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SIMULATED HUMANOID ROBOT CONTROL WITH REINFORCEMENTE LEARNING

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This publication was accepted like Final Work of Undergraduation Study

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To God, my parents and all my good friends.

Acknowledgments

make it later

Resumo

Abstract

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List of Abbreviations and Acronyms

AI	Artificial Intelligence
API	Application Programming Interface
ANN	Artificial Neural Network
CMA-ES	Covariance Matrix Adaptation Evolution Strategy
CL	Curriculum Learning
CoM	Center of Mass
CNN	Convolutional Neural Network
DNN	Deep Neural Network
DDPG	Deep Deterministic Policy Gradients
DPG	Deterministic Policy Gradients
DQN	Deep Q-Network
DRL	Deep Reinforcement Learning
GPU	Graphics Processing Unit
KL	Kullback?Leibler
IK	Inverse Kinematics
MC	Monte-Carlo
MDP	Markov Decision Process
ML	Machine Learning
MLP	Multilayer Perceptron
NN	Neural Network
PPO	Proximal Policy Optimization
ReLU	Rectified Linear Unit
RL	Reinforcement Learning
RNN	Recurrent Neural Network
RPC	Remote Procedure Call
SS3D	Soccer Simulation 3D
Soccer3D	Soccer Simulation 3D
SGD	Stochastic Gradient Descent
TD	Temporal-Difference

List of Symbols

$\mathbb{A}$	A set
$\mathbb{R}$	The set of real numbers
a_i	Element i of vector a, with indexing starting at 1
A^T	Transpose of matrix A
$\frac{dy}{dx}$	Derivative of y with respect to x
$\frac{\partial y}{\partial x}$	Partial derivative of y with respect to x
∇y	Gradient of y
$\int_a^b f(x)dx$	Definite integral with respect to x over [a, b]
$\mathbb{I}^{\text{condition}}$	conditional unit function
$f : \mathbb{A} \rightarrow \mathbb{B}$	The function f with domain $\mathbb{A}$ and range $\mathbb{B}$
$f(x, \theta)$	A function of x parameterized by θ
$\mathbb{P}(x)$	Probability distribution over a continuous variable
$\mathbb{E}[X]$	Expectation of random variable X
$\mathrm{KL}[P, Q]$	KL divergence between P and Q
$\log x$	Natural logarithm of x
Reinforcement Learning	
$s, s\prime$	States
a	Action
r	Reward
t	Discrete timestep
A_t	Action at timestep t
S_t	State at timestep t
R_t	Reward at timestep t
G_t	Return (cumulative discounted reward) following time t
π	Policy, agent behavior rule
$\pi(s)$	Action taken in state s under policy π

$v_\pi(s)$	Value of state s under policy π (expected return)
$v_*(s)$	Value of state s under the optimal policy
$q_\pi(s, a)$	Value of taking action a in state s under policy π
$q_\pi(s, a)$	Value of taking action a state s under policy π
V, V_t	Estimate of state-value function v_π or v_*
Q, Q_t	Estimate of action-value function q_π or q_*

