

Data Driven Science & Engineering

Machine Learning, Dynamical Systems, and Control

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Chapter 11

Reinforcement Learning

Reinforcement learning (RL) is a major branch of machine learning that is concerned with how to learn control laws and policies to interact with a complex environment from experience [695, 369]. Thus, RL is situated at the growing intersection of control theory and machine learning [601], and it is among the most promising fields of research towards generalized artificial intelligence and autonomy. Both machine learning and control theory fundamentally rely on optimization, and likewise, RL involves a set of optimization techniques within an experiential framework for learning how to interact with the environment.

In reinforcement learning, an *agent*¹ senses the state of its environment and learns take appropriate actions to optimize future rewards. The ultimate goal in RL is to learn an effective control strategy or set of actions through positive or negative reinforcement. This search may involve trial-and-error learning, model-based optimization, or a combination of both. In this way, reinforcement learning is fundamentally biologically inspired, mimicking how animals learn to interact with their environment through positive and negative reward feedback from trial-and-error experience. Much of the history of reinforcement learning, and machine learning more broadly, has been linked to studies of animal behavior and the neurological basis of decisions, control, and learning [521, 657, 201, 199]. For example, Pavlov's dog is an illustration that animals learn to associate environmental cues with a food reward [563]. The term *reinforcement* refers to the rewards, such as food, used to reinforce desirable actions in humans and animals. However, in animal systems reinforcement is ultimately achieved through cellular and molecular learning rules.

Multiple textbooks have been written on this topic, which spans almost a century of progress. Major advances in deep reinforcement learning are also rapidly changing the landscape. This chapter is not meant to be comprehensive; rather, it aims to provide a solid foundation, to introduce key concepts and leading approaches, and to lower the barrier to entry in this exciting field.

¹Ironically, from the perspective of reinforcement learning, in *The Matrix*, Neo is actually the agent learning to interact with his environment.

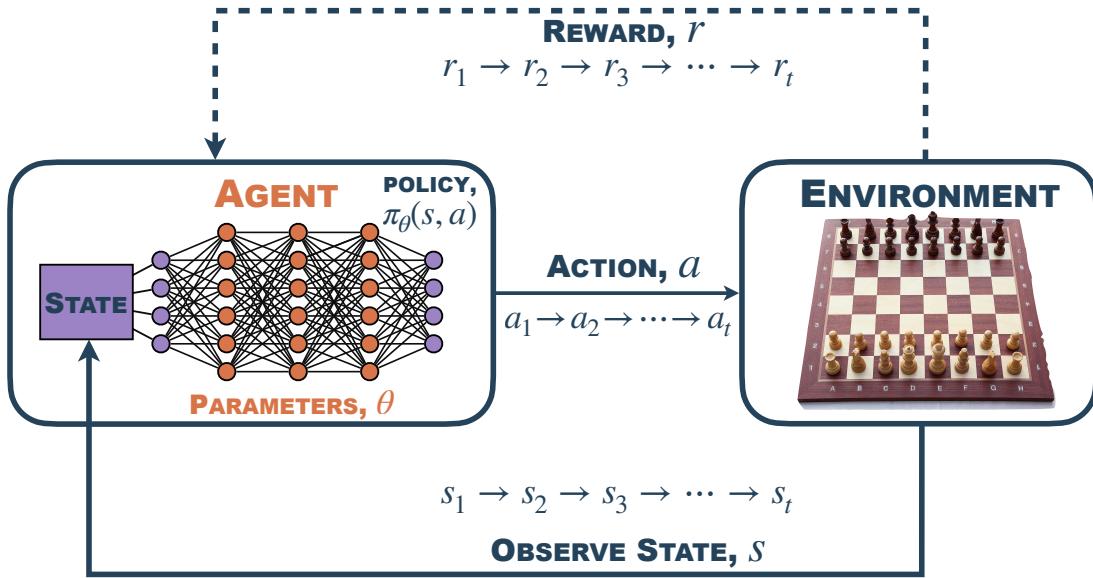


Figure 11.1: Schematic of reinforcement learning, where an agent senses its environmental state s and takes actions a according to a policy π that is optimized through learning to maximize future rewards r . In this case, a deep neural network is used to represent the policy π . This is known as a *deep policy network*.

11.1 Overview and Mathematical Formulation

Figure 11.1 provides a schematic overview of the reinforcement learning framework. An RL agent senses the state of its environment and learns to take appropriate actions to achieve optimal immediate or delayed rewards. Specifically, the RL agent arrives at a sequence of different states $s_k \in \mathcal{S}$ by performing actions $a_k \in \mathcal{A}$, with the selected actions leading to positive or negative rewards r_k used for learning. The sets \mathcal{S} and \mathcal{A} denote the sets of possible states and actions, respectively. Importantly, the RL agent is capable of learning delayed rewards, which is critical for systems where the optimal solution involves a multi-step procedure. Rewards may be thought of as sporadic and time-delayed labels, leading to RL being considered a third major branch of machine learning, called *semi-supervised* learning, which complements the other two branches of supervised and unsupervised learning. One canonical example is learning a set of moves, or a long term strategy, to win a game of chess. As is the case with human learning, RL often begins with an unstructured *exploration*, where trial-and-error are used to learn the rules, followed by *exploitation*, where a strategy is chosen and optimized within the learned rules.

The Policy

An RL agent senses the state of its environment s and takes actions a through a policy π that is optimized through learning to maximize future rewards r . Reinforcement learning is often formulated as an optimization problem to learn the policy $\pi(s, a)$,

$$\pi(s, a) = \Pr(a = a | s = s), \quad (11.1)$$

which is the probability of taking action a given state s , to maximize the total future rewards. In the simplest formulation, the policy may be a look-up table that is defined on the discrete state and action spaces S and A , respectively. However, for most problems, representing and learning this policy becomes prohibitively expensive, and π must instead be represented as an approximate function that is parameterized by a lower-dimensional vector θ :

$$\pi(s, a) \approx \pi(s, a, \theta). \quad (11.2)$$

Often, this parameterized function will be denoted $\pi_\theta(s, a)$. Function approximation is the basis of deep reinforcement learning in Sec. 11.4, where it is possible to represent these complex functions using deep neural networks.

Note that in the literature, there is often an abuse of notation, where $\pi(s, a)$ is used to denote the action taken, rather than the *probability* density of taking an action a given a state observation s . In the case of a deterministic policy, such as a greedy policy, then it may be possible to use $a = \pi(s)$ to represent the action taken. We will attempt to be clear throughout when choosing one convention over another.

The Environment: a Markov Decision Process (MDP)

In general, the measured state of the system may be a partial measurement of a higher-dimensional environmental state that evolves according to a stochastic, nonlinear dynamical system. However, for simplicity, most introductions to RL assume that the state evolves according to a Markov decision process (MDP), so that the probability of the system occurring in the current state is determined only by the previous state. We will begin with this simple formulation. However, even though it is often assumed that the state evolves according to an MDP, it is often the case that this model is not known, motivating the use of “*model-free*” RL strategies discussed in Sec. 11.3. Similarly, when a model is not known, it may be possible to first learn an MDP using data-driven methods and then use this for “*model-based*” reinforcement learning, as in Sec. 11.2.

An MDP consists of a set of states S , a set of actions A , and a set of rewards R , along with the probability of transitioning from state s_k at time t_k to state s_{k+1} at time t_{k+1} given action a_k ,

$$P(s', s, a) = \Pr(s_{k+1} = s' | s_k = s, a_k = a), \quad (11.3)$$

and a reward function R

$$R(s', s, a) = \Pr(r_{k+1} | s_{k+1} = s', s_k = s, a_k = a). \quad (11.4)$$

Sometimes the transition probability $P(s', s, a)$ will be written as $P(s' | s, a)$. Again, sometimes there will be an abuse of notation, where a chosen policy π will be used instead of the action a in the argument of either P or R above. In this case, it is assumed that this applies a sum over states, as in

$$P(s', s, \pi) = \sum_{a \in \mathcal{A}} \pi(s, a) P(s', s, a). \quad (11.5)$$

Thus, an MDP generalizes the notion of a Markov process to include actions and rewards, making it suitable for decision making and control. A simple Markov process is a set of states \mathcal{S} and a probability of transitioning from one state to the next. The defining property of a Markov process and an MDP is that the probability of being in a future state is entirely determined by the current state, and not by previous states or hidden variables. The MDP framework is closely related to transition state theory and the Perron-Frobenius operator, which is the adjoint of the Koopman operator from Section 7.4.

In the case of a simple Markov process with a finite set of states \mathcal{S} , then it is possible to let $s \in \mathbb{R}^n$ be a vector of the probability of being in each of the n states, in which case the Markov process $P(s', s)$ may be written in terms of a transition matrix, also known as a stochastic matrix, or a probability matrix, T :

$$s' = Ts, \quad (11.6)$$

where each column of T must add up to 1, which is a statement of conservation of probability that given a particular state s , *something* must happen after the transition to s' . Similarly, for an MDP, given a policy π , the transition process may be written as

$$s' = \sum_{a \in \mathcal{A}} \pi(s, a) T_a s. \quad (11.7)$$

Now for each action a , T_a is a Markov process with all columns summing to 1.

One of the defining properties of a Markov process is that the system asymptotically approaches a steady state μ , which is the eigenvector of T corresponding to eigenvalue 1. Similarly, given a policy π , an MDP asymptotically approaches a steady state $\mu_\pi = \sum_a \pi(s, a) \mu_a$.

This brings up another notational issue, where for continuous processes, $s \in \mathbb{R}^n$ describes the continuous state vector in an n -dimensional vector space, as in Chapters 7 and 8, while for discrete state spaces, $s \in \mathbb{R}^n$ denotes a vector of probabilities of belonging to one of n finite states. It is important to carefully consider which notation is being used for a given problem, as these formulations have different dynamics (i.e., differential equation versus MDP) and interpretations (i.e., deterministic dynamics versus probabilistic transitions).

The Value Function

Given a policy π , we next define a value function that quantifies the desirability of being in a given state:

$$V_\pi(s) = \mathbb{E} \left(\sum_k \gamma^k r_k \mid s_0 = s \right), \quad (11.8)$$

where \mathbb{E} is the expected reward over the time steps k , subject to a *discount rate* γ . Future rewards are discounted, reflecting the economic principle that current rewards are more valuable than future rewards. Often, the subscript π is omitted from the value function, in which case we refer to the value function for the best possible policy:

$$V(s) = \max_{\pi} \mathbb{E} \left(\sum_{k=0}^{\infty} \gamma^k r_k \mid s_0 = s \right). \quad (11.9)$$

One of the most important properties of the value function is that the value at a state s may be written recursively as

$$V(s) = \max_{\pi} \mathbb{E} \left(r_0 + \sum_{k=1}^{\infty} \gamma^k r_k \mid s_1 = s' \right), \quad (11.10)$$

which implies that

$$V(s) = \max_{\pi} \mathbb{E} (r_0 + \gamma V(s')), \quad (11.11)$$

where $s' = s_{k+1}$ is the next state after $s = s_k$ given action a_k , and the expectation is over actions selected from the optimal policy π . This expression, known as *Bellman's equation*, is a statement of Bellman's principle of optimality, and it is a central result that underpins modern RL.

