bottom. Curiously, attention head 1 does not appear to be focusing on anything obviously interesting, in fact it is focusing on grid cells in empty space. Note that while we're only looking at 3 of the 49 nodes, even after looking at all of the nodes, the attention weights are quite sparse, only a few grid cells at most are assigned any significant attention. But perhaps this isn't surprising as the attention heads appear to be specializing. Attention head 1 may be focusing on a small subset of landmarks in the environment to get an understanding of location and orientation. The fact that it can do this with just a few grid cells is impressive.

Attention heads 2 and 3 (rows 2 and 3 in Figure 10.23) are more interesting and are doing close to what we expect. Look at attention head 2 for the agent node, it is strongly attending

to the key (and essentially nothing else), which is exactly what we would hope given that at this initial state its first job is to pick up the key. Reciprocally, the key is attending to the agent, suggesting there is a bidirectional relation from agent to key and key to agent. The door is also attending to the agent most strongly, but there's also a small amount of attention given to the key and the space directly in front of the door.

Attention head 3 for the agent is attending to a few landmark grid cells, again, probably to establish a sense of position and orientation. Attention head 3 for the key is attending to door and the door is reciprocally attending to the key. Putting it all together we get that the agent is related to the key which is related to the door. If the goal square was in view, we might see that the door is also related to the goal. While this is a simple environment, it has relational structure that we can learn with a relational neural network, and we can inspect the relations that it learns. It is interesting how sparse the attention is assigned. Each node prefers to attend strongly to a single other node, with sometimes a couple other nodes that it weakly attends to.

Since this is a Gridworld, it is easy to partition the state into discrete objects, but in many cases such as the Atari games, the state is a big RGB pixel array and the objects we would want to focus on are collections of these pixels. In this case it becomes difficult to map the attention weights back to specific objects in the video frame, but we can still see which parts of the image the relational module as a whole is using to make its decisions. We tested a similar architecture on the Atari game Alien (we just used 4x4 kernel convolutions instead of 1x1 and added some maxpooling layers), and we can see that it indeed learns to focus on salient objects in the video frame (code not shown).

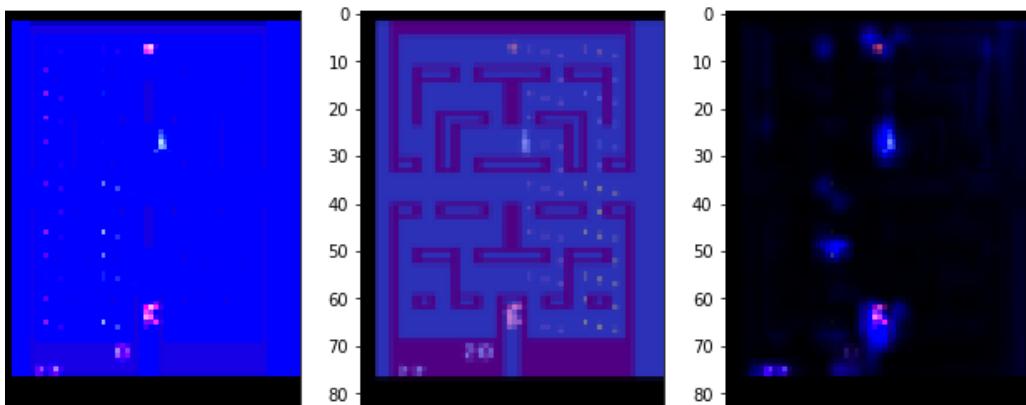


Figure 10.25 Left: preprocessed state given to the DQN. Middle: Raw video frame. Right: Attention map over state. We can see that the attention map is focused on the alien in the bottom center of the screen, the player in the center, and the bonus at the top, which are the most salient objects in the game.

Relational modules using the self-attention mechanism are powerful tools in the machine learning toolkit, and can be very useful for training RL agents where we want some idea of

how they're making decisions. Self-attention is one mechanism for performing message passing on a graph as we discussed and is part of the broader field of graph neural networks, which we encourage the reader to explore further. There are many implementations of graph neural networks (GNNs) but particularly relevant for us after this chapter is the Graph Attention Network that uses the same self-attention mechanism we just implemented but with the added ability to operate on more general graph structured data.

10.7 Summary

- Graph neural networks are machine learning models that operate on graph-structured data. Graphs are data-structures composed of a set of objects (called nodes) and relations between objects (called edges). A natural graph type is a social network in which the nodes are individuals and the edges between nodes represent friendships.
- An adjacency matrix is a matrix with dimensions $A:N \times N$ where N is the number of nodes in the graph that encodes the connectivity between each pair of nodes.
- Message passing is an algorithm for computing updates to node features by iteratively aggregating information from a node's neighbors.
- Inductive biases are the prior information we have about some set of data that we use to constrain our model toward learning certain kinds of patterns. In this chapter we employed a relational inductive bias, for example.
- We say a function f is invariant to some transformation g when the function's output remains unchanged when the input is first transformed by g , i.e. $f(g(x)) = f(x)$.
- We say a function f is equivariant to some transformation g when applying the transformation to the input is the same as applying the transformation to the output, i.e. $f(g(x)) = g(f(x))$.
- Attention models are designed to increase the interpretability and performance of machine learning models by forcing the model to only "look at" (attend to) a subset of the input data. By examining what the model learns to attend to, we can have a better idea of how it is making decisions.
- Self-attention models model attention between objects (or nodes) in an input rather than just the model attending to different parts of the input. This naturally leads to a form of graph neural network, since the attention weights can be interpreted as edges between nodes.
- Multi-head self-attention allows the model to have independent attention mechanisms that can each attend to a different subset of the input data. This allows us to still get interpretable attention weights but increases the bandwidth of information that can flow through the model.
- Relational reasoning is a form of reasoning based on objects and relationships between objects rather than using absolute frames of reference. E.g., "a book is on the top" relates the book to the table, rather than saying the book is at position 10 and the table is at position 8 (an absolute reference frame).
- Inner (dot) product is a product between two vectors that results in a single scalar

value.