Contents

1 Introduction

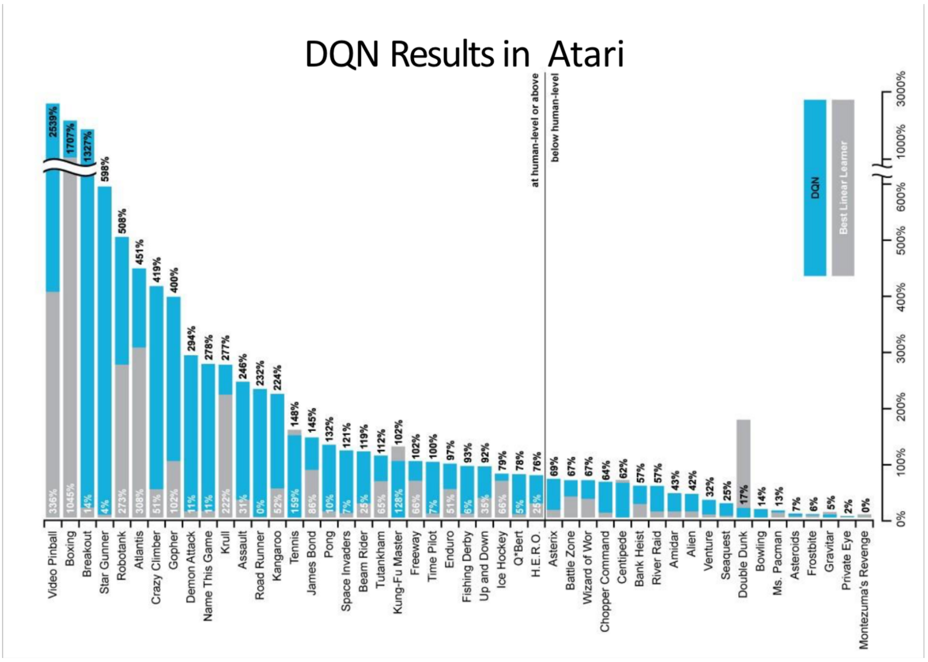
1.1 Motivation

In the last decades, the advances in computers architecture and computer science have pushed the research frontier to produce super intelligent algorithms, capable of dealing with difficult classification problems of subtle and inherently human concepts, or even hard decision making tasks in challenge situations. We can see intelligent algorithms applied to speech and image recognition, email spam classification, advertising, fraud detection, autonomous self-driving cars, virtual assistants, security, finance and several other applications in our lives. Never in the history we have witness such a great bet in the future of machines.

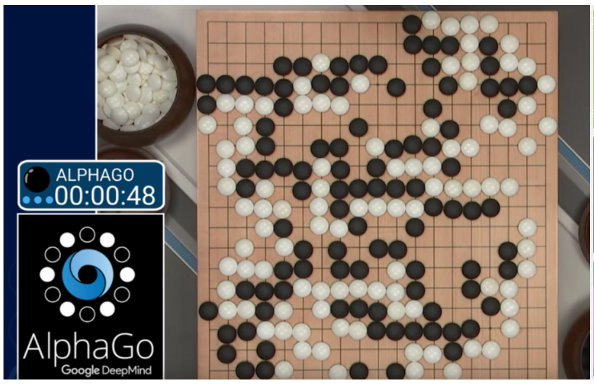
Besides, most recently, the cutting edge achievements in AI have shown algorithms capable of overcome top human intelligence in difficult problems. In 2015, Google DeepMind created an AI that learned how to play 49 Atari games using the same learning algorithm (including the same hyper parameters), using as the input only the pixels from the screen. The algorithm, called Deep Q-Learning (MNIH *et al.*, 2015), was a breakthrough achievement in the mission of accomplishing a general purpose machine learning agent in a wide variety of games.

In the same year, DeepMind left another big mark in the human history. A computer program called AlphaGo defeated the best human Go player for the first time. Go consists of a very complex board game, with more than 10^170 configurations, and represents one of the biggest challenges to human intelligence and an unconceivable problem to a computer until then. Going even further, in 2017, Silver *et al.* (2017) introduced AlphaGo Zero, an evolution of the previous version, capable of leaning how to play without any outside data from human games, but just playing with itself. Figure 1.1 illustrates these successful examples.

Another big field in Computer Science is mobile robotics, which plays a major role in the future of the industry and the forefront of academic research recently. Robotics can address state of the art challenges in different domains, such as Electronics Engineering, Mechanical Engineering, Control Theory and, of course, Machine Learning.



(a) DQN results in Atari games



(b) AlphaGo against Lee Sedol

(c) Different Atari games

FIGURE 1.1 – DeepMind recent achievements.

AI finds in Robotics several applications, as computer vision, path planning and even locomotion, and in this last one we can find one of its biggest challenges. In Atari and board games we can easily define a goal, win, but how can we define the agility and flexibility of a walk or a jump movement? In this sense, several works have been conducted in the problem of trying to reproduce human movements in humanoid robotics agents, and more specifically, in a simulated scenario.

One of the biggest initiatives of the research community to foster the study of robotics is RoboCup. RoboCup established itself as one of the main international robotics competition in the world, and a powerful scientific conference. It pushes state-of-the-art research in robotics by maintaining different technical challenges with one thing in common, making robots play soccer, with the mission of developing a humanoid robot team capable of win the champion of FIFA World Cup in 2050.

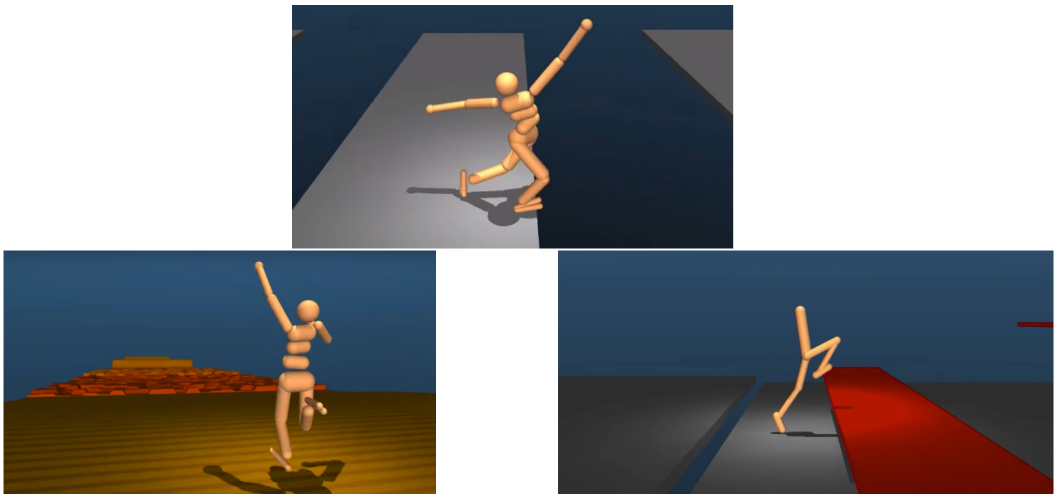


FIGURE 1.2 – Simulated humanoid agent movements and AI.