Given the value function, it is possible to extract the optimal policy as

$$\pi = \operatorname{argmax}_{\pi} \mathbb{E} (r_0 + \gamma V(s')), \quad (11.12)$$

Goals and Challenges of Reinforcement Learning

Learning the policy π , the value function V , or jointly learning both, is the central challenge in RL. Depending on the assumed structure of π , the size and evolution dynamics of S , and the reward landscape R , determining an optimal policy may range from a closed form optimization to a rather high-dimensional unstructured optimization. Thus, a large number of trials must often be evaluated in order to determine an optimal policy. In practice, reinforcement learning may be very expensive to train, and it might not be the right strategy for

problems where testing a policy is expensive or potentially unsafe. Similarly, in many cases, there are simpler control strategies than RL, such as LQR or MPC; when these approaches are effective, they are often preferable. Reinforcement learning is, therefore, well-suited for situations where some combination of the following are true: evaluating a policy is inexpensive, as in board games; there are sufficient resources to perform a near brute-force optimization, as in evolutionary optimization; no other control strategy works.

Although RL is typically formulated within the mathematical framework of MDPs, many real world applications do not satisfy these assumptions. For example, the dynamics may depend on the state history or on hidden or latent variables. Similarly, the evolution dynamics may be entirely deterministic, yet chaotic. However, as we will see, it is often possible to develop approximate probabilistic transition state models for chaotic dynamics or to augment the environment state to include past states for systems with memory or hidden variables. Often, the underlying MDP transition probability and reward functions are not known *a priori*, and must either be learned ahead of time through some exploration phase, or alternative model-free optimization techniques must be used. Finally, many of the theoretical convergence results, and indeed many of the fundamental RL algorithms, only apply to *finite* MDPs, which are characterized by finite actions \mathcal{A} and states \mathcal{S} . Games, such as chess, fall into this category, even though the number of states may be combinatorially large. Even continuous dynamical systems, such as a pendulum on a cart, may be approximated by a finite MDP through a discretization or quantization process.

There is typically much less supervisory information available to an RL agent than is available in classical supervised learning. One of the central challenges of reinforcement learning is that rewards are often extremely rare and may be significantly delayed from a sequence of good control actions. This challenge leads to the so-called credit assignment problem, coined by Minsky [514] to describe the challenge of knowing what action sequence was responsible for the reward ultimately received. These sparse and delayed rewards have been a central challenge in RL for six decades, and they are still a focus of research today. The resulting optimization problem is computationally expensive and data intensive, requiring considerable trial and error.

Today, reinforcement learning is being used to learn sophisticated control policies for complex open-world problems in autonomy and propulsion (e.g., self-driving cars, learning to swim and fly, etc.) and as a general learning environment for rule-constrained games (e.g., checkers, backgammon, chess, go, Atari, etc.). Much of the history of RL may be traced through the success on increasingly challenging board games, from checkers [628] to backgammon [712] and more recently to chess and go [671]. These games serve to illustrate many of the central challenges that are still faced in RL, including the curse of dimensionality and the credit assignment problem.



Figure 11.2: Reinforcement learning is inspired by biological learning with sparse rewards. Mordecai is trained to balance a treat on his nose until a command is given, after which he grabs it out of the air. *Credit: Bing Brunton for image and training.*

Motivating examples

It is helpful to understand RL through simple examples. Consider a mouse in a maze. The mouse is the agent, and the environment is the maze. The mouse measures the local state in its environment; it does not have access to a full top-down view of the maze, but instead it knows its current local environment and what past actions it has taken. The mouse has *agency* to take some action about what to do next, for example whether to turn left, turn right, or go forward. Typically, the mouse does not receive a reward until the end of the maze. If the mouse received a reward after each correct turn, it would have a much simpler learning task. Setting such a curriculum is a strategy to help teach animals, whereby initially dense rewards are sparsified throughout the learning process.

More generally, RL may be used to understand animal behavior, ranging from semi-supervised training to naturalistic behaviors. Figure 11.2 shows a trained behavior where a treat is balanced on Mordecai’s nose until a command is given, after which he is able to grab it out of the air. Often, training animals to perform complex tasks involves expert human guidance to provide intermediate rewards or secondary reinforcers, such as using a clicker to indicate a future reward. In animal training and in RL, the more proximal the reward is in time to the action, the easier it is to learn the task. The connection between learning and temporal proximity is the basis of *temporal difference* learning, which is a powerful concept in RL, and this is also important to our understanding of the chemical basis for addiction [605].

It is also helpful to consider two-player games, such as tic-tac-toe, checkers, backgammon, chess, and go. In these games, the agent is one of the players, and the environment encompasses the rules of the game along with an adversarial opponent. These examples are also interesting because there is an element of randomness or stochasticity in the environment, either because of the fundamental rules (e.g., a dice-roll in backgammon) or because of an opponent’s probabilistic strategy. Thus, it may be advantageous for the agent to also adopt a probabilistic policy, which is in contrast to much of the theory of classical control for deterministic systems. Similarly, a probabilistic strategy may be

important when learning how to play.

In most games, the reward signal comes at the end of the game after the agent has won or lost. Again, this makes the learning process exceedingly challenging, as it is initially unclear which subsequence of actions were particularly important in driving the outcome. For example, an agent may play an excellent chess opening and midgame and then lose at the end because of a few bad moves. Should the agent discard the entire first half of the game, or worse yet, attribute this to a negative reward? Thus, it is clear that a major part of learning an effective policy is understanding the value of being in a given state s . In a game like chess, where the number of states is combinatorially large, there are too many states to count, and it is intractable to map out the exact value of all board states. Instead, players create simple heuristic rules-of-thumb about what are good board positions, e.g. assigning points to the various pieces to keep track of a rough score. This intermediate score provides a denser reward structure throughout the game. However, these heuristics are sub-optimal and may be susceptible to gambits, where the opponent sacrifices a piece for an immediate point loss in order to eventually move to a more favorable global state s . In backgammon, an intermediate point total may be more explicitly computed as the total number of *pips*, or points that a player must roll to move all pieces home and off the board. Although this makes it relatively simple to estimate the strength of a board position, the discrete nature of the die roll and game mechanics makes this a sub-optimal approximation, as the number of required *dice-rolls* or *turns* may also be a useful measure.

Thinking through games like these illustrates many of the modern strategies to improve the learning rates and sample efficiency of RL, including hindsight replay, temporal difference learning, look ahead, and reward shaping, which we will discuss in the following sections. For example, playing against a skilled teacher can dramatically improve the learning rate, as the teacher provides guidance about whether or not a move is good, and why, adding information to help shape proxy metrics that can be used as intermediate rewards and models that can accelerate the learning process.

Categorization of RL Techniques

Nearly all problems in machine learning and control theory involve challenging optimization problems. In the case of machine learning, the parameters of a model are optimized to best fit the training data, as measured by a loss function. In the case of control, a set of control performance metrics are optimized subject to the constraints of the dynamics. Reinforcement learning is no different, as it is at the intersection of machine learning and control theory.

There are many approaches to learn an optimal policy π , which is the ultimate goal of RL. A major dichotomy in reinforcement learning is that of *model-*

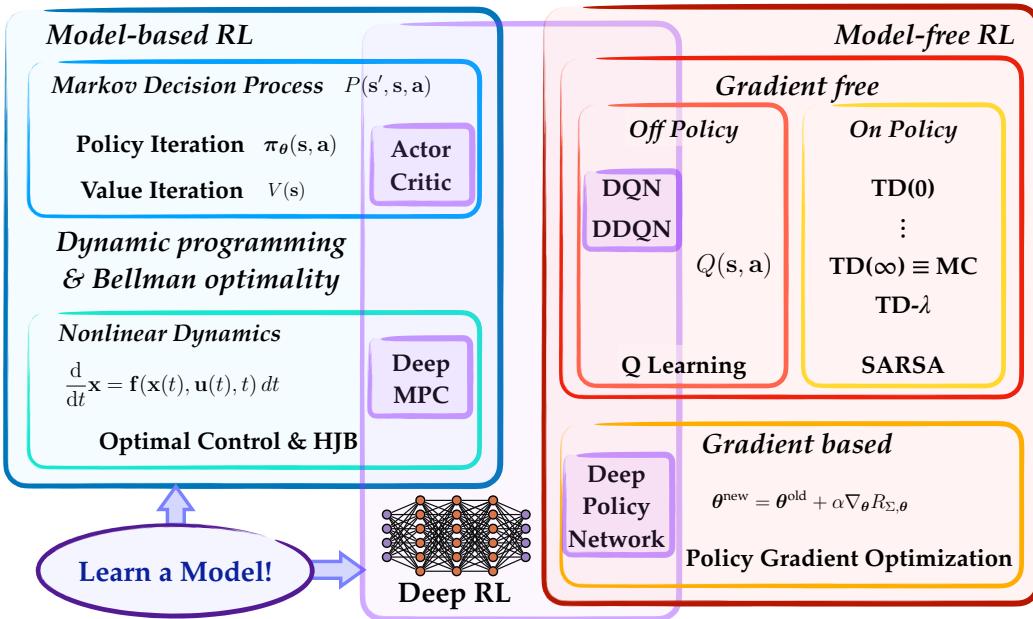


Figure 11.3: Rough categorization of reinforcement learning techniques. This organization is not comprehensive, and some of the lines are becoming blurred. The first major dichotomy is between model-based and model-free RL techniques. Next, within model-free RL, there is a dichotomy between gradient-based and gradient-free methods. Finally, within gradient-free methods, there is a dichotomy between on-policy and off-policy methods.

based RL versus *model-free RL*. When there is a known model for the environment, there are several strategies for learning either the optimal policy or value function through what is known as *policy iteration* or *value iteration*, which are forms of dynamic programming using the Bellman equation. When there is no model for the environment, alternative strategies, such as Q-learning, must be employed. The reinforcement learning optimization problem may be particularly challenging for high-dimensional systems with unknown, nonlinear, stochastic dynamics and sparse and delayed rewards. All of these techniques may be combined with function approximation techniques, such as neural networks, for approximating the policy π , the value function V , or the quality function Q (discussed in subsequent sections), making them more useful for high-dimensional systems. These model-based, model-free, and deep learning approaches will be discussed below. Note that this section only provides a glimpse of the many optimization approaches used to solve RL problems, as this is a vast and rapidly growing field.