- Outer product is a product between two vectors that results in a matrix.
- Einstein notation or Einsum lets us describe generalized tensor-tensor products called tensor contractions using a simple syntax based on labeling the indices of a tensor.
- Double Q-learning stabilizes training by separating action-selection and action-value updating.

11

In Conclusion: A Review and Roadmap

In this final chapter we first take a moment to briefly review what we've learned, highlighting and distilling what we think are the most important skills and concepts to take away. We have covered the fundamentals of reinforcement learning and if you have made it this far and have engaged with the projects, you're well-positioned to implement many other algorithms and techniques.

This book is a *course* on the fundamentals of Deep Reinforcement Learning, not a textbook or reference. That means we could not possibly have introduced all there is to know about DRL, and we had to make tough choices about what to leave out. There are a number of exciting topics in DRL we wished we could have included, and there are some topics that, despite being "industry standards," were inappropriate to include in a project-focused introductory book like this one. However, we wanted to leave you with a roadmap for where to go from here with your new skills. In the second part of this chapter we introduce at a high-level some topics, techniques and algorithms in DRL that are worth knowing if you're serious about continuing in the DRL field. Most of these areas were excluded because they involved advanced mathematics that we do not expect readers of this book to be familiar with and we did not have the space to teach more mathematics.

11.1 What did we learn?

Deep Reinforcement Learning is the combination of Deep Learning and Reinforcement Learning. Reinforcement learning is a framework for solving control tasks, which are problems in which an agent can take actions that lead to positive or negative rewards given some environment. The environment is the universe in which the agent acts. The agent can either have full access to the state (i.e. an instantaneous snapshot) of the environment or it may

only have partial access to the state of the environment, which is called partial observability. The environment evolves in discrete time steps according to some dynamical rules and at each time step the agent takes an action which may influence the next state. After taking each action, the agent receives feedback in the form of a reward signal. We described a mathematical formalization of this called the Markov Decision Process (MDP).

An MDP is a mathematical structure that includes a set of states S that the environment can be in, and a set of actions A that the agent can take, which may depend on the particular state of the environment. There is a reward function $R(s_t, a_t, s_{t+1})$ that produces the reward signal given the transition from the current state to the next state and the agent's action. The environment may evolve deterministically or stochastically, but in either case, agent initially does not know the dynamical rules of the environment and thus all state transitions must be described probabilistically from the perspective of the agent.

We therefore have a conditional probability distribution over next states s_{t+1} given the current state and the action taken by the agent at the current time step, denoted $\Pr(s_{t+1} | s_t, a_t)$. The agent follows some policy π which is a function that maps a probability distribution over actions given the current state s_t , i.e. $\pi: S \rightarrow \Pr(A)$. The objective of the agent is to take actions that maximize the time-discounted cumulative rewards over some time horizon. The time-discounted cumulative reward is termed the return (often denoted with the character G or R), and is equal to:

$$G_t = \sum_t \gamma^t r_t$$

The return G_t at time t is equal to the sum of discounted rewards for each time step until the end of the episode (for episodic environments) or until the sequence converges for non-episodic environments. The γ factor is a parameter in the interval $(0,1)$ and is the discount rate that determines how quickly the sequence will converge, and thus how much the future is discounted. A discount rate close to 1 will mean that future rewards are given similar weight to immediate rewards (optimizing over the long-term), whereas a low discount rate leads to preferring only short-term time horizons.

A derived concept from this basic MDP framework is that of a value function. A value function assigns a value to either states or state-action pairs (i.e. a value for taking an action in a given state), with the former being called a state-value function (or often just the value function) and the latter being the action-value or Q -function. The value of a state is simply the expected return given the agent starts in that state and follows some policy π , hence value functions implicitly depend on the policy. Similarly, the action-value or Q -value of a state-action pair is the expected return given the agent takes the action in that state and follows the policy π until the end. A state that puts the agent in close position to win a game, for example, would be assigned a high state-value assuming the underlying policy was reasonable. We denote the value function as $V_\pi(s)$ with the subscript π indicating the dependence of the value on the underlying policy, and the Q -function as $Q_\pi(s, a)$, although we often drop the π subscript for convenience.

Right now we understand the function $Q_\pi(s,a)$ as being some sort of black-box that tells you the exact expected rewards for state action a in state s , but of course, we do not have access to such an all-knowing function, we have to estimate it. In this book we used neural networks to estimate value functions and policy functions although any suitable function could work. In the case of a neural-based $Q_\pi(s,a)$, we trained neural networks to predict the expected rewards. The value functions are defined and approximated recursively, such that $Q_\pi(s,a)$ is updated as:

$$V_\pi(s) = r_t + \gamma V_\pi(s')$$

Where s' refers to the next state, or s_{t+1} . For example, in Gridworld landing on the goal tile results in +10, landing on the pit results in -10 and losing the game, and all other non-terminal moves are penalized at -1. If the agent was 2 steps away from the winning goal tile, then the final state reduces to $V_\pi(s_3)=10$. Then if $\gamma=0.9$, the previous state is valued at $V_\pi(s_2) = r_2 + 0.9 V_\pi(s_3) = -1 + 9 = 8$. And the move before that must be $V_\pi(s_1) = r_1 + 0.9 V_\pi(s_2) = -1 + 0.9 \cdot 8 = 5.4$. As you can see, states farther from the winning state are valued less. Training a reinforcement learning agent then just amounts to successfully training a neural network to either approximate the value function (so the agent will choose actions that lead to high-value states) or directly approximate the policy function by observing rewards after actions and reinforcing actions based on the rewards received. Both approaches have their pros and cons, but often times we combine learning both a policy and a value function together, which is called an actor-critic algorithm where the actor refers to the policy and the critic refers to the value function.