One RoboCup's particular league is the RoboCup 3D Soccer Simulation League, consisting of a soccer match between two teams, each one composed by up to 11 simulated NAO robots from Aldebaran Robotics. This league address both high level and low level robotics challenges, like path planning and locomotion, and greatly helped improving our understand of human movements like walk and kick the ball.

FIGURE 1.3 – Robocup symbol and Soccer 3D Simulation league match.

1.2 Problem Statement

Inspired by the RoboCup Soccer Simulation 3D (Soccer3D or SS3D) league, this dissertation's objective is to learn a high level soccer behavior for simulated humanoid robots, more specifically, the behavior of kicking the ball towards a planned final distance from the agent. In this sense, the algorithm should input the current game state, including agent's and ball's positions, and output a sequential movement for each robot's joint.

1.3 Approach

Instead of employing a deterministic and off-line built single movement, called Keyframe movement, we intend to use a model-free deep reinforcement learning based approach that tries to learn the desired behavior by interacting with an environment (the simulation server) and receiving rewards depending on which actions it chooses.

1.4 Literature Review

Reinforcement Learning techniques have been in increasingly study in the past 30 years. In this time, some specific works have established famous breakthroughs in this field. For instance, Temporal-Difference (TD) learning algorithms (BARTO *et al.*, 1983) created the groundwork for many future RL algorithms, making use of value function estimation and policy and value iteration methods. In the same way, Q-Learning (WATKINS, 1989) introduced off-policy model-free learning with *Sarsa*, estimating action-value functions and making room to future DRL algorithms.

After these works, Wiliams (1992) created a new paradigm presenting the REINFORCE algorithm, which introduces policy search methods. This technique estimate the optimal-policy function π_* directly, without the need of value or action-value functions and works way better in continuous action space, as we see in the robotics world. The most recent approaches developed make use and improve this method, such as the Deep Deterministic Policy Gradients (DDPG) algorithm, introduced by (LILLICRAP *et al.*, 2015), the Trust Region Policy Optimization (TRPO) algorithm, presented in (SCHULMAN *et al.*, 2015), and the Proximal Policy Optimization (PPO) algorithm, given in (SCHULMAN *et al.*, 2017).

Another recent breakthrough in the RL field was given by Deep Neural Networks, making possible to escalate the classical algorithms to high dimensional problems. This process was marked by the incredible results of the Deep Q-Networks (DQN) algorithm (MNIH *et al.*, 2015). This technique was able to learn 49 Atari games directly from raw pixels of the screen. It introduces the idea of modeling the action-value function as a neural network, and handle the inherently instability problem from value function approximation by introducing also two techniques: Experience Replay (LIN, 1992) and Target Networks Mnih *et al.* (2015).

Some recent works started to address humanoid movements in the RL field. However, the main problem which comes with that endeavor is that simple rewards functions or naÃ¯vely selected ones, such as the score for the games problems, can lead to results that do not match the expectations. This is the common case in continuous control tasks, like locomotion. In this sense, (HEESS *et al.*, 2017) proposed that rich and robust behaviors can emerge from simple reward functions, if the environment itself contains sufficient richness and diversity. This work introduces scenarios with a lot of obstacles and varying levels of difficulty, which are presented to the agent as an implicit curriculum, making possible to overcome increasingly hard challenges. A similar idea was also introduced by (BENGIO *et al.*, 2009)

Others DeepMind's papers introduced methods to learn to imitate human movements, like (MEREL *et al.*, 2017) and (WANG *et al.*, 2017), which combines supervised learning and Generative Adversarial Imitation Learning (GAIL) ((HO; ERMON, 2016)), in a way that accentuates their individual strengths and address their limitations.

Another recent state-of-the-art work in imitation learning is (PENG *et al.*, 2018). This work makes possible for a motion capture actor to supply a set of reference motions for style, and then generate goal-directed and physically realistic behaviors from them. The approach used for this is designing a reward function which combines rewarding motions that resemble reference animation data, and also achieving additional task objectives.