11.2 Model-Based Optimization and Control

This section provides a high-level overview of some essential model-based optimization and control techniques. Some don't consider these techniques to be reinforcement learning, as they don't involve learning an optimal strategy through trial-and-error experience. However, they are closely related. It is possible to learn a model through trial-and-error, and then use this model with these techniques, which would be considered RL.

For the simplified case of a known model that is a finite MDP, it is possible to learn either the optimal policy or value function through what is known as *policy iteration* or *value iteration*, which are forms of dynamic programming using the Bellman equation. Dynamic programming [70, 71, 83, 735, 81, 82, 618] is a powerful approach that is used for general optimal nonlinear control and reinforcement learning, among other tasks. These algorithms provide a mathematically simplified optimization framework that helps to introduce essential concepts used throughout.

More generally, RL optimization is related to the field of optimal nonlinear control, which has deep roots in variational theory going back to Bernoulli and the Brachistochrone problem nearly four centuries ago. We will explore this connection to nonlinear control theory in Sec. 11.6.

Dynamic programming

Dynamic programming is a mathematical framework introduced by Richard E. Bellman [70, 71] to solve large multi-step optimization problems, such as those found in decision making and control. Policy iteration and value iteration, discussed below, are two examples of the use of dynamic programming in reinforcement learning. To solve these multi-step optimizations, dynamic programming reformulates the large optimization problem as a recursive optimization in terms of smaller sub-problems, so that only a local decision need be optimized. This approach relies on Bellman's principle of optimality, which states that a large multi-step control policy must also be locally optimal in every sub-sequence of steps.

The Bellman equation in (11.11) indicates that the large optimization problem over an entire state-action trajectory (s_k, a_k) may be broken into a recursive optimization at each point along the trajectory. As long as the value function is known at the next point s' , it is possible to solve the optimization at point s simply by optimizing the policy $\pi(s, a)$ at this point. Of course, this assumes that the value function is known at *all* possible next states s_{k+1} , which is a function of the current state s_k , the current action a_k , and the dynamics governing the system; this becomes even more complex for non-MDP dynamics, such as the nonlinear control formulation in the next subsection. For even moderately

large problems, this suffers from the curse of dimensionality, and approximate solution methods must be employed.

When tractable, dynamic programming (i.e., the process of breaking a large problem into smaller overlapping sub-problems) provides a globally optimal solution. There are two main approaches to dynamic programming, referred to as *top down* and *bottom up*:

Top down: The top-down approach involves maintaining a table of sub-problems that are referred to when solving larger problems. For a new problem, the table is checked to see if the relevant sub-problem has been solved. If so, it is used, and if not, the sub-problem is solved. This tabular storage is called *memoization* and becomes combinatorially complex for many problems.

Bottom up: The bottom-up approach involves starting by solving the smallest sub-problems first, and then combining these to form the larger problems. This may be thought of as working backwards from every possible goal state, finding the best previous action to get there, then going back two steps, then going back three steps, etc.

Although dynamic programming still represents a brute-force search through all sub-problems, it is still more efficient than a naive brute-force search. In some cases, it reduces the computational complexity to an algorithm that scales linearly with the number of sub-problems, although this may still be combinatorially large, as in the example of the game of chess. Dynamic programming is closely related to divide-and-conquer techniques, such as quick sort, except that divide-and-conquer applies to *non-overlapping* or *non-recursive* (i.e., independent) sub-problems, while dynamic programming applies to overlapping, or recursively interdependent sub-problems.

However, the recursive strategy suggests approximate solution techniques, such as the alternating directions method, where a sub-optimal solution is initialized and the value function is iterated over. This will be discussed next.

Policy iteration

Policy iteration is a two step optimization procedure to simultaneously find an optimal value function V_π and the corresponding optimal policy π .

First, a candidate policy π is evaluated, resulting in the value function for this fixed policy. This typically involves a brute force calculation of the value function for this policy starting at many or all initial states. The policy may need to be simulated for a long time depending on the reward delay and discounting factor γ .

Next, the value function is fixed, and the policy is optimized to improve the expected rewards by taking different actions at a given state. This optimization

relies on the alternative recursive formulation of the value function in (11.8) due to Bellman's equation (11.11):

$$V_\pi(s) = \mathbb{E}(R(s', s, \pi(s)) + \gamma V_\pi(s')) \quad (11.13a)$$

$$= \sum_{s'} P(s' | s, \pi(s)) (R(s', s, \pi(s)) + \gamma V_\pi(s')). \quad (11.13b)$$

Note that in this expression, we have assumed a deterministic policy $a = \pi(s)$, otherwise, (11.13b) would involve a second summation over $a \in \mathcal{A}$, with the expression multiplied by $\pi(s, a)$.

It is then possible to fix $V_\pi(s')$ and optimize over the policy in the first term. In particular, the new deterministic optimal policy at the state s is given by:

$$\pi(s) = \operatorname{argmax}_{a \in \mathcal{A}} \mathbb{E}(R(s', s, a) + \gamma V_\pi(s')). \quad (11.14)$$

Once the policy is updated, the process repeats, fixing this policy to update the value function, and then using this updated value function to improve the policy. The process is repeated until both the policy and the value function converge to within a specified tolerance. It is important to note that this procedure is both expensive and prone to finding local minima. It also resembles the alternating descent method that is widely used in optimization and machine learning.

The formulation in (11.13b) makes it clear that it may be possible to optimize backwards from a state known to give a reward with high probability. Additionally, this approach requires having a model for P and R to predict the next state s' , making this a *model-based* approach.

Value iteration

Value iteration is similar to policy iteration, except that at every iteration only the value function is updated, and the optimal policy is extracted from this value function at the end. First, the value function is initialized, typically either with zeros or at random. Then, for all states $s \in \mathcal{S}$, the value function is updated by returning the maximum value at that state across all actions $a \in \mathcal{A}$, holding the value function fixed at all other states $s' \in \mathcal{S} \setminus s$:

$$V(s) = \max_a \sum_{s'} P(s' | s, a) (R(s', s, a) + \gamma V(s')). \quad (11.15)$$

This iteration is repeated until a convergence criterion is met.

After the value function converges, it is possible to extract the optimizing policy π :

$$\pi(s, a) = \operatorname{argmax}_a \sum_{s'} P(s' | s, a) (R(s', s, a) + \gamma V(s')). \quad (11.16)$$

Although value iteration typically requires fewer steps per iteration, policy iteration often converges in fewer iterations. This may be due to the fact that the value function is often more complex than the policy function, requiring more parameters to optimize over.

Note that the value function in RL typically refers to a discounted sum of future rewards that should be maximized, while in nonlinear control it refers to an integrated cost that should be minimized. The phrase *value function* is particularly intuitive when referring to accumulated rewards in the economic sense, as it quantifies the *value* of being in a given state. However, in the case of nonlinear control theory, the *value function* is more accurately thought of as quantifying the *numerical value* of the cost function evaluated on the optimal trajectory. This notation can be confusing and is worth careful consideration depending on the context.

Quality function

Both policy iteration and value iteration rely on the quality function $Q(s, a)$, which is defined as

$$Q(s, a) = \mathbb{E} (R(s', s, a) + \gamma V(s')) \quad (11.17a)$$

$$= \sum_{s'} P(s' | s, a) (R(s', s, a) + \gamma V(s')). \quad (11.17b)$$

In a sense, the optimal policy $\pi(s, a)$ and the optimal value function $V(s, a)$ contain redundant information, as one can be determined from the other via the quality function $Q(s, a)$:

$$\pi(s, a) = \operatorname{argmax}_a Q(s, a) \quad (11.18a)$$

$$V(s) = \max_a Q(s, a). \quad (11.18b)$$

This formulation will be used for model-free Q-learning [757, 734, 244] in Section 11.3.

11.3 Model-Free Reinforcement Learning and Q-Learning

Both policy iteration and value iteration above rely on the *quality* function $Q(s, a)$, which describes the joint desirability of a given state/action pair. Policy iteration (11.14) and value iteration (11.15) are both model-based reinforcement learning strategies, where it is assumed that the MDP model is known: each iteration requires a one-step look ahead, or model-based prediction of the next state s' given the current state and action s and a . Based on this model, it is possible to forecast and maximize over all possible actions.

When a model is not available, there are several reinforcement learning approaches to learn effective decision and control policies to interact with the environment. Perhaps the most straightforward approach is to first learn a model of the environment using some data-driven active learning strategy, and then use the standard model-based approaches discussed earlier. However, this may be infeasible for very large or particularly unstructured systems.

Q -learning is a leading model-free alternative, which learns the Q function directly from experience, without requiring access to a model. Thus, it is possible to generalize many of the model-based optimization strategies above to more unstructured settings, where a model is unavailable. The Q function has the one-step look ahead implicitly built into its representation, without needing to explicitly refer to a model. From this learned Q function, the optimal policy and value function may be extracted as in (11.18).

Before discussing the mechanics of Q -learning in detail, it is helpful to introduce several concepts, including Monte Carlo based learning and temporal difference learning.

Monte Carlo learning

In the simplest approach to learning from experience, the value function V or quality function Q may be learned through a Monte Carlo random sampling of the state-action space through repeated evaluation of many policies. Monte Carlo approaches require that the RL task is *episodic*, meaning that the task has a defined start and terminates after a finite number of actions, resulting in a total cumulative reward at the end of the episode. Games are good examples of episodic RL tasks.

In Monte Carlo learning, the total cumulative reward at the end of the task is used to estimate either the value function V or the quality function Q by dividing the final reward equally among all of the intermediate states or state-action pairs, respectively. This is the simplest possible approach to deal with the credit assignment problem, as credit is shared equally among all intermediate steps. However, for this reason, Monte Carlo learning is typically quite sample inefficient, especially for problems with sparse rewards.

Consider the case of Monte Carlo learning of the value function. Given a new episode consisting of n steps, the cumulative discounted reward R_Σ is computed

$$R_\Sigma = \sum_{k=1}^n \gamma^k \mathbf{r}_k \quad (11.19)$$

and used to update the value function at every state \mathbf{s}_k visited in this episode:

$$V^{\text{new}}(\mathbf{s}_k) = V^{\text{old}}(\mathbf{s}_k) + \frac{1}{n} (R_\Sigma - V^{\text{old}}(\mathbf{s}_k)) \quad \forall k \in [1, \dots, n]. \quad (11.20)$$

This incremental update, weighted by $1/n$, is equivalent to waiting until the end of the episode and then updating the value function at all states along the trajectory with an equal share of the reward. Similarly, in the case of Monte Carlo learning of the Q function, the discounted reward R_Σ is used to update the Q function at every state-action pair $(\mathbf{s}_k, \mathbf{a}_k)$ visited in this episode:

$$Q^{\text{new}}(\mathbf{s}_k, \mathbf{a}_k) = Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k) + \frac{1}{n} (R_\Sigma - Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k)) \quad \forall k \in [1, \dots, n]. \quad (11.21)$$

In the limit of infinite data and infinite exploration, this approach will eventually sample all possible state-action pairs and converge to the true quality function Q . However, in practice, this often amounts to an intractable brute-force search.