11.2 The Uncharted Topics in Deep Reinforcement Learning

The Markov decision process framework and value and policy functions we just reviewed were detailed in chapters 2-5. We then spent the rest of the book implementing more sophisticated techniques for successfully training value and policy functions in difficult environments (e.g. environments with sparse rewards) and environments with multiple interacting agents. Unfortunately, there were many exciting things we didn't have the space to cover, so we end the book with a brief tour of some other areas in deep reinforcement learning you might want to explore. We only give a taste of a few topics we think are worth exploring more and hope you will look into these areas more deeply on your own.

11.2.1 Prioritized Experience Replay

We briefly mentioned the idea of prioritized replay earlier in the book when we decided to add multiple copies of the same experience to the replay memory if the experience led to a winning state. Since winning states are rare and we want our agent to learn from these informative events, we thought that adding multiple copies would ensure that each training epoch would include a few of these winning events. This was a very unsophisticated means of prioritizing experiences in the replay based on how informative they are in training the agent.

The term prioritized experience replay generally refers to a specific implementation introduced in an academic paper called *Prioritized Experience Replay* by Schaul et al 2015 and uses a much more sophisticated mechanism to prioritize experiences. In their implementation, all experiences are recorded just once unlike our approach, however, rather than selecting a minibatch from the replay completely randomly (i.e. uniformly), they preferentially select experiences that are more informative. They defined informative experiences as not merely those that led to a winning state like we did, but rather those where the DQN had a high error in predicting the reward. In essence, the model preferentially trains on the most surprising experiences. As the model trains, however, the once surprising experiences become less surprising, and the preferences get continually re-weighted. This leads to substantially improved training performance. This kind of prioritized experience replay is a standard practice for value-based reinforcement learning, whereas policy-based reinforcement learning still tends to rely on using multiple parallelized agents and environments.

11.2.2 Proximal Policy Optimization (PPO)

We mostly implemented Deep Q-networks (DQN) in this book rather than policy functions, and this is for good reason. The (deep) policy function we implemented in chapters 4 and 5 were rather unsophisticated and would not work very well for more complex environments. The problem is not with the policy networks themselves but with the training algorithm. The simple REINFORCE algorithm we used is fairly unstable. When the rewards vary significantly from action to action the REINFORCE algorithm does not lead to stable results. We need a training algorithm that enforces smoother, more constrained updates to the policy network.

Proximal Policy Optimization (PPO) is a more advanced training algorithm for policy methods that allows for far more stable training. It was introduced in the paper *Proximal Policy Optimization Algorithms* by Schulman et al 2017 at OpenAI. We did not cover PPO in this book because, while the algorithm itself is relatively simple, understanding it requires more mathematical machinery that is outside the scope of this introductory book. Making Deep Q-learning more stable required only a few intuitive upgrades like adding a target network and implementing double Q-learning, so that is why we preferred to use value learning over policy methods in this book. However, in many cases directly learning a policy function is more advantageous than a value function such as for environments with a continuous action space, since we cannot create a DQN that returns an infinite number of Q-values for each action.

11.2.3 Hierarchical Reinforcement Learning and the Options Framework

When a child learns to walk she isn't thinking about which individual muscle fibers to activate and for how long, or when a businessperson is debating a business decision with colleagues they aren't thinking about the individual sequences of sounds they need to make for the other people to understand their business strategy. Our actions exist at various levels of abstraction down from moving individual muscles up to grand schemes. This is just like noticing that a story is made up of individual letters, but those letters are composed into words that are

composed into sentences and paragraphs and so on. The writer may be thinking of a general next scene in her story and only once decided on this will she actually get to typing out individual characters.

All the agents we've implemented in this book are operating at the level of typing out individual characters so to speak; they are incapable of thinking at a higher-level. Hierarchical reinforcement learning is an approach to solving this problem, allowing agents to build up higher-level actions from lower ones. Rather than our Gridworld agent deciding one step at a time what to do, it might survey the board and decide on a higher-level sequence of actions. It might learn re-usable sequences such as "move all the way up" or "move around obstacle" that can be implemented in a variety of game states.

The success of deep learning in reinforcement learning is due to their ability to represent complex high-dimensional states into a hierarchical of higher-level state representations. In hierarchical reinforcement learning, the goal is to extend this to representing states *and* actions hierarchically. One popular approach to this is called the options framework.

Consider Gridworld, it has 4 primitive actions of up, right, left, down and each action lasts one time step. In the options framework, there are options rather than just primitive actions. An option is the combination of an option-policy (which just like a regular policy takes a state and returns a probability distribution over actions), a termination condition, and an input set (which is a subset of states). The idea is that a particular option gets triggered when the agent encounters a state in the option's input set, and then that particular option's policy is run until the termination condition is met, at which point a different option may be selected. These option policies might be simpler policies than a single big deep neural network policy that we have implemented in this book. But by intelligently selecting these more high-level options efficiencies can be gained by not having to use a more computationally intensive policy for taking each primitive step.

11.2.4 Model-Based Planning

We already discussed the idea of models in reinforcement learning in two contexts. In the first, a model is simply another term for an approximating function like a neural network. We sometimes just refer to our neural network as a model since it approximates or models the value function or the policy function. The other context is when we refer to model-based versus model-free learning. In both cases we are using a neural network as a model of the value function or a policy, but in this case model-based means the agent is making decisions based on an explicitly constructed model of the dynamics of the environment itself rather than just its value function. In model-free learning all we care about is learning to accurately predict rewards which may or may not require a deep understanding of how the environment actually works. In model-based, we actually want to learn how the environment works. Metaphorically, in model-free learning we are satisfied knowing that there is something called gravity that makes things fall and we make use of this phenomenon but in model-based learning we want to actually approximate the laws of gravity.

Our model-free DQN worked surprisingly well, especially when combined with other advances like curiosity, so what is the advantage of explicitly learning a model of the environment? With an explicit and accurate environment model, the agent can learn to make long-term plans rather than just deciding which next action to take. By using its environment model to predict the future several time steps ahead, it can evaluate the long-term consequences of its immediate actions and this can lead to faster learning (due to increased sample efficiency). This is related to but not necessarily the same as the hierarchical reinforcement learning we discussed since hierarchical reinforcement learning does not necessarily depend on an environment model. But with an environment model, the agent can plan out a sequence of primitive actions to accomplish some higher-level goal.