1.5 Contributions

This work's major contribution is successfully applying deep reinforcement learning (DRL) algorithms in the task of learning a behavior to kick a ball towards a planned final distance from the agent in the Soccer3D environment domain. To the best of our knowledge, this work is the first that makes use of a DRL approach to address this specific challenge.

1.6 Outline of this Dissertation

This dissertation is organized as follows:

- **Chapter 1** introduces this dissertation by describing the motivation behind the problem we address, by the Literature review and by summarizing the contributions.
- **Chapter 2** describes a brief theoretical background of reinforcement learning and neural networks.
- **Chapter ??** describes some experiments using OpenAI gym frameworks

2 Reinforcement Learning

Reinforcement Learning (RL) is an area of machine learning that studies how an agent interacts with an environment receiving instant rewards (SUTTON; BARTO, 1998). The standard RL setup consists of an agent interacting with an environment E in discrete timesteps. At each timestep t, an agent receives an observation S_t, takes action A_t and ends up in state S_{t+1}, receiving an scalar reward R_{t+1}. Figure 2.1 illustrates this notion.

RL is a simple yet powerful framework that defines the interaction between the agent and the environment. The agent learns from the environment in order to achieve long-term goals.

When modelling a problem with RL, there are 3 main components that must be carefully modeled:

- **State space**: set of values that define the state of the agent in the environment. This represents the information available to the agent.
- **Action space**: set of values that define the possible actions the agent can take in the environment.
- **Reward signal**: defines how the agent is rewarded in regards to the goal.

The agent's goal is to maximize the cumulative reward it gets when interacting with the environment. Note that normally these interactions are episodic, which means that

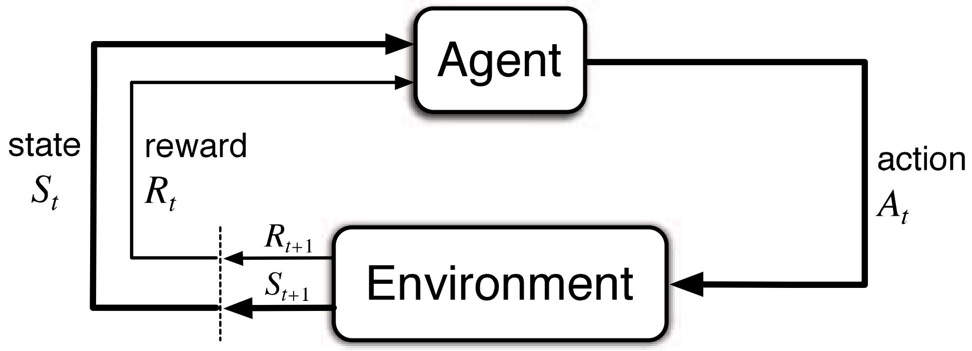


FIGURE 2.1 – Agent interacting with environment.

the task restarts after some number of steps.

The following sections will describe the theory behind RL.

2.1 Markov Decision Process

A Markov Decision Processes (MDP) defines a mathematical framework that formally describes this interaction with the environment. It is said that if the state of the agent contains all the necessary information from the past, it has the Markov Property and can be defined formally as:

$$\mathcal{P}(S_{t+1}|S_t) = \mathcal{P}(S_{t+1}|S_1, S_2, ..., S_t) \tag{2.1}$$

Therefore, a RL problem is an MDP if it has the Markov Property.

A particular MDP is defined by

- State set, $\mathcal{S}$.
- Action set, $\mathcal{A}$.
- Initial state distribution $P(S_1)$.
- One-step transition dynamics of the environment E, denoted as $\mathcal{P}(S_{t+1}|S_t, A_t)$.

In general, the environment may be partially observed so that the entire history of state-action pairs would be required to fully describe the state.

2.2 Return

The return from state S is defined as the sum of discounted future reward from timestep t:

$$G_t = R_{t+1} + \gamma R_{t+2} + ... = \sum_{k=0}^{\infty} \gamma^k R_{t+k+1} \tag{2.2}$$

Notice that $\gamma \in [0, 1]$ introduces the concept of discounting so that the agent prefers to gain instant rewards instead of long term rewards. Also, the return depends on the actions being chosen (therefore on the policy *pi* as well) and may be stochastic.

2.3 Policies

A policy π maps the states to a probability distribution over the actions $\pi : \mathcal{S} \to \mathcal{P}(\mathcal{A})$. It is represented by Equation (2.3).

$$\pi(a|s) = \mathcal{P}[A_t = a|S_t = s] \tag{2.3}$$

The policy fully describes the behavior of the agent and can also be deterministic formalized as $\mu_\theta : \mathcal{S} \to \mathcal{A}$ with parameter vector $\theta \in \mathbb{R}^2$ and $A_t = \mu_\theta(S_t)$.

2.4 Value functions

The value functions are estimates of the agent's current return.