It is also possible to discount past experiences by introducing a learning rate $\alpha \in [0, 1]$ and using this to update the Q function:

$$Q^{\text{new}}(\mathbf{s}_k, \mathbf{a}_k) = Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k) + \alpha (R_\Sigma - Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k)) \quad \forall k \in [1, \dots, n]. \quad (11.22)$$

Larger learning rates $\alpha > 1/n$ will favor more recent experience.

There is a question about how to initialize the many episodes required to learn with Monte Carlo. When possible, the episode will be initialized randomly at every initial state or state-action pair, providing a random sampling; however, this might not be possible for many learning tasks. Typically, Monte Carlo learning is performed *on-policy*, meaning that the optimal policy is enacted, based on the current value or quality function, and the information from this locally optimal policy is used for the update. It is also possible to promote exploration by adding a small probability of taking a random action, rather than the action dictated by the optimal policy. Finally, there are off-policy Monte Carlo methods, but in general, they are quite inefficient or unfeasible.

Temporal difference (TD) learning

Temporal different learning [694, 711, 202, 712, 105], known as TD learning, is another sample-based learning strategy. In contrast to Monte Carlo learning, TD learning is not restricted to episodic tasks, but instead learns continuously by bootstrapping based on current estimates of the value function V or quality function Q , as in dynamic programming (e.g., as in value iteration in (11.15)). TD learning is designed to mimic learning processes in animals, where time delayed rewards are often learned through environmental cues that act as secondary reinforcers preceding the delayed reward; this is most popularly understood through Pavlov's dog [563]. Thus, TD learning is typically more sample efficient than Monte Carlo learning, resulting in decreased variance, but at the cost of a bias in the learning due to the bootstrapping.

TD(0): 1-step look ahead

To understand TD learning, it is helpful to begin with the simplest algorithm: TD(0). In TD(0), the estimate of the one-step-ahead future reward is used to update the current value function.

Given a control trajectory generated through an optimal policy π , the value function at state s_k is given by

$$V(s_k) = \mathbb{E} (r_k + \gamma V(s_{k+1})) . \quad (11.23)$$

Thus, in the language of Bayesian statistics, $r_k + \gamma V(s_{k+1})$ is an *unbiased estimator* for $V(s_k)$.

For non-optimal policies π , this same idea may be used to update the value function based on the value function one step in the future:

$$V^{\text{new}}(s_k) = V^{\text{old}}(s_k) + \alpha \underbrace{\left(\underbrace{r_k + \gamma V^{\text{old}}(s_{k+1})}_{\text{TD target estimates } R_\Sigma} - V^{\text{old}}(s_k) \right)}_{\text{TD error}} . \quad (11.24)$$

Instead of using a model to predict s_{k+1} , which is required to evaluate $V(s_{k+1})$, it is possible to wait until the next step is actually taken and retroactively adjust the value function. Notice that this is very similar to optimization of the Bellman equation using dynamic programming but with retroactive updates based on sampled data rather than proactive updates based on a model prediction.

In the TD(0) update above, the expression $R_\Sigma = r_k + \gamma V(s_{k+1})$ is known as the *TD target*, as it is the estimate for the future reward, analogous to R_Σ in Monte Carlo learning of the Q function in (11.22). The difference between this target and the previous estimate of the value function is the TD error, and it is used to update the value function, just as in Monte Carlo learning, with a learning rate α .

TD(n): n -step look ahead

Other temporal difference algorithms can be developed, based on multi-step look-aheads into the future. For example, TD(1) uses a TD target based on two steps into the future

$$r_k + \gamma r_{k+1} + \gamma^2 V(s_{k+2}) \quad (11.25)$$

and, TD(n) uses a TD target based on $n + 1$ steps into the future

$$R_\Sigma^{(n)} = r_k + \gamma r_{k+1} + \gamma^2 r_{k+2} + \cdots + \gamma^n r_{k+n} + \gamma^{n+1} V(s_{k+n+1}) \quad (11.26a)$$

$$= \sum_{j=0}^n \gamma^j r_{k+j} + \gamma^{n+1} V(s_{k+n+1}). \quad (11.26b)$$

Again, there does not need to be a model for these future states, but instead, the value function may be retroactively adjusted based on the actual sampled trajectory and rewards. Note that in the limit that an entire episode is used, TD(n) converges to the Monte Carlo learning approach.

TD- λ : Weighted look ahead

An important variant of the TD learning family is TD- λ , which was introduced by Sutton [694]. TD- λ creates a TD target R_{Σ}^{λ} that is a weighted average of the various TD(n) targets $R_{\Sigma}^{(n)}$. The weighting is given by:

$$R_{\Sigma}^{\lambda} = (1 - \lambda) \sum_{k=1}^{\infty} \lambda^{n-1} R_{\Sigma}^{(n)} \quad (11.27)$$

and the update equation is

$$V^{\text{new}}(\mathbf{s}_k) = V^{\text{old}}(\mathbf{s}_k) + \alpha (R_{\Sigma}^{\lambda} - V^{\text{old}}(\mathbf{s}_k)) . \quad (11.28)$$

TD- λ was used for an impressive demonstration in the game of Backgammon by Tesauro in 1995 [712].

TD learning provides one of the strongest connections between reinforcement learning and learning in biological systems. These neural circuits are believed to estimate the future reward, and feedback is based on the difference between the expected reward and the actual reward, which is closely related to the TD error. In fact, there are specific neurotransmitter feedback loops that strengthen connections based on proximity of their firing to a dopamine reward signal [657]. The closer the proximity in time between an action and a reward, the stronger the feedback.

Bias-variance tradeoff

Monte Carlo learning and TD learning exemplify the *bias-variance tradeoff* in machine learning. Monte Carlo learning typically has high variance but no bias, while TD learning has lower variance but introduces a bias because of the bootstrapping. Although the *true* TD target $\mathbf{r}_k + \gamma V(\mathbf{s}_{k+1})$ is an unbiased estimate of $V(\mathbf{s}_k)$ for an optimal policy π , the sampled TD target is a biased estimate, because it uses sub-optimal actions and the current imperfect estimate of the value function.

SARSA: State-action-reward-state-action learning

SARSA is a popular TD algorithm that is used to learn the Q function *on-policy*. The Q update equation in SARSA(0) is nearly identical to the V update equation

(11.24) in TD(0):

$$Q^{\text{new}}(\mathbf{s}_k, \mathbf{a}_k) = Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k) + \alpha (\mathbf{r}_k + \gamma Q^{\text{old}}(\mathbf{s}_{k+1}, \mathbf{a}_{k+1}) - Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k)). \quad (11.29)$$

There are SARSA variants for all of the TD(n) algorithms, based on the n step TD target:

$$R_{\Sigma}^{(n)} = \mathbf{r}_k + \gamma \mathbf{r}_{k+1} + \gamma^2 \mathbf{r}_{k+2} + \cdots + \gamma^n \mathbf{r}_{k+n} + \gamma^{n+1} Q(\mathbf{s}_{k+n+1}, \mathbf{a}_{k+n+1}) \quad (11.30a)$$

$$= \sum_{j=0}^n \gamma^j \mathbf{r}_{k+j} + \gamma^{n+1} Q(\mathbf{s}_{k+n+1}, \mathbf{a}_{k+n+1}). \quad (11.30b)$$

In this case, the SARSA(n) update equation is given by

$$Q^{\text{new}}(\mathbf{s}_k, \mathbf{a}_k) = Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k) + \alpha \left(R_{\Sigma}^{(n)} - Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k) \right). \quad (11.31)$$

Note that this is on-policy because the actual action sequence $\mathbf{a}_k, \mathbf{a}_{k+1}, \dots, \mathbf{a}_{k+n+1}$ has been used to receive the rewards \mathbf{r} and evaluate the $n+1$ step Q function $Q(\mathbf{s}_{k+n+1}, \mathbf{a}_{k+n+1})$.

Q-Learning

We are now ready to discuss Q -learning [757, 734, 244], which is one of the most central approaches in model-free RL. Q -learning is essentially an off-policy TD learning scheme for the Q function. In Q -learning, the Q update equation is

$$Q^{\text{new}}(\mathbf{s}_k, \mathbf{a}_k) = Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k) + \alpha \left(\mathbf{r}_k + \gamma \max_{\mathbf{a}} Q(\mathbf{s}_{k+1}, \mathbf{a}) - Q^{\text{old}}(\mathbf{s}_k, \mathbf{a}_k) \right). \quad (11.32)$$

Notice that the only difference between Q -learning and SARSA(0) is that SARSA(0) uses $Q(\mathbf{s}_{k+1}, \mathbf{a}_{k+1})$ for the TD target, while Q -learning uses $\max_{\mathbf{a}} Q(\mathbf{s}_{k+1}, \mathbf{a})$ for the TD target. Thus, SARSA(0) is considered *on-policy* because it uses the action \mathbf{a}_{k+1} based on the actual policy: $\mathbf{a}_{k+1} = \pi(\mathbf{s}_{k+1})$. In contrast, Q -learning is *off-policy* because it uses the optimal \mathbf{a} for the update based on the current estimate for Q , while taking a different action \mathbf{a}_{k+1} based on a different behavior policy. Thus, Q -learning may take sub-optimal actions \mathbf{a}_{k+1} to explore, while still using the optimal action \mathbf{a} to update the Q function.

Generally, Q -learning will learn a more optimal solution faster than SARSA, but with more variance in the solution. However, SARSA will typically yield more cumulative rewards during the training process, since it is on-policy. In safety critical applications, such as self-driving cars or other applications where there can be catastrophic failure, SARSA will typically learn less optimal solutions, but with a better safety margin, since it is maximizing on-policy rewards.

Q -learning applies to discrete action spaces \mathcal{A} and state spaces \mathcal{S} governed by a finite MDP. The Q function is classically represented as a table of Q values that is updated through some iteration based on new information as a policy is tested and evaluated. However, this tabular approach doesn't scale well to large state spaces, and so typically function approximation is used to represent the Q function, such as a neural network in deep Q -learning. Even if the action and state spaces are continuous, as in the pendulum on a cart system, it is possible to discretize and then apply Q -learning. In addition to being model free, Q -learning is also referred to as *off-policy* RL, as it does not require that an optimal policy is enacted, as in policy iteration and value iteration. Off-policy learning is more realistic in real-world applications, enabling the RL agent to improve when its policy is sub-optimal and by watching and imitating other more skilled agents. Q -learning is especially good for games, such as backgammon, chess, and go. In particular, deep Q -learning, which approximates the Q function using a deep neural network, has been used to surpass the world champions in these challenging games.