The simplest way to train an environment model is to just have a separate deep learning module that predicts future states. In fact we did just that in Chapter 8 on curiosity-based learning, however, we did not use the environment model to plan or look into the future, we only used it to explore surprising states. But with a model $M(s_t)$ that takes a state and returns a predicted next state s_{t+1} , we could then take that predicted next state and feed it back into the model to get the predicted state s_{t+2} and so on. The distance into the future we could predict depends on the inherent randomness in the environment and the accuracy of the model, but even if we could only accurately predict out to a few time steps into the future this would be immensely useful.

11.2.5 Monte Carlo Tree Search (MCTS)

Many games have a finite set of actions and a finite length such as Chess, Go and Tic-Tac-Toe. The Deep Blue algorithm that IBM developed to play Chess didn't use machine learning at all, it was a brute force algorithm that used a form of tree-search. Consider the game of Tic-Tac-Toe. It is a two-player game typically played on a square 3x3 grid where player 1 places an X-shaped token and player 2 places an O-shaped token. The goal of the game is to be the first to get 3 of your tokens lined up in a row, column or diagonal.

The game is so simple that the human strategy also generally involves limited tree search. If you're player 2 and there's already one opposing token on the grid, you can consider all possible responses to all possible open spaces you have and you can keep doing this until the end of the game. Of course, even for a 3x3 board, the first move has 9 possible actions, and there are 8 possible actions by player 2, and then 7 possible actions for player 1 again, so the number of possible trajectories (the game tree) becomes quite large, but a brute force exhaustive search like this could be guaranteed win at tic-tac-toe assuming the opponent isn't using the same approach.

For a game like Chess, the game tree is far too large to use a completely brute force search of the game tree; one must necessarily limit the number of potential moves to consider. Deep Blue used a tree search algorithm that is more efficient than exhaustive search but still involved no learning. It still amounted to searching possible trajectories and just computing which ones led to winning states.

Another approach is Monte Carlo Tree Search, in which you use some mechanism of randomly sampling a set of potential actions and expanding the tree from there, rather than consider *all* possible actions. The AlphaGo algorithm developed by DeepMind to play the game Go used a deep neural network to evaluate which actions are worth doing a tree search on and also to decide the value of selected moves. Therefore Alpha Go combined brute-force search with deep neural networks to get the best of both. These types of combination algorithms are currently state-of-the-art for games in the class of Chess and Go.

11.3 The End

Thank you for reading our book! We really hope you have learned a satisfying amount of deep reinforcement learning. Please reach out to us in the forums at Manning.com for any questions or comments. We look forward to hearing from you.

A

Mathematics, Deep Learning, PyTorch

While the intended reader already has some basic knowledge of deep learning (i.e. has actually implemented a simple neural network before), we include this appendix that serves as a rapid review of deep learning, the relevant mathematics we use in this book, and how to implement deep learning models in PyTorch. We cover these topics by demonstrating how to implement a deep learning model in PyTorch to classify images of handwritten digits from the famous MNIST dataset.

A.1 Mathematics of Deep Learning

Deep Learning algorithms, which are also called artificial neural networks, are relatively simple mathematical functions and mostly just require an understanding of vectors and matrices. Training a neural network, however, requires an understanding of the basics of calculus, namely the derivative. The fundamentals of *applied* deep learning therefore require only knowing how to multiply vectors and matrices and take the derivative of multivariable functions, which we review here. *Theoretical* machine learning refers to the field that rigorously studies the properties and behavior of machine learning algorithms and yields new approaches and algorithms. Theoretical machine learning involves advanced graduate-level mathematics that covers a wide variety of mathematical disciplines that are outside the scope of this book. In this book we only utilize informal mathematics in order to achieve our practical aims, not rigorous proof-based mathematics.

A.1.1 Linear Algebra

Linear algebra is the study of linear transformations. A linear transformation is a transformation (e.g. a function) in which the sum of the transformation of two inputs separately, e.g. $T(a)$ and $T(b)$, is the same as summing the two inputs and transforming them together, i.e. $T(a+b)=T(a)+T(b)$. A linear transformation also has the property that $T(a \cdot b)=a \cdot T(b)$. Linear transformations are said to preserve the operations of addition and multiplication since you can apply these operations either before or after the linear transformation and the result is the same.

One informal way to think of this is that linear transformations do not have "economies of scale." Think of a linear transformation as converting money as the input into some other resources like gold, so that $T(\$100)=1$ unit of gold, for example. The unit price of gold will be constant no matter how much money you put in. In contrast, non-linear transformations might give you a "bulk discount" so that if you buy 1000 units of gold or more the price would be less on a per unit basis than if you buy less than 1000 units.

Another way to think of linear transformations is to make a connection to calculus (which we review in more detail later). A function or transformation takes some input value x and maps it to some output value y . A particular output y may be a larger or smaller value than the input x , or more generally a neighborhood around an input x will be mapped to a larger or smaller neighborhood around the output y . Here a neighborhood means the set of points arbitrarily close to x or y . For a single-variable function like $f(x)=2x+1$ a neighborhood is actually an interval. For example, the neighborhood around an input point $x=2$ would be all the points arbitrarily close to 2, such as 2.000001 and 1.9999999.

One way to think of the derivative of a function at a point is as the ratio of the size of the output interval around that point to the size of the input interval around the input point. Linear transformations will always have some constant ratio of output to input intervals for all points, whereas non-linear transformations will have a varying ratio.