- State-value function
$$v_\pi(s) = \mathbb{E}[G_t|S_t = s] \tag{2.4}$$
- Action-value function
$$q_\pi(s, a) = \mathbb{E}[G_t|S_t = s, A_t = a] \tag{2.5}$$

The value function estimates how good the agent's current state is (or how good it is for it to take a given action at that state).

2.5 Goal of RL

The goal of RL is to learn the optimal behavior (described by the policy) of the agent. This policy maximizes the expected return $\mathbb{E}_{R_i,S_i\sim E,A_i\sim\pi}[G_1]$. We will now define optimality for the value function and policy:

2.5.1 Optimal Value Function

The value functions are optimal if they are the highest value for all states (or state-action pairs).

- Optimal State-value function: $v_*(s) = \max\limits_\pi v_\pi(s)$.
- Optimal Action-value function: $q_*(s, a) = \max\limits_\pi q_\pi(s, a)$.

Therefore, solving an MDP means finding the optimal value function (or optimal policy).

2.5.2 Optimal Policy

Let the partial ordering of policies be

$$\pi \geq \pi\prime \text{ if } v_{\pi}(s) \geq v_{\pi\prime}(s)$$

The optimal policy is better than any other, $\pi_* \geq \pi, \forall \pi$ and achieves the optimal value functions.

An interesting property of the optimal policy is that it can be implicitly defined with q_*. The optimal policy can be defined as the following deterministic policy

$$\pi_*(a|s) = \begin{cases} 1, & \text{if } a = \underset{a'}{\operatorname{argmax}}\ q_*(s, a') \\ 0, & \text{otherwise} \end{cases}$$

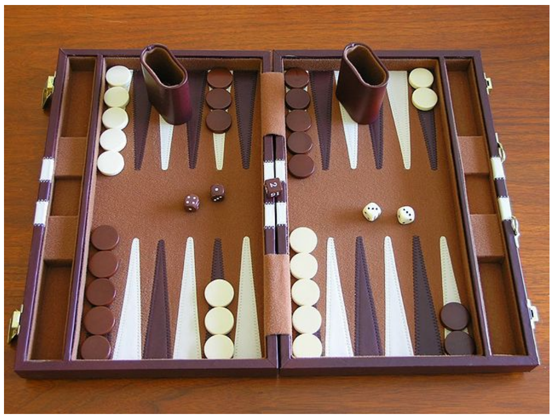
2.6 Function Approximation

Many classic tabular RL algorithms work by estimating the value functions for each state, for example, Value Iteration methods. A problem arises when the state/action spaces are extremely large, or if the state/action spaces are continuous. Some examples of large discrete state spaces are board games. This is known as the *curse of dimensionality* (BENGIO *et al.*, 2012). Backgammon has over 10^{20} board states (LEVNER, 1976) and the game of Go (with board size of 19x19) has over 10^{170} states (TROMP; FARNEBÃ¤CK, 2016). Figure 2.2 illustrates these games.

There are 2 problems of having so many states in realistic situations:

- It will be impossible to store all the states in memory.
- It will be impossible to visit all the states in training.

For continuous domains, we have an analogous situation since it is possible to discretize the state or action space and then apply tabular methods. Figure 2.3 illustrates 3 continuous control problems and the number of states resulting from one possible discretization.


(a) Game of Backgammon.

(b) Game of Go.

FIGURE 2.2 – Example of board games that have large discrete state spaces.

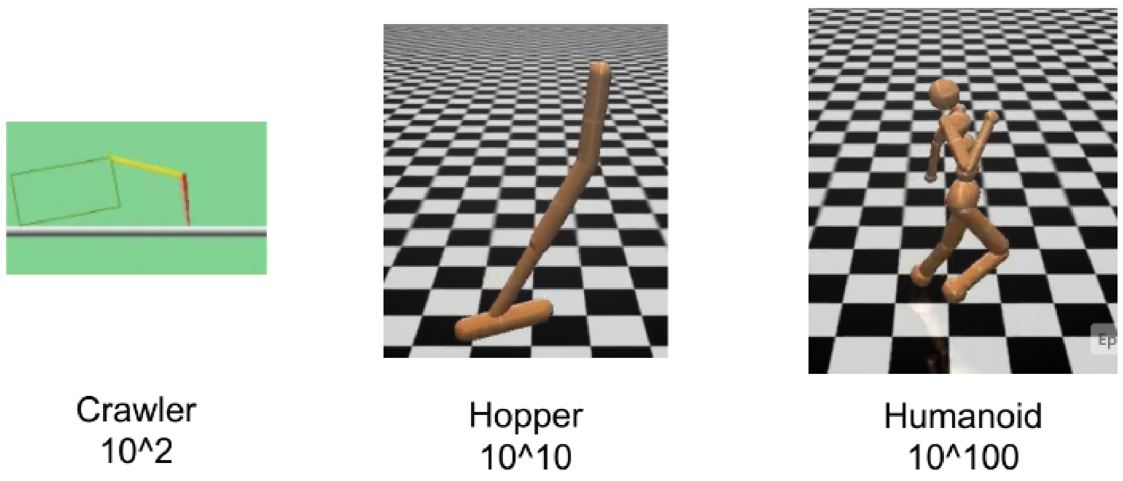


FIGURE 2.3 – Sample control tasks from the (BROCKMAN *et al.*, 2016) toolkit.