Experience replay and imitation learning

Because Q -learning is off-policy, it is possible to learn from action-state sequences that do not use the current optimal policy. For example, it is possible to store past experiences, such as previously played games, and *replay* these experiences to further improve the Q function.

In an on-policy strategy, such as SARSA, using actions that are sub-optimal, based on the current optimal policy, will degrade the Q function, since the TD target will be a flawed estimate of future rewards based on a sub-optimal action. However, in Q -learning, since the action is optimized over the current Q function in the update, it is possible to learn from experience resulting from sub-optimal actions. This also makes it possible to learn from watching other, more experienced agents, which is related to imitation learning [637, 337, 351, 222].

Experience replay is deeply intuitive, as it is closely related to how we learn, through recalling past experiences in the light of new knowledge (i.e., an updated Q function). Similarly, imitation learning is perhaps one of the most fundamental first steps in biological learning.

Exploration vs exploitation: ϵ -greedy actions

It is important to introduce an element of random exploration into Q -learning, and there are several techniques. One approach is the ϵ -greedy algorithm to select the next action. In this approach, the agent takes the current optimal action $a_k = \max_a Q(s_k, a)$, based on the current Q function, with probability $1 - \epsilon$, where $\epsilon \in [0, 1]$. With probability ϵ , the agent takes a random action.

Thus, the agent balances exploration with the random actions and exploitation with the optimal actions. Larger ϵ promote more random exploration.

Typically, the value of ϵ will be initialized to a large value, often $\epsilon = 1$. Throughout the course of training, ϵ decays so that as the Q function improves, the agent increasingly takes the current optimal action. This is closely related to simulated annealing from optimization, which mimics the process of metal finding a low-energy state through a specific cooling schedule.

Policy Gradient Optimization

Policy gradients [696, 377, 672] are one of the most common and powerful techniques to optimize a policy that is parameterized, as in (11.2). When the policy π is parameterized by θ , it is possible to use gradient optimization on the parameters to improve the policy much faster than through traditional iteration. The parameterization may be a multi-layer neural network, in which case this would be a *deep policy network*, although other representations and function approximations may be useful. In any case, instead of extracting the policy as the argument maximizing the value or quality functions, it is possible to directly optimize the parameters θ , for example through gradient descent or stochastic gradient descent. The value function $V_\pi(s)$, depending on a policy π then becomes $V(s, \theta)$ and a similar modification is possible for the quality function Q .

The total estimated reward is given by

$$R_{\Sigma, \theta} = \sum_{s \in \mathcal{S}} \mu_\theta(s) \sum_{a \in \mathcal{A}} \pi_\theta(s, a) Q(s, a), \quad (11.33)$$

where μ_θ is the asymptotic steady state of the MDP given a policy π_θ parameterized by θ . It is then possible to compute the gradient of the total estimated reward with respect to θ

$$\nabla_\theta R_{\Sigma, \theta} = \sum_{s \in \mathcal{S}} \mu_\theta(s) \sum_{a \in \mathcal{A}} Q(s, a) \nabla_\theta \pi_\theta(s, a) \quad (11.34a)$$

$$= \sum_{s \in \mathcal{S}} \mu_\theta(s) \sum_{a \in \mathcal{A}} \pi_\theta(s, a) Q(s, a) \frac{\nabla_\theta \pi_\theta(s, a)}{\pi_\theta(s, a)} \quad (11.34b)$$

$$= \sum_{s \in \mathcal{S}} \mu_\theta(s) \sum_{a \in \mathcal{A}} \pi_\theta(s, a) Q(s, a) \nabla_\theta \log(\pi_\theta(s, a)) \quad (11.34c)$$

$$= \mathbb{E}(Q(s, a) \nabla_\theta \log(\pi_\theta(s, a))). \quad (11.34d)$$

Then the policy parameters may be updated as

$$\theta^{\text{new}} = \theta^{\text{old}} + \alpha \nabla_\theta R_{\Sigma, \theta}, \quad (11.35)$$

where α is a the learning weight; note that α may be replaced with a vector of learning weights for each component of θ . There are several approaches to approximating this gradient, including through finite differences, the REINFORCE algorithm [770], and natural policy gradients [377].

11.4 Deep Reinforcement Learning

Deep reinforcement learning is one of the most exciting areas of machine learning and of control theory, and it is one of the most promising avenues of research towards generalized artificial intelligence. Deep learning has revolutionized our ability to represent complex functions from data, providing a set of architectures for achieving human level performance in complex tasks such as image recognition and natural language processing. Classic reinforcement learning suffers from a representation problem, as many of the relevant functions, such as the policy π , the value function V , and the quality function Q , may be exceedingly complex functions defined over a very high dimensional state and action space. Indeed, even for simple games, such as the 1972 Atari game Pong, the black and white screen at standard resolution 336×240 has over $10^{24,000}$ possible discrete states, making it infeasible to represent any of these functions exactly without approximation. Thus, deep learning provides a powerful tool for improving these representations.

It is possible to use deep learning in several different ways to approximate the various functions used in RL, or to model the environment more generally. Typically the central challenge is in identifying and representing key features in a high-dimensional state space. For example, the policy $\pi(a, s)$ may now be approximated by

$$\pi(s, a) \approx \pi(s, a, \theta), \quad (11.36)$$

where θ represent the weights of a neural network.

This pairing of deep learning for representations with reinforcement learning for decision making and control has resulted in dramatic improvements to our capabilities of reinforcement learning. For example, Fig. 11.4 shows a simple policy network designed to play Pong, and Fig. 11.5 shows a more general deep convolutional neural network architecture used to develop a deep Q network to play Atari games [519].

Much of what is discussed in this section is also relevant for other function approximation techniques besides deep learning. For example, policy gradients may be computed and used for gradient-based optimization using other representations, and there is a long history before deep learning [696, 377]. That said, many of the most exciting and impressive recent demonstrations of RL leverage the full power of deep learning, and so we present these innovations in this context.

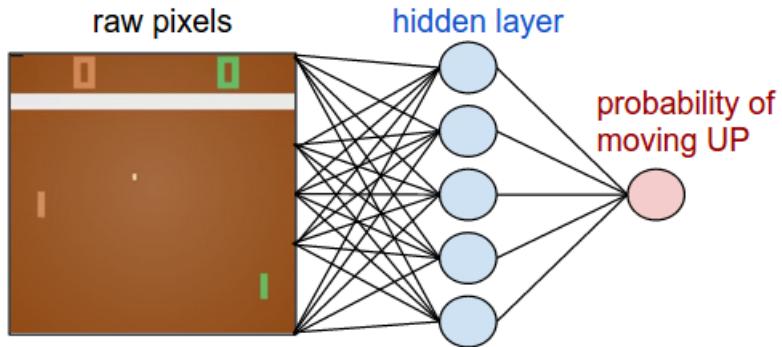


Figure 11.4: Deep policy network to encode the probability of moving up in the game of Pong. Reproduced with permission from Andrej Karpathy's Blog "Deep Reinforcement Learning: Pong from Pixels" at <http://karpathy.github.io/2016/05/31/r1/>.

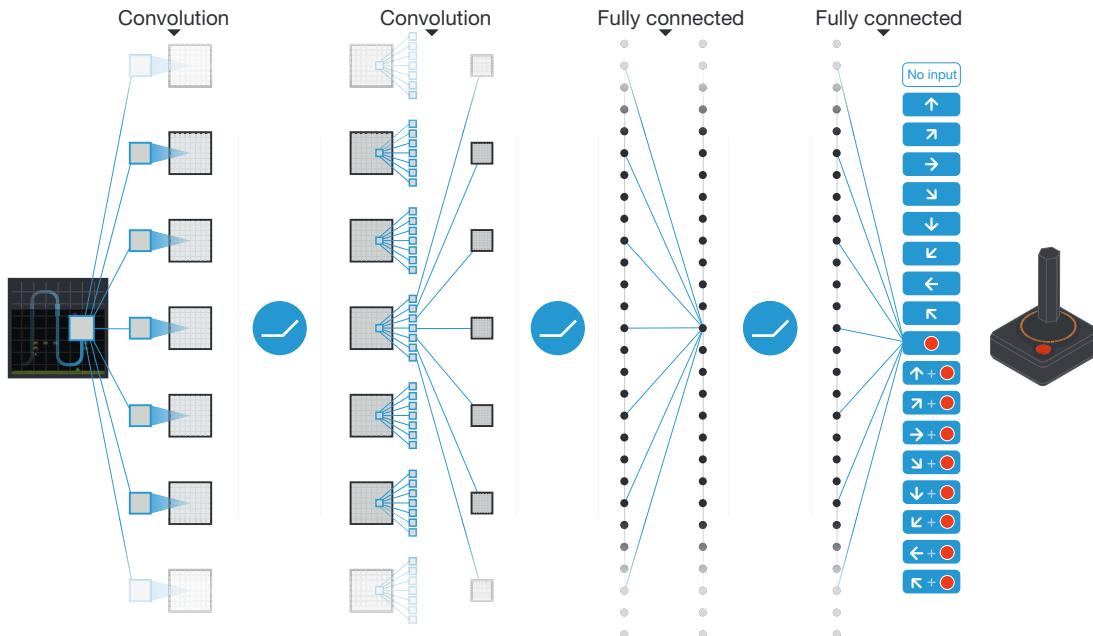


Figure 11.5: Convolutional structure of deep Q network used to play Atari games. Reproduced with permission from [519].

Deep Q-learning

Many of the most exciting advances in the past decade have involved some variation of deep Q -learning, which uses deep neural networks to represent the quality function Q . As with the policy in (11.36), it is possible to approximate

the Q function through some parameterization θ

$$Q(\mathbf{s}, \mathbf{a}) \approx Q(\mathbf{s}, \mathbf{a}, \theta), \quad (11.37)$$

where θ represents the weights of a deep neural network. In this representation, the training loss function is directly related to the standard Q -learning update in (11.32):

$$\mathcal{L} = \mathbb{E} \left[\left(\mathbf{r}_k + \gamma \max_{\mathbf{a}} Q(\mathbf{s}_{k+1}, \mathbf{a}_{k+1}, \theta) - Q(\mathbf{s}_k, \mathbf{a}_k, \theta) \right)^2 \right]. \quad (11.38)$$

The first part of the loss function, $\mathbf{r}_k + \gamma \max_{\mathbf{a}} Q(\mathbf{s}_{k+1}, \mathbf{a}_{k+1}, \theta)$, is the temporal difference target from before, and the second part, $Q(\mathbf{s}_k, \mathbf{a}_k, \theta)$, is the prediction.

Deep reinforcement learning based on a deep Q network (DQN) was introduced by Mnih et al. [519] to play Atari games. Specifically, this network used a deep convolutional neural network to represent the Q function, where the inputs were the Atari screen, as shown in Fig. 11.5. In this original paper, both the Q functions in (11.38) were represented by the same network weights θ . However, in a double DQN [742], different networks are used to represent the target and prediction Q functions, which reduces bias due to inaccuracies early in training. In double DQN, it may be necessary to fix the target network for multiple training iterations of the prediction network before updating to improve stability and convergence [264].