Linear transformations are often represented as matrices, which are rectangular grids of numbers. Matrices encode the coefficients for multivariable linear functions such as:

$$f_x(x, y) = Ax + By$$

$$f_y(x, y) = Cx + Dy$$

While this appears to be two functions, this is really a single function that maps a 2-dimensional point (x, y) to a new 2-dimensional point (\hat{x}, \hat{y}) using the coefficients A, B, C, D . To find \hat{x} you use the f_x function and to find \hat{y} you use the f_y function. We could have written this as a single line:

$$f(x, y) = (Ax + By, Cx + Dy)$$

This makes it more clear the output is a 2-tuple or 2-dimensional vector. In any case, it is useful to think of each of this function in two separate pieces since the computations for the x

and y components are independent. While the mathematical notion of a vector is very general and abstract, for machine learning, a vector is just a 1-dimensional array of numbers. This linear transformation takes a 2-vector (has 2 elements) and turns it into another 2-vector, and to do this it requires 4 separate pieces of data, the 4 coefficients. There is a difference between a linear transformation like $Ax+By$ and something like $Ax+By+C$ which adds a constant; the latter is called an **affine** transformation. In practice, we use affine transformations in machine learning, but for this discussion we will stick with just linear transformations.

Matrices are a convenient way to store these coefficients. We can package these data into a 2-by-2 matrix:

$$F = \begin{bmatrix} A & B \\ C & D \end{bmatrix}$$

The linear transformation is now represented completely by this matrix and an implicit understanding of how to use it. We can apply this linear transformation by juxtaposing the matrix with a vector, e.g. Fx .

$$F = \begin{bmatrix} A & B \\ C & D \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$

We compute the result of this transformation by multiplying each row in F with each column (only one here) of x . If you do this you get the same result as the explicit function definition above. Matrices do not need to be square, they can be any rectangular shape.



We can graphically represent matrices as boxes with two strings coming out on each end with labeled indices. We call this a string diagram. The n represents the dimensionality of the input vector and the m is the dimensionality of the output vector. You can imagine a vector flowing into the linear transformation from the left and a new vector is produced on the right side. For the practical deep learning we use in this book, you only need to understand this much linear algebra, i.e. the principles of multiplying vectors by matrices. Any additional math will be introduced in the respective chapters.

A.1.2 Calculus

Calculus is essentially the study of differentiation and integration. In deep learning, we only really need to use differentiation. Differentiation is the process of getting a derivative of a

function. We already introduced one notion of derivative, i.e. the ratio of an output interval to the input interval. It tells you how much the output space is stretched or squished. Importantly, these intervals are oriented intervals so they can be negative or positive, and thus the ratio can be negative or positive. For example, take the function $f(x)=x^2$. Take a point x and its neighborhood $(x-\epsilon, x+\epsilon)$ where ϵ is some arbitrarily small value and we get an interval around x . To be concrete, let $x=3, \epsilon=0.1$. So the interval around $x=3$ is $(2.9, 3.1)$. The size (and orientation) of this interval is $3.1-2.9=+0.2$. This interval gets mapped to $f(2.9)=8.41$ and $f(3.1)=9.61$. This output interval is $(8.41, 9.61)$ and its size is $9.61-8.41=1.2$. As you can see, the output interval is still positive so the ratio $df/dx=1.2/0.2=6$, which is the derivative of the function f at $x=3$. We denote the derivative of a function f with respect to an input variable x as df/dx , but this is not to be thought as a literal fraction; it's just a notation. We don't need to take an interval on both sides of the point; an interval on one side will do as long as its small, i.e. we can define an interval as $(x, x+\epsilon)$ and the size of the interval is just ϵ whereas the size of the output interval is $f(x+\epsilon) - f(x)$.

Using concrete values like we did only yields approximations in general, to get absolutes we'd need to use infinitely small intervals. We can do this symbolically by imagining that ϵ really is an infinitely small number such that it is bigger than 0 but smaller than any number other number in our number system. Now differentiation becomes an algebra problem.

$$f(x) = x^2 \tag{1}$$

$$\frac{df}{dx} = \frac{f(x + \epsilon) - f(x)}{\epsilon} \tag{2}$$

$$= \frac{(x + \epsilon)^2 - x^2}{\epsilon} \tag{3}$$

$$= \frac{x^2 + 2x\epsilon + \epsilon^2 - x^2}{\epsilon} \tag{4}$$

$$= \frac{\epsilon(2x + \epsilon)}{\epsilon} \tag{5}$$

$$= 2x + \epsilon \tag{6}$$

$$2x \approx 2x + \epsilon \tag{7}$$

Here we simply take the ratio of the output interval to the input interval, both of which are infinitely (or arbitrarily) small (infinitesimal) because ϵ is an infinitesimal number. We can algebraically reduce the expression to $2x+\epsilon$ and since ϵ is infinitesimal, $2x+\epsilon$ is infinitely close to just $2x$ which we take as the true derivative of the original function $f(x)=x^2$. Remember, we're taking ratios of oriented intervals that can be positive or negative. We not only want to know how much a function stretches (or squeezes) the input but whether it changes the direction of the interval. There is a lot of advanced mathematics justifying all of this (see non-standard analysis) but this process works just fine for practical purposes.