If the discretized space is large, we still have the problem described above. An approach to deal with this problem is to use a function approximation that estimates the value function. The approximate value function, $\hat{v}(s, \theta)$ will be defined by a parameter weight vector $\theta \in \mathbb{R}^n$ and

$$\hat{v}(s, \theta) \approx v_\pi(s)$$

The interesting part of function approximation is that this function estimator can be any function, ranging from a simple linear function of the states to a complex NNs. Normally the number of weights is much less than the number of states.

In this work, we focused on using neural networks as function approximators; Chapter 3 lays the groundwork for the theory regarding Neural Networks.

2.7 RL algorithms

There are 3 classes of RL algorithms: methods based on value functions, methods based on policy search and a hybrid approach which combines value functions and policy search (SUTTON; BARTO, 1998).

2.7.1 Value Function Methods

Value function methods are based on estimating v or q functions. Monte-Carlo (MC) methods and TD Learning are the two methods generally used for predicting the value function (SUTTON; BARTO, 1998).

2.7.1.1 Monte-Carlo

MC prediction are model-free (i.e. they do not require knowledge of the underlying dynamics) methods that learn directly from complete episodes of experience. They estimate the value functions by averaging sample returns and therefore can only be applied to episodic MDPs.

2.7.1.2 Temporal-Difference Learning

TD Learning are model-free and can learn from incomplete episodes. TD Learning updates the estimate by *bootstrapping*, which means it updates the value function using an existing estimate.

The simplest TD method, known as TD(0), updates the value function as

$$V(S_t) = V(S_t) + \alpha[R_{t+1} + \gamma V(S_{t+1}) - V(S_t)] \tag{2.6}$$

TD has some advantages in comparison to MC: TD can learn before the end of that episode (or in non episodic MDPS) and have low variance and some bias. MC on the other hand has high variance, zero bias, having good convergence properties (even with function approximation).

2.7.2 Policy Search Methods

Policy search methods do not have an estimate of the value function. These algorithms typically maintain a parameterized policy π_θ whose parameters are updated to maximize the expected return. The Policy Gradient Theorem defines that for any differentiable policy $\pi_\theta(s, a)$ the policy gradient is

$$\nabla_\theta J(\theta) = \mathbb{E}_{\pi_\theta}[\nabla_{\pi_\theta} \log \pi_\theta(s, a) Q^{\pi_\theta}(s, a)] \tag{2.7}$$

An example usage of this theorem is seen in the REINFORCE algorithm that uses Equation (2.7) to update the policy's weight using gradient ascent (WILIAMS, 1992).

2.7.3 Actor-Critic Methods

Actor-critic methods also work by updating a parameterized policy π_θ but instead use a *critic* to estimate the action-value function Q^{π_θ},

$$Q_w(s, a) \approx Q^{\pi_\theta}(s, a)$$

where w is the weight vector that parameterizes Q. Therefore actor-critic algorithms maintain two sets of parameters: the *critic* that updates that action-value function parameters w and the *actor* that updates the policy parameters θ in the direction suggested by the *critic*.

Figure 2.4 illustrates the architecture of actor-critic algorithms.