Experience replay is a critical component of training a DQN, which is possible because it is an off-policy RL algorithm. Short segments of past experiences are used in batches for the stochastic gradient descent during training. Moreover, to place more importance on experiences with large model mismatch, it is possible to weight past experiences by the magnitude of the TD error. This process is known as prioritized experience replay [642].

Dueling deep Q networks (DDQNs) [756] are another important deep Q learning architecture that are used to improve training when actions have a marginal affect on the quality function. In particular, a DDQN splits the quality function into the sum of a value function and an *advantage* function $A(\mathbf{s}, \mathbf{a})$, which quantifies the additional benefit of a particular action over the value of being in that state:

$$Q(\mathbf{s}, \mathbf{a}, \theta) = V(\mathbf{s}, \theta_1) + A(\mathbf{s}, \mathbf{a}, \theta_2). \quad (11.39)$$

The value and advantage networks have separate networks that are combined to estimate the Q function.

There are a variety of other useful architectures for deep Q learning, with more introduced regularly. For example, deep recurrent Q networks are promising for dynamic problems [323]. Advantage actor-critic networks, discussed in the next section, combine the DDQN with deep policy networks.

Actor-critic networks

Actor-critic methods in reinforcement learning simultaneously learn a policy function and a value function, with the goal of taking the best of both value-based and policy-based learning. The basic idea is to have an actor, which is policy-based, and a critic, which is value-based, and to use the temporal difference signal from the critic to update the policy parameters. There are many actor-critic methods that predate deep learning. For example, a simple actor-critic approach would update the policy parameters θ in (11.36) using the temporal difference error $r_k + \gamma V(s_{k+1}) - V(s_k)$:

$$\theta_{k+1} = \theta_k + \alpha (r_k + \gamma V(s_{k+1}) - V(s_k)). \quad (11.40)$$

It is rather straightforward to incorporate deep learning into an actor-critic framework. For example, in the advantage actor critic (A2C) network, the actor is a deep policy network, and the critic is a DDQNs. In this case, the update is given by

$$\theta_{k+1} = \theta_k + \alpha \nabla_\theta ((\log \pi(s_k, a_k, \theta)) Q(s_k, a_k, \theta_2)). \quad (11.41)$$

Challenges and Additional Techniques

There are several important innovations that are necessary to make reinforcement learning tractable for even moderately challenging tasks. Two of the biggest challenges in RL are: 1) high-dimensional state and action spaces, and 2) sparse and delayed rewards.

Many games, such as chess and go, have exceedingly large state spaces. For example, Claude Shannon estimated the number of games of chess, known as the Shannon number, at around 10^{120} in his famous paper “Programming a computer for playing chess” [666]; this paper was a major inspiration for modern dynamic programming and reinforcement learning. Representing a value or quality function, let alone sampling over these states, is beyond astronomically difficult. Thus, approximate representations of the value or quality functions using approximation theory, such as deep neural networks, are necessary.

Sparse and delayed rewards represent the central challenge of reinforcement learning, leading to the well-known credit assignment problem, which we have seen multiple times at this point. The following techniques, including reward shaping and hindsight experience replay, are leading techniques to overcome the credit assignment problem.

Reward shaping

Perhaps the most standard approach for systems with sparse rewards is a technique called reward shaping. This involves designing customized proxy fea-

tures that are indicative of a future reward and that may be used as an intermediate reward signal. For example, in the game of chess, the relative point count, where each piece is assigned a numeric value and added up (e.g., a queen is worth 10 points, rooks are worth 5, knights and bishops are worth 3, and pawns are worth 1 point), is an example of a shaped reward that gives an intermediate reward signal each time a piece is taken.

Reward shaping is quite common and can be very effective. However, these rewards require expert human guidance to design, and this requires customized effort for each new task. Thus, reward shaping is not a viable strategy for a generalized artificial intelligence agent capable of learning multiple games or tasks. In addition, reward shaping generally limits the upper end of the agent’s performance to that of the human expert.

Hindsight experience replay

In many tasks, such as robotic manipulation, the goal is to move the robot or an object from one location to another. For example, consider a robot arm that is required to slide an object on a table from point *A* to point *B*. Without a detailed physical model, or other prior knowledge, it is extremely unlikely that a random control policy will result in the object actually reaching the desired destination, so the rewards may be very sparse. It is possible to shape a reward based on the distance of the object to the goal state, although this is not a general strategy and suffers from the limitations discussed above.

Hindsight experience replay (HER) [22, 438] is a strategy that enriches the reward signal by taking failed trials and pretending that they were successful at a different task. This approach makes the reward structure much more dense, and has the benefit of enabling the simultaneous learning of a whole family of motion tasks.

HER is quite intuitive in the context of human learning, for example in the case of tennis. Initially, it is difficult to aim the ball, shots often go wild when learning. However, this provides valuable information about those muscle actions, which might be useful for future tasks. After lots of practice, it then becomes possible to pick from different shots and place the ball more deliberately.

Curiosity driven exploration

Another challenge with RL for large open-world environments is that the agent may easily get stuck in a local minima, where it over-optimizes for a small region of state space. One approach to this problem is to augment the reward signal with a *novelty* reward that is large in regions of state space that are not well modeled. This is known as curiosity driven exploration [562], and it involves an intrinsic curiosity module (ICM), which compares a forward model

of the evolution of the state, or a latent representation of the state, with the actual observed evolution. The discrepancy between the model and the actual dynamics is the novelty reward. When this difference is large, the agent becomes *curious* and explores this region more. There are similarities between this approach and TD learning, and in fact, many of the same variations may be implemented for curiosity driven exploration. The main difference is that in TD learning, the reward discrepancy is used as feedback to improve the value or quality function, while in curiosity driven exploration the discrepancy is explicitly used as an additional reward signal. This is a clever approach to embedding this fundamental behavior of intelligent biological learning systems, to be curious and explore.

There are challenges when using this novelty reward for chaotic and stochastically driven systems, where there are aspects of the state evolution that are fundamentally unpredictable. A naive novelty reward would constantly provide positive incentive to explore these regions, since the forward model will not improve. Instead, the authors in [562] overcome this challenge by predicated novelty on the predictability of an outcome given the action using latent features in an autoencoder, so only aspects of the future state that can be affected by the agent's actions are included in the novelty signal.

11.5 Applications and Environments

Here we provide a brief overview of some of the modern applications and success stories of RL, along with some common environments.

OpenAI Gym

The OpenAI Gym is an incredible open source resource to develop and test reinforcement learning algorithms in a wide range of environments. Fig. 11.6 shows a small selection of these systems. Example environments include

- Classic Atari video games: over 100 tasks on Atari 2600 games, including asteroids, breakout, space invaders, and many others.
- Classic control benchmarks: tasks include balancing an inverted pendulum on a cart; swing-up of a pendulum; swing-up of a double pendulum; and driving up a hill with an underactuated system.
- Goal-based robotics [780]: tasks include pushing or fetching a block to a goal position with a robot arm, with and without sliding after loss of contact; robotic hand manipulation for reaching a pose or orienting various objects.

- MuJoCo [718]: tasks include multi-legged locomotion, running, hopping, swimming, etc. within a fast physics simulator environment.

This wide range of environments and tasks provides an invaluable resource for RL researchers, dramatically lowering the barrier to entry and facilitating the benchmarking and comparison of innovations.

Classic board games

As discussed throughout this chapter, RL has developed tremendously over the past half century, from a biologically inspired idea to a major field pushing the forefront of efforts in generalized artificial intelligence. This progress can be largely traced through the success of RL on increasingly challenging games, where RL has learned to interact with and mimic humans, and eventually to defeat our greatest grandmasters.

Many of the most fundamental advances in RL were either developed for the purpose of playing games, or demonstrated on the most challenging games of the time. These simple board games also make the struggles of machine learning and artificial intelligence more relatable to humans² as we can reflect on our own experiences learning first how to play tic-tac-toe, then checkers, and then eventually “real” games, such as backgammon, chess, and go. The progression of RL capabilities roughly follows this progression of complexity, with tic-tac-toe being essentially a homework exercise, checkers being the earliest real demonstration of RL by Arthur Samuel [628], and more complex games such as backgammon [712] and eventually chess and go [670, 673] following. Interestingly, about three decades passed between each of these definitive landmarks. One of the next major landmarks is a generalist RL agent that can learn to play multiple games [671], rather than specializing in only one task.

The success of DeepMind’s AlphaGo and AlphaGo Zero, depicted in Fig. 11.7, demonstrates the remarkable power of modern RL. This system was a major breakthrough in RL research, learning to beat the Grandmaster Lee Sedol 4-1 in 2016. However, AlphaGo relied heavily on reward shaping and expert guidance, making it a custom solution, rather than a generalized learner. Its successor, AlphaGo Zero, relied entirely on self-play, and was able to eventually defeat the original AlphaGo decisively. AlphaGo was based largely on CNNs, while AlphaGo Zero used a residual network (ResNet). ResNets are easier to train, and AlphaGo Zero was one of the first concrete success stories that cemented ResNets as a competitive architecture. AlphaGo Zero was trained in 40 days on 4 tensor processing units, in contrast to many advanced ML algorithms that are trained for months on thousands of GPUs. Both AlphaGo and

²“A strange game. The only winning move is not to play. How about a nice game of chess?”
– WarGames, 1983