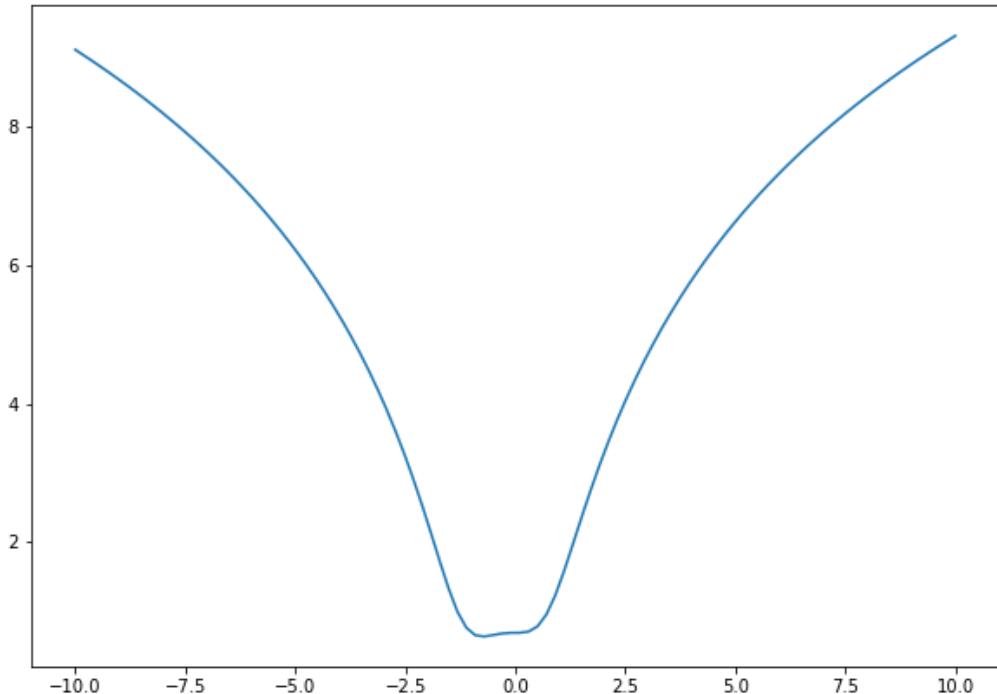
Why is differentiation a useful concept in deep learning? Well, in machine learning we are trying to **optimize** a function, which means either find the input points to the function such that the output of the function is a maximum or minimum over all possible inputs. That is, given some function $f(x)$, we want to find an x such that $f(x)$ is smaller than any other choice of x , we generally denote this as $\text{argmin}(f(x))$. Usually we have a loss (aka cost or error) function that takes some input vector, a target vector and parameter vector and returns the degree of error between the predicted output and the true output and our goal is to find the set of parameters that minimizes this error function. There are many possible ways to minimize this function, not all of which depend on using derivatives but in most cases the most effective and efficient way to optimize loss functions in machine learning is to use derivative information.

Since deep learning models are non-linear (i.e. they do not preserve addition and scalar multiplication), the derivatives are not constant like in linear transformations. The amount and direction of squishing or stretching that is happening from input to output points varies from point to point. In another sense, it tells us which direction the function is curving, so we can follow the curve downward to the lowest point. Multivariable functions like deep learning models don't just have a single derivative but a set of *partial* derivatives that describe the curvature of the function with respect to each individual input component. This way we can figure out which sets of parameters for a deep neural network lead to the smallest error.

The simplest example of using derivative information to minimize a function is to see how it works for a simple compositional function. The function we will try to find the minimum of is:

$$f(x) = \log(x^4 + x^3 + 2)$$

Whose graph looks like:



You can see visually that the minimum of this function appears to be near around -1.0. This is a compositional function because it contains a polynomial expression “wrapped” in a logarithm, so we need to use the chain rule from calculus to compute the derivative. We want the derivative of this function with respect to x . This function only has one “valley” therefore it will only have one minimum; however, deep learning models are high-dimensional and highly compositional and tend to have many minima. Ideally, we’d like to find the global minimum which is the lowest point in the function. A global or local minimum are points on the function where the slope (i.e. derivative) at those points are 0. Some functions like this simple example we can compute the minimum analytically, i.e. using algebra. Deep learning models are generally too complex for algebraic calculations and we must use iterative techniques.

The chain rule in calculus gives us a way of computing derivatives of compositional functions by decomposing it into pieces. If you’ve heard of backpropagation, it’s basically just the chain rule applied to neural networks with some tricks to make it more efficient. For our example case, let’s re-write the above function as two functions:

$$h(x) = x^4 + x^3 + 2$$

$$f(x) = \log(h(x))$$

We first compute the derivative of the “outer” function which is $f(x)=\log(h(x))$, but this just gives us df/dh and what we really want is df/dx . You may have learned that the derivative of natural-log is:

$$\frac{d}{dx} \log(x) = \frac{1}{x}$$

And the derivative of the inner function $h(x)$ is:

$$\frac{d}{dx}(x^4 + x^3 + 2) = 4x^3 + 3x^2$$

To get the full derivative of the compositional function, we notice that:

$$\frac{df}{dx} = \frac{df}{dh} \cdot \frac{dh}{dx}$$

That is, the derivative we want, df/dx is obtained by multiplying the derivative of the outer function with respect to its input and the inner function (the polynomial) with respect to x .

$$\frac{df}{dh} = \frac{1}{h(x)} \cdot \frac{dh}{dx}$$

$$\frac{df}{dh} = \frac{1}{x^4 + x^3 + 2} \cdot (4x^3 + 3x^2)$$

$$\frac{df}{dh} = \frac{4x^3 + 3x^2}{x^4 + x^3 + 2}$$

You can set this derivative to 0 calculate the minima algebraically, $4x^2+3x=0$. This function has two minima at $x=0$ and $x=-3/4=-0.75$. But only $x=-0.75$ is the global minimum since $f(-0.75)=0.638971$ whereas $f(0)=0.693147$ which is slightly larger.

Let’s see how we can solve this using gradient descent, which is an iterative algorithm to find the minima of a function. The idea is we first start with a random x as a starting point. We then compute the derivative of the function at this point which tells us the magnitude and direction of curvature at this point. We then choose a new x point based on the old x point, it’s derivative, and a step size parameter to control how fast we move. That is,

$$x_{new} = x_{old} - \alpha \frac{df}{dx}$$

Let’s see how to do this in code.

Listing A.1: Gradient Descent

```

import numpy as np

def f(x): #A
    return np.log(np.power(x,4) + np.power(x,3) + 2)

def dfdx(x): #B
    return (4*np.power(x,3) + 3*np.power(x,2)) / f(x)

x = -9.41 #C
lr = 0.001 #D
epochs = 5000 #E
for i in range(epochs):
    deriv = dfdx(x) #F
    x = x - lr * deriv #G

#A The original function
#B The derivative function
#C Random starting point
#D Learning rate (step size)
#E Number of iterations to optimize over
#F Calculate derivative of current point
#G Update current point

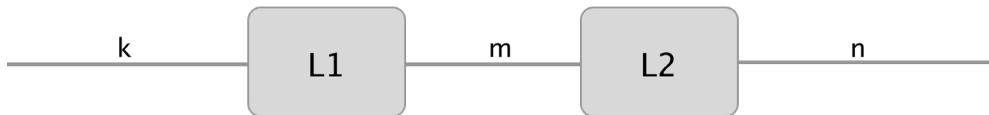
```

If you run this gradient descent algorithm, you should get $x=-0.750000000882165$, which is (if rounded) exactly what you get when calculated algebraically. This simple process is the same one we use when training deep neural networks, except that deep neural networks are multivariable compositional functions and so we are using partial derivatives. A partial derivative is no more complex than a normal derivative.