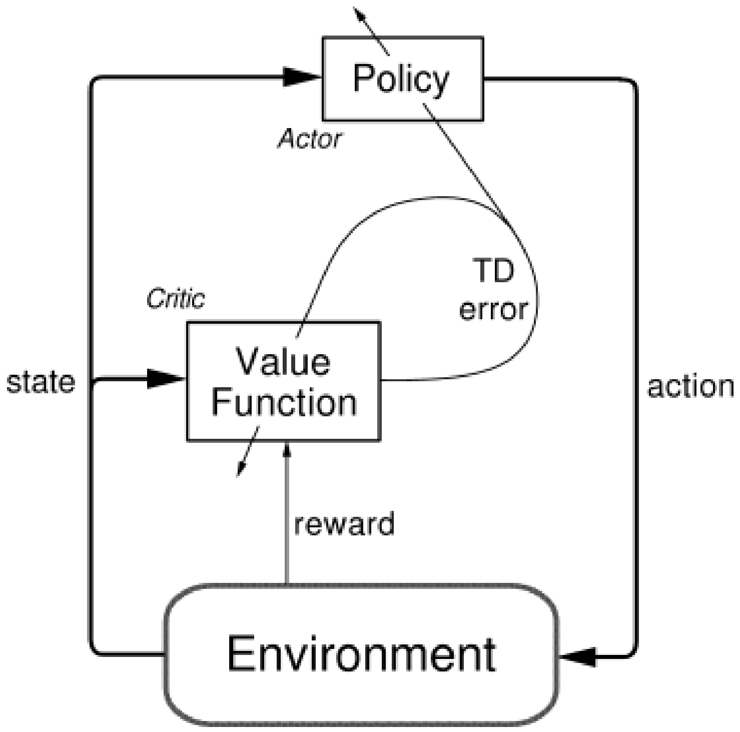


FIGURE 2.4 – Actor-critic architecture from (SUTTON; BARTO, 1998).

2.8 Curriculum Learning

Reinforcement learning has been used to solve non-trivial tasks in locomotion (SCHULMAN *et al.*, 2015) and video games (MNIH *et al.*, 2015).

However, there are many tasks that are hard to design a reward function that is easily maximized and that when optimized yields the expected behavior (FLORENSA *et al.*, 2017). For example, tasks with sparse rewards are still challenging since it is very hard to achieve the goal following random exploration (MATIISEN *et al.*, 2017). One approach to overcome this problem is to use curriculum learning (BENGIO *et al.*, 2009).

Curriculum learning is a sequence of training criteria where tasks are ordered by increasing difficulty and training moves from to a harder task only when it has mastered the easier tasks. Usually, to apply curriculum learning to a task, the researcher must be able to order the subtasks by difficulty and decide the heuristics for when a subtask has been mastered (MATIISEN *et al.*, 2017).

Curriculum learning is a recent idea that has been applied to a wide range of RL problems. An interesting result is Zaremba e Sutskever (2014) that applies a variant of curriculum learning to evaluate short computer programs. Some other examples include (BANSAL *et al.*, 2017; MATIISEN *et al.*, 2017).

3 Deep Learning

In the last chapter we described the mathematical background behind reinforcement learning and how a problem can be modeled with it. We also saw that for problems with continuous state and/or action spaces, it can be necessary to use function approximators such as neural networks. In this chapter we will describe the theoretical background of NNs, as function approximators.

Deep learning is a field of Machine Learning that in part studies deep neural networks and how they learn.

3.1 History

Today, Deep learning is a very significant topic for the scientific community yet its history goes back since the 1940s (GOODFELLOW; COURVILLE, 2016).

There has been a major resurgence of deep learning mainly because computers today became faster. Training large deep learning models are computationally very expensive and could be sped up with the use of graphics processing units (GPUs).

Artificial Neural Networks are one of the earliest learning algorithms. The novel concept behind it was to create mathematical models that tried to mimic the brain. NNs were based on the human brain's neurological structure, more specifically neurons and how they connect with other neurons. Figure 3.1 illustrates a single neuron cell.

A neuron cell is capable of transmitting information by sending electrical and chemical signals through axons and they connect to other neurons forming neural networks. The human brain, for example, has billions of connected neurons. NNs, therefore, are a simplified mathematical representation of neurons: essentially, a neuron can be viewed as a cell that receives one or more inputs and produces one or more outputs.