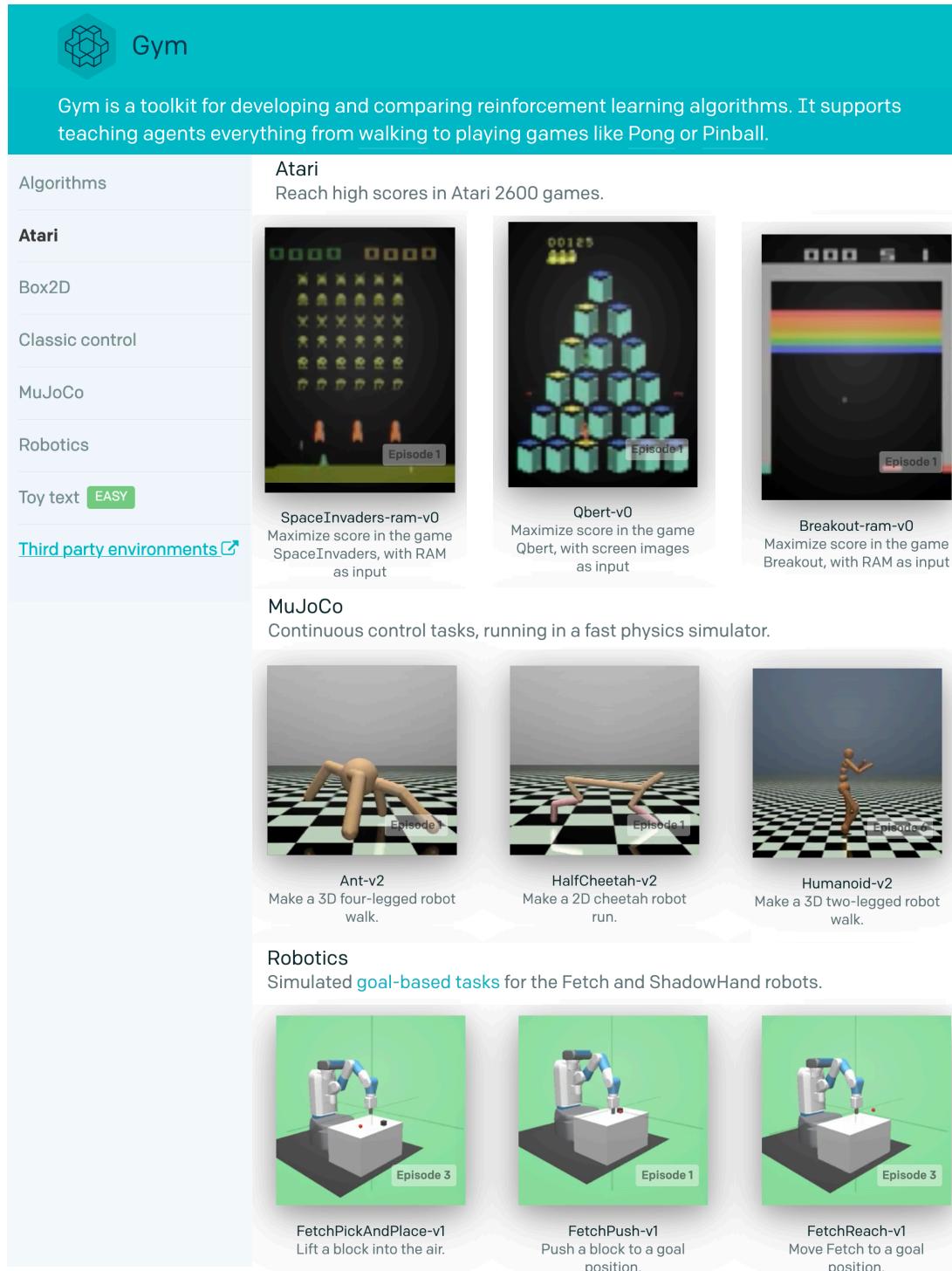


Figure 11.6: The OpenAI Gym [121] (gym.openai.com) provides a flexible simulation environment to test learning strategies. Examples include classic Atari 2600 video games and simulated rule-based control environments, including open world physics [718], and robotics [780]. Other examples include classic control benchmarks.



Figure 11.7: Reinforcement learning has demonstrated incredible performance in recent expert tasks, such as AlphaGo defeating world champion Lee Sedol in the game of Go [671] on March 19, 2016.

AlphaGo Zero are based on using deep learning to improve a Monte Carlo tree search.

Video games

Some of the most impressive recent innovations in RL have involved scaling up to larger input spaces, which are well-exemplified by the ability of RL to master classic Atari video games [519]. In the case of Atari games, the pixel space is processed using a CNN architecture, with human-level performance being achieved mere years after the birth of modern deep learning for image classification [423]. More recently, RL has been demonstrated on more sophisticated games, such as StarCraft [747], which is a real-time strategy game; DeepMind’s AlphaStar became a Grandmaster in 2019.

General artificial intelligence is one of the grand challenge problems in modern machine learning, whereby a learning agent is able to excel at multiple tasks, as in biological systems. What is perhaps most impressive about recent RL agents that learn video games is that the learning approach is *general*, so that the same RL framework can be used to learn multiple tasks. There is evidence that video games may improve performance in human surgeons [619, 478], and it may be that future RL agents will master both robotic manipulation and video games in a next stage of generalized AI.

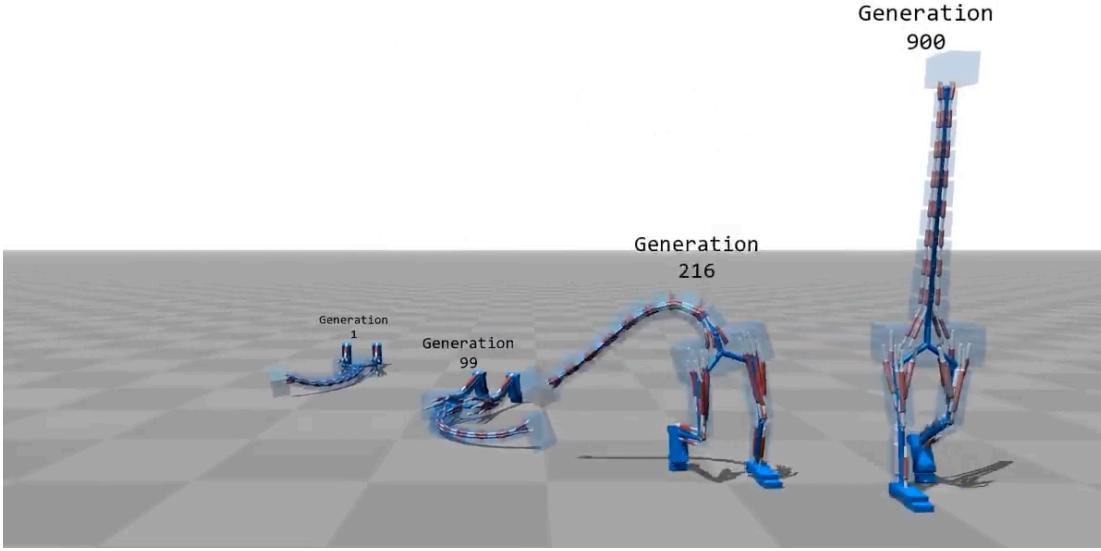


Figure 11.8: Illustration of improved bipedal locomotion performance with more generations of learning. *Reproduced from Geijtenbeek et al. [277].*

Physical systems

Although much of RL has been developed for board games and video games, it is increasingly being used for various advanced modeling and control tasks in physical systems. Physical systems, such as lasers [690] and fluids [595], often require additional considerations, such as continuous state and action spaces [601], and the need for certifiable solutions, such as trust regions [656], for safety critical applications (e.g., transportation, autonomous flight, etc.).

There has been considerable work applying RL in the field of fluid dynamics [132] for fluid flow control [308, 577, 594, 595], for example for bluff body control [247] and controlling Rayleigh-Bénard convection [67]. RL has also been applied to the related problem of navigation in a fluid environment [184, 86, 310], and more recently for turbulence modeling [543].

In addition to studying fluids, there is an extensive literature using RL to develop control policies for real and simulated robotic systems that operate primarily in a fluid environment, for example to learn how to fly and swim. For example, some of the earliest work has involved optimizing the flight of uninhabited aerial vehicles [395, 2, 710, 1, 785, 551, 603] with especially impressive helicopter aerobatics [2]. Controlling the motion of fish [274, 275, 545, 745] is another major area of development, including individual [274] and collective motion [275, 545, 745]. Gliding and perching is another large area of development [602, 603, 544].

Robotics and Autonomy

Robotics [404, 306] and autonomy [664, 627, 558, 604] are two of the largest areas of current research in RL. These both count as *physical systems*, as in the section above, but deserve their own treatment, as these are major areas of innovation. In fact, both robotics and autonomy may be viewed as two of the most pressing societal applications of machine learning in general, and reinforcement learning in particular, with self driving cars alone promising to remake the modern transportation and energy landscape. As with the discussion of physical systems above, these are typically safety critical applications with physical constraints [440, 708]. Figure 11.8 shows a virtual locomotion task that involves learning physics in a robot walker.

11.6 Optimal Nonlinear Control

Reinforcement learning has considerable overlap with optimal nonlinear control, and historically they were developed in parallel under the same optimization framework. Here we provide a brief overview of optimal nonlinear control theory, which will provide a connection between the classic linear control theory from Chapter 8 and dynamic programming to solve Bellman's equations used in this chapter. We have already seen optimal control in context of linear dynamics and quadratic cost functions in Section 8.4, resulting in the linear quadratic regulator (LQR). Similarly, we have used Bellman's equations to find optimal policies in RL for systems governed by MDPs. A major goal of this section is to provide a more general mathematical treatment of Bellman's equations, extending these approaches to fully nonlinear optimal control problems. However, this section is very technical and departs from the MDP notation used throughout the rest of the chapter; it may be omitted on a first reading. For more details, see the excellent text by Stengel [687].

Hamilton-Jacobi-Bellman equation

In optimal control, the goal is often to find a control input $\mathbf{u}(t)$ to drive a dynamical system

$$\frac{d}{dt} \mathbf{x} = \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t), t) dt \quad (11.42)$$

to follow a trajectory $\mathbf{x}(t)$ that minimizes a cost function

$$J(\mathbf{x}(t), \mathbf{u}(t), t_0, t_f) = Q(\mathbf{x}(t_f), t_f) + \int_{t_0}^{t_f} \mathcal{L}(\mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau. \quad (11.43)$$

Note that this formulation in (11.43) generalizes the LQR cost function in (8.47); now the immediate cost function $\mathcal{L}(\mathbf{x}, \mathbf{u})$ and the terminal cost $Q(\mathbf{x}(t_f), t_f)$ may be non-quadratic functions. Often there are also constraints on the state \mathbf{x} and control \mathbf{u} , which determine what solutions are admissible.

Given an initial state $\mathbf{x}_0 = \mathbf{x}(t_0)$ at t_0 , an optimal control $\mathbf{u}(t)$ will result in an optimal cost function J . We may define a *value* function $V(\mathbf{x}, t_0, t_f)$ that describes the total integrated cost starting at this position \mathbf{x} assuming the control law is optimal:

$$V(\mathbf{x}(t_0), t_0, t_f) = \min_{\mathbf{u}(t)} J(\mathbf{x}(t), \mathbf{u}(t), t_0, t_f), \quad (11.44)$$

where $\mathbf{x}(t)$ is the solution to (11.42) for the optimal $\mathbf{u}(t)$. Notice that the value function is no longer a function of the control $\mathbf{u}(t)$, as this has been optimized over, and it is also not a function of a trajectory $\mathbf{x}(t)$, but rather of an initial state \mathbf{x}_0 , as the remainder of the trajectory is entirely specified by the dynamics and the optimal control law. The value function is often called the *cost-to-go* in control theory, as the value function evaluated at any point $\mathbf{x}(t)$ on an optimal trajectory will represent the remaining cost associated with continuing to enact this optimal policy until the final time t_f . In fact, this is a statement of Bellman's optimality principle, that the value function V remains optimal starting with any point on an optimal trajectory.