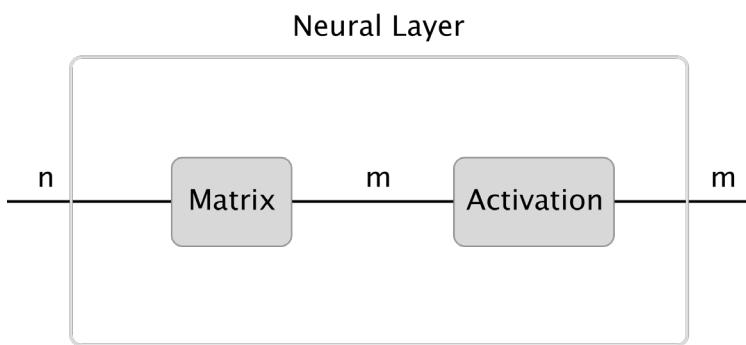
Consider the multivariable function $f(x,y)=x^4+y^2$. There is no longer a single derivative of this function since it has two input variables. We can take the derivative with respect to x or y or both. When we take the derivative of a multivariable function with respect to all of its inputs and package this into a vector, we call it the **gradient**, which is denoted by the nabla symbol ∇ , i.e. $\nabla f(x) = [df/dx, df/dy]$. To compute the partial derivative of f with respect to x , i.e. df/dx we simply set the other variable y to be a constant and differentiate as usual. In this case, $df/dx=4x^3$ and $df/dy=2y$. So the gradient $\nabla f(x)=[4x^3,2y]$, which is the vector of partial derivatives. Then we can run gradient descent as usual, except now we find the vector associated with the lowest point in an error function of the deep neural network.

A.1.3 Deep Learning

A deep neural network is simply a composition of multiple layers of simpler functions called layers. Each layer function consists of a matrix multiplication followed by a non-linear **activation function**. The most common activation function is $f(x)=\max(0,x)$ which returns 0 if x is negative or returns x otherwise. A simple neural network might be:



Read this diagram from left to right as if data flows in from the left into the L1 function then L2 function and then becomes the output on the right. The symbols k, m, n refer to the dimensionality of the vectors. A k-length vector is input to function L1, which produces an m-length vector then gets passed to L2, which finally produces an n-dimensional vector. Now let's look and see what each of these L functions are doing.



A neural network layer, generically, consists of two parts: a matrix multiplication and an activation function. An n-length vector comes in from the left, gets multiplied by a matrix (often called a parameter or weight matrix) which may change the dimensionality of the resulting output vector. The output vector now of length m gets passed through an non-linear activation which does not change the dimensionality of the vector. A deep neural network is just stacking these layers together and we train it by applying gradient descent on the weight matrices which are the parameters of the neural network. Here's a simple 2-layer neural network in Numpy.

Listing A.2: Simple Neural Network

```
def nn(x,w1,w2):
    l1 = x @ w1 #A
    l1 = np.maximum(0,l1) #B
    l2 = l1 @ w2
    l2 = np.maximum(0,l2)
    return l2

w1 = np.random.randn(784,200) #C
w2 = np.random.randn(200,10)
x = np.random.randn(784) #D
nn(x,w1,w2)

array([326.24915523,     0.          ,     0.          , 301.0265272 ,
```

```
188.47784869,    0.        ,    0.        ,    0.        ,
 0.        ,    0.        ])
```

#A Matrix multiplication
#B Non-linear activation function
#C Weight (parameter) matrix, initialized randomly
#D Random input vector

In the next section learn how to use the PyTorch library to automatically compute gradients for us to easily train neural networks.

A.1.4 PyTorch

In the previous sections we learned how to use gradient descent to find the minimum of a function, but in order to do that we needed the gradient. With our simple example we could compute the gradient with paper and pencil. With deep learning models that is impractical, so we rely on libraries like PyTorch that provide **automatic differentiation** capabilities to make it much easier. The basic idea is that in PyTorch we create a **computational graph** similar to the diagrams we used above, where relations between inputs, outputs and connections between different functions are made explicit and kept track of so we can easily apply the chain rule automatically to compute gradients. Fortunately, switching from numpy to PyTorch is simple, and most of the time we can just replace `numpy` with `torch.` Let's translate our neural network from above into PyTorch:

Listing A.3: PyTorch Neural Network

```
import torch

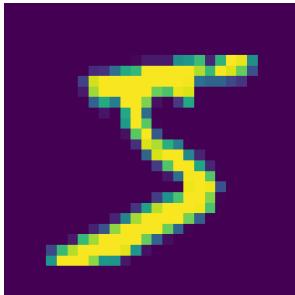
def nn(x,w1,w2):
    l1 = x @ w1 #A
    l1 = torch.relu(l1) #B
    l2 = l1 @ w2
    return l2

w1 = torch.randn(784,200,requires_grad=True) #C
w2 = torch.randn(200,10,requires_grad=True)
```

#A Matrix multiplication
#B Non-linear activation function
#C Weight (parameter) matrix, with gradients tracked

This looks almost identical to the numpy version except that we use `torch.relu` instead of `np.maximum` but they are the same function. We also added a `requires_grad=True` parameter to the weight matrix setup. This tells PyTorch that these are trainable parameters that we want to track gradients for, whereas `'x'` is an input not a trainable parameter. We also got rid of the last activation function for reasons that will become clear.

For this example, we will use the famous MNIST data set that contains images of handwritten digits from 0 to 9, such as this:



We want to train our neural network to recognize these images and classify them as their respective digits 0 through 9. PyTorch has a related library that lets us easily download this data set.