The Hamilton-Jacobi-Bellman³ (HJB) equation establishes a partial differential equation that must be satisfied by the value function $V(\mathbf{x}(t), t, t_f)$ at every intermediate time $t \in [t_0, t_f]$:

$$-\frac{\partial V}{\partial t} = \min_{\mathbf{u}(t)} \left(\left(\frac{\partial V}{\partial \mathbf{x}} \right)^T \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t)) + \mathcal{L}(\mathbf{x}(t), \mathbf{u}(t)) \right). \quad (11.45)$$

To derive the HJB equation, we may compute the total time derivative of

³Kalman recognized that the Bellman optimal control formulation was a generalization of the Hamilton-Jacobi equation from classical mechanics to handle stochastic input-output systems. These formulations all involve the calculus of variations, which traces its roots back to the Brachistochrone problem of Johann Bernoulli.

the value function $V(\mathbf{x}(t), t, t_f)$ at some intermediate time t :

$$\frac{d}{dt}V(\mathbf{x}(t), t, t_f) = \frac{\partial V}{\partial t} + \left(\frac{\partial V}{\partial \mathbf{x}} \right)^T \frac{d\mathbf{x}}{dt} \quad (11.46a)$$

$$= \min_{\mathbf{u}(t)} \frac{d}{dt} \left(\int_0^{t_f} \mathcal{L}(\mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau + Q(\mathbf{x}(t_f), t_f) \right) \quad (11.46b)$$

$$= \min_{\mathbf{u}(t)} \left(\underbrace{\frac{d}{dt} \int_0^{t_f} \mathcal{L}(\mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau}_{-\mathcal{L}(\mathbf{x}(t), \mathbf{u}(t))} \right) \quad (11.46c)$$

$$\implies -\frac{\partial V}{\partial t} = \min_{\mathbf{u}(t)} \left(\left(\frac{\partial V}{\partial \mathbf{x}} \right)^T \mathbf{f}(\mathbf{x}, \mathbf{u}) + \mathcal{L}(\mathbf{x}, \mathbf{u}) \right). \quad (11.46d)$$

Note that the terminal cost does not vary with t , so it has zero time derivative. The derivative of the integral of the instantaneous cost $\int_t^{t_f} \mathcal{L}(\mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau$ is equal to $-\mathcal{L}(\mathbf{x}(t), \mathbf{u}(t))$ by the first fundamental theorem of calculus. Finally, the term $(\partial V / \partial \mathbf{x})^T \mathbf{f}(\mathbf{x}, \mathbf{u})$ may be brought into the minimization argument, since V is already defined as the optimal cost over \mathbf{u} . The LQR optimal Riccati equation is a special case of the HJB equation, and the vector of partial derivatives in $(\partial J / \partial \mathbf{x})$ serves the same role of the Lagrange multiplier co-state λ . The HJB equation may also be more intuitive in vector calculus notation

$$-\frac{\partial V}{\partial t} = \min_{\mathbf{u}(t)} (\nabla V \cdot \mathbf{f}(\mathbf{x}(t), \mathbf{u}(t)) + \mathcal{L}(\mathbf{x}(t), \mathbf{u}(t))). \quad (11.47)$$

The HJB formulation above relies implicitly on Bellman's principle of optimality, that for any point on an optimal trajectory $\mathbf{x}(t)$, the value function V is still optimal for the remainder of the trajectory:

$$V(\mathbf{x}(t), t, t_f) = \min_{\mathbf{u}} \left(\int_t^{t_f} \mathcal{L}(\mathbf{x}(\tau), \mathbf{u}(\tau)) d\tau + Q(\mathbf{x}(t_f), t_f) \right). \quad (11.48)$$

One outcome is that the value function can be decomposed as:

$$V(\mathbf{x}(t_0), t_0, t_f) = V(\mathbf{x}(t_0), t_0, t) + V(\mathbf{x}(t), t, t_f). \quad (11.49)$$

This makes it possible to take the total time derivative above. A more rigorous derivation is possible using the calculus of variations.

The HJB equation is incredibly powerful, providing a PDE for the optimal solution of general nonlinear control problems. Typically, the HJB equation is solved numerically as a two-point boundary value problem, with boundary conditions $\mathbf{x}(0) = \mathbf{x}_0$ and $V(\mathbf{x}(t_f), t_f) = Q(\mathbf{x}(t_f), t_f)$, for example using a shooting method. However, a nonlinear control problem with a three-dimensional

state vector $\mathbf{x} \in \mathbb{R}^3$ will result in a three-dimensional PDE. Thus, optimal nonlinear control based on the HJB equation typically suffers from the curse of dimensionality. Phase-space clustering techniques have shown great promise in reducing the effective state-space dimension for systems that evolve on a low-dimensional attractor [376].

Discrete-time HJB and the Bellman equation

Bellman's optimal control is especially intuitive for discrete-time systems, where instead of optimizing over a function, we optimize over a discrete control sequence. Consider a discrete-time dynamical system

$$\mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k, \mathbf{u}_k). \quad (11.50)$$

The cost is now given by

$$J(\mathbf{x}_0, \{\mathbf{u}_k\}_{k=0}^n, n) = \sum_{k=0}^n \mathcal{L}(\mathbf{x}_k, \mathbf{u}_k) + Q(\mathbf{x}_n, t_n). \quad (11.51)$$

Similarly, the value function is defined as the value of the cumulative cost function, starting at a point \mathbf{x}_0 assuming an optimal control policy \mathbf{u} :

$$V(\mathbf{x}_0, n) = \min_{\{\mathbf{u}_k\}_{k=0}^n} J(\mathbf{x}_0, \{\mathbf{u}_k\}_{k=0}^n, n). \quad (11.52)$$

Again, Bellman's principle of optimality states that an optimal control policy has the property that at any point along the optimal trajectory $\mathbf{x}(t)$, the remaining control policy is optimal with respect to this new initial state. Mathematically,

$$V(\mathbf{x}_0, n) = V(\mathbf{x}_0, k) + V(\mathbf{x}_k, n) \quad \forall k \in (0, n). \quad (11.53)$$

Thus, the value at an intermediate time step k may be written as

$$V(\mathbf{x}_k, n) = \left(\min_{\mathbf{u}_k} \mathcal{L}(\mathbf{x}_k, \mathbf{u}_k) \right) + \underbrace{V(\mathbf{x}_{k+1}, n)}_{\text{s.t. } \mathbf{x}_{k+1} = \mathbf{F}(\mathbf{x}_k, \mathbf{u}_k)} \quad (11.54a)$$

$$= \min_{\mathbf{u}_k} (\mathcal{L}(\mathbf{x}_k, \mathbf{u}_k) + V(\mathbf{F}(\mathbf{x}_k, \mathbf{u}_k), n)). \quad (11.54b)$$

It is also possible, given a value function $V(\mathbf{x}_k, n)$, to determine the next optimal control action \mathbf{u}_k by returning the \mathbf{u}_k that minimizes the above expression. This defines an *optimal policy* $\mathbf{u} = \pi(\mathbf{x})$. Dropping the functional dependence of V on the end time, we then have

$$V(\mathbf{x}) = \min_{\mathbf{u}} (\mathcal{L}(\mathbf{x}, \mathbf{u}) + V(\mathbf{F}(\mathbf{x}, \mathbf{u}))) \quad (11.55a)$$

$$\pi(\mathbf{x}) = \operatorname{argmin}_{\mathbf{u}} (\mathcal{L}(\mathbf{x}, \mathbf{u}) + V(\mathbf{F}(\mathbf{x}, \mathbf{u}))). \quad (11.55b)$$

These form the Bellman equations.

Note that we have explicitly include the terminal time t_f in the terminal cost $Q(\mathbf{x}_n, t_n)$ and $Q(\mathbf{x}(t_f), t_f)$, as it there are situations when the arrival time should be minimized. However, it is also possible to include the time explicitly in the immediate cost $\mathcal{L}(\mathbf{x}, \mathbf{u}, t)$, for example to include a discount function $e^{-\gamma t}$ for future costs or rewards.

Suggested reading

Texts

- (1) **Reinforcement learning: An introduction**, by R. S. Sutton and A. G. Barto, 1998 [695].

Papers and reviews

- (1) ***Q*-learning**, by C. Watkins and P. Dayan, *Machine Learning*, 1992 [757].
- (2) **TD (λ) converges with probability 1**, by P. Dayan and T. J. Sejnowski, *Machine Learning*, 1994 [202].
- (3) **Human-level control through deep reinforcement learning**, by V. Mnih et al., *Nature*, 2015 [519].
- (4) **Mastering the game of go without human knowledge**, by D. Silver et al., *Nature*, 2017 [673].
- (5) **A tour of reinforcement learning: The view from continuous control**, by B. Recht, *Annual Review of Control, Robotics, and Autonomous Systems*, 2019 [601].

Blogs and lectures

- (1) **Deep Reinforcement Learning: Pong from Pixels**, by A. Karpathy, <http://karpathy.github.io/2016/05/31/r1/>.
- (2) **Introduction to Reinforcement Learning with David Silver**, by D. Silver, https://www.youtube.com/playlist?list=PLqYmG7hTraZBiG_XpjnPrSNw-1XQaM_gB

Homework

Exercise RL-1. This example will explore reinforcement learning on the game of tic-tac-toe. First, describe the states, actions, and rewards.

Next, design a policy iteration algorithm to optimize the policy π . Begin with a randomly chosen policy. Plot the value function on the board and describe the optimal policy.

How many policy iterations are required before the policy and value function converge? How many games were played at each policy iteration? Is this consistent with what you would expect a human learning would do?

Is there any structure or symmetry in the game that could be used to improve the learning rate? Implement a policy iteration that exploits this structure, and determine how many policy iterations are required before converging and how many games played per policy iteration.

Exercise RL-2. Repeat the above example using value iteration instead of policy iteration. Compare the number of iterations in both methods, along with the total training time.

Exercise RL-3. This exercise will develop a reinforcement learning controller for the fluid flow past a cylinder. There are several open-source codes that can be used to simulate simple fluid flows, such as the IBPM code at <https://github.com/crowley/ibpm/>.

Use reinforcement learning to develop a control law to force the cylinder wake to be symmetric. Describe the reward structure and what learning framework you chose. Also plot your results, including learning rates, performance, etc. How long did it take to train this controller (i.e., how many computational iterations, how much CPU time, etc.)?

Now, assume that the RL agent only has access to the lift and drag coefficients, C_L and C_D . Design an RL scheme to track a given reference lift value, say $C_L = 1$ or $C_L = -1$. See if you can make your controller track a reference that switches between these values. What if the reference lift is much larger, say $C_L = 2$ or $C_L = 5$?

Exercise RL-4. Install the AI Gym API and develop an RL controller for the classic control example of a pendulum on a cart. Explore different RL strategies.

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