Listing A.4: Classifying MNIST using a neural network

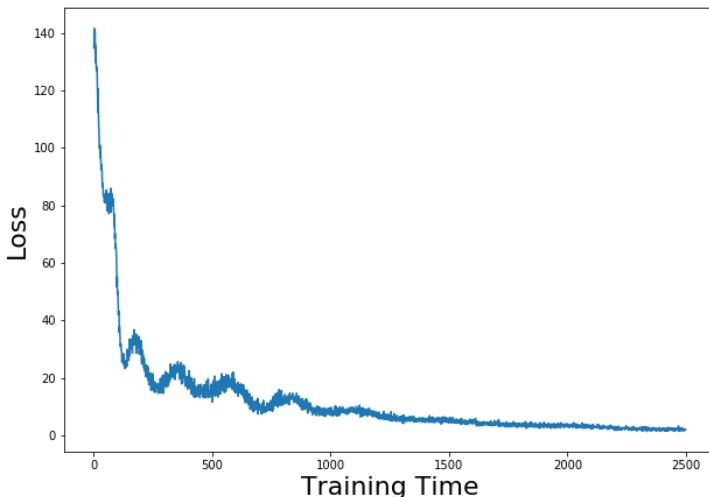
```

mnist_data = TV.datasets.MNIST("MNIST", train=True, download=False) #A

lr = 0.001
epochs = 2000
batch_size = 100
lossfn = torch.nn.CrossEntropyLoss() #B
for i in range(epochs):
    rid = np.random.randint(0,mnist_data.train_data.shape[0],size=batch_size) #C
    x = mnist_data.train_data[rid].float().flatten(start_dim=1) #D
    x /= x.max() #E
    pred = nn(x,w1,w2) #F
    target = mnist_data.train_labels[rid] #G
    loss = lossfn(pred,target) #H
    loss.backward() #I
    with torch.no_grad(): #J
        w1 -= lr * w1.grad #K
        w2 -= lr * w2.grad

```

#A Download and load the MNIST dataset
#B Setup a loss function
#C Get a set of random index values
#D Subset the data and flatten the 28x28 images into 784 vectors
#E Normalize the vector to be between 0 and 1
#F Make a prediction using the neural network
#G Get the ground-truth image labels
#H Compute the loss
#I Backpropagate
#J Do not compute gradients in this block
#K Gradient descent over the parameter matrices



Believe it or not but this short code snippet trains a complete neural network to successfully classify MNIST digits at around 70% accuracy. We just implemented gradient descent exactly the same way we did with our toy log-polynomial function, but PyTorch handled the gradients for us. Since the gradient of the neural network's parameters depends on the input data, each time we run the neural network "forward" with a new random sample of images, the gradients will be different. So we run the neural network forward with a random sample of data, PyTorch keeps track of the computations that occur, and when we're done, we call the `backward()` method on the last output, in this case it is generally the loss. The backward method uses automatic differentiation to compute all gradients for all PyTorch variables that have `requires_grad=True` set. Then we can update the model parameters using gradient descent. We wrap the actual gradient descent part in the `torch.no_grad()` context because we don't want it to keep track of these computations.

We can easily achieve greater than 95% accuracy by improving the training algorithm by using a more sophisticated version of gradient descent. We implemented our own version of **stochastic gradient descent**, the stochastic part because we are randomly taking subsets from the dataset and computing gradients based on that, which gives us noisy estimates of the true gradient given the full set of data. PyTorch includes built-in optimizers, of which stochastic gradient descent (SGD) is one. The most popular alternative is called Adam, which is a more sophisticated version of SGD. We just need to instantiate the optimizer with the model parameters.

Listing A.5: Using the Adam Optimizer

```
mnist_data = TV.datasets.MNIST("MNIST", train=True, download=False)

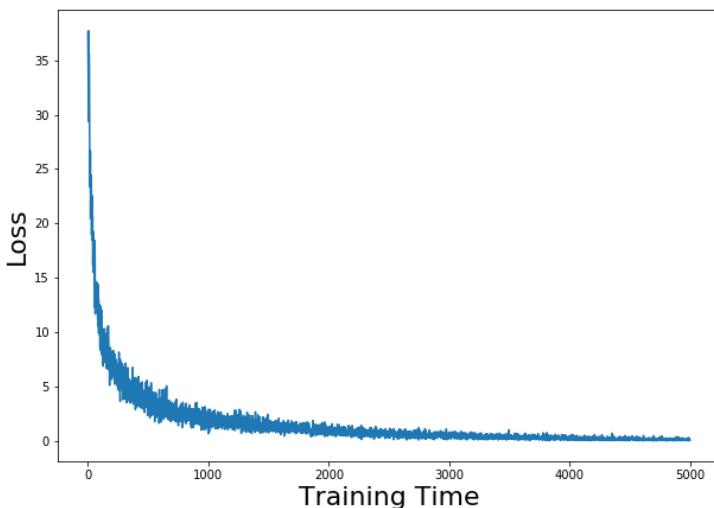
lr = 0.001
epochs = 5000
batch_size = 500
```

```

lossfn = torch.nn.CrossEntropyLoss() #A
optim = torch.optim.Adam(params=[w1,w2],lr=lr) #B
for i in range(epochs):
    rid = np.random.randint(0,mnist_data.train_data.shape[0],size=batch_size)
    x = mnist_data.train_data[rid].float().flatten(start_dim=1)
    x /= x.max()
    pred = nn(x,w1,w2)
    target = mnist_data.train_labels[rid]
    loss = lossfn(pred,target)
    loss.backward() #C
    optim.step() #D
    optim.zero_grad() E

```

#A Setup the loss function
#B Setup the ADAM optimizer
#C Backpropate
#D Update the parameters
#E Reset the gradients



You can see that the loss function is much smoother now with the Adam optimizer and it dramatically increases the accuracy of our neural network classifier. And that is the fundamental idea behind deep learning.