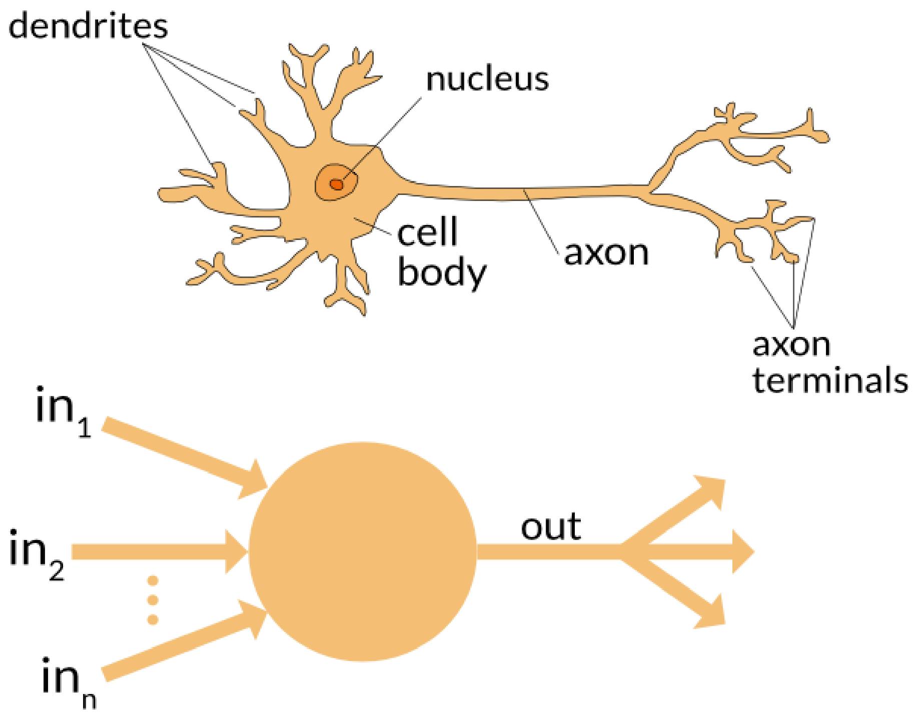


FIGURE 3.1 – Neuron unit cell structure.

3.2 Neural Networks

3.2.1 Representation

In simple terms, a neural network is a mathematical structure that receives an input and calculates an output. We will describe a simple NN known as feedforward neural network or Multi Layer Perceptron (MLP).

A neural network is composed of multiple layers where each layer has one or more nodes (neurons). The NN receives an input and computes the output according to the network architecture and parameters θ. Each input, called sample or example, is a n-dimensional feature vector x, and is represented as a column vector:

$$x = \begin{bmatrix} x_1 & x_2 & x_3 & x_4 & \dots & x_{n-1} & x_n \end{bmatrix}^\intercal \tag{3.1}$$

x is known as the input layer, and each coordinate represents each of the sample's features. The output is a k-dimensional vector y, known as the output layer. Every other layer that is not the input nor the output layer is known as a hidden layer.

In this work, note that every time we refer to an element $z^{[l]}$ we are referring to an element of the l-th layer.

Figure 3.2 illustrates a very simple NN with a 3-dimensional feature vector, 1-dimensional output vector and only one hidden layer.

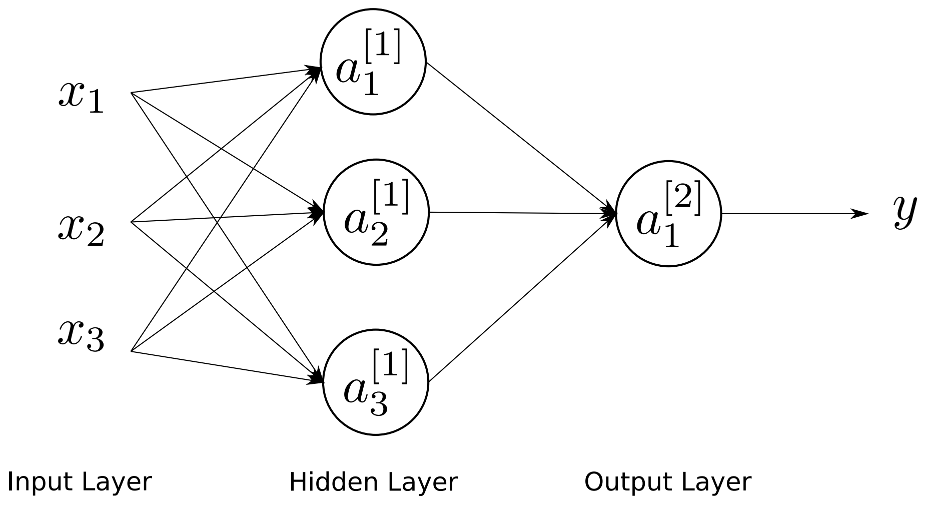


FIGURE 3.2 – Simple neural network.

Every node of the network is computed using the values from the previous layer. For the MLP, the node computation model is done through a linear model $f(x;\theta)$, with θ consisting of internal parameters w (weights) and b (bias). w has the same dimensions as the input and b is a scalar. In this work, we treat w as a column vector.

$$w = \begin{bmatrix} w_1 & w_2 & w_3 & w_4 & \dots & w_{n-1} & w_n \end{bmatrix}^{\mathsf{T}} \tag{3.2}$$

The model is defined as

$$z = w^T x + b \tag{3.3}$$

The output of the node a, also known as the activation, is calculated with x, b and a function $\sigma : \mathbb{R} \to \mathbb{R}$:

$$a = \sigma(z) = \sigma(w^T x + b) = \sigma\left(\sum_{i=1}^{n} w_i x_i + b\right) \tag{3.4}$$

Figure 3.3 illustrates the output of a single neuron.

σ is called activation function, applied to the model output (z). The activation function normally is a non-linear function and its most used common choice today is the **rectified linear unit** (NAIR; HINTON, 2010) or ReLU and is defined as $\sigma(z) = max\{z, 0\}$, shown in 3.4.

Other examples of popular activation functions are $\sigma(z) = \frac{1}{1+e^{-z}}$, known as the sigmoid function and $tanh(z)$ (XU; LI, 2016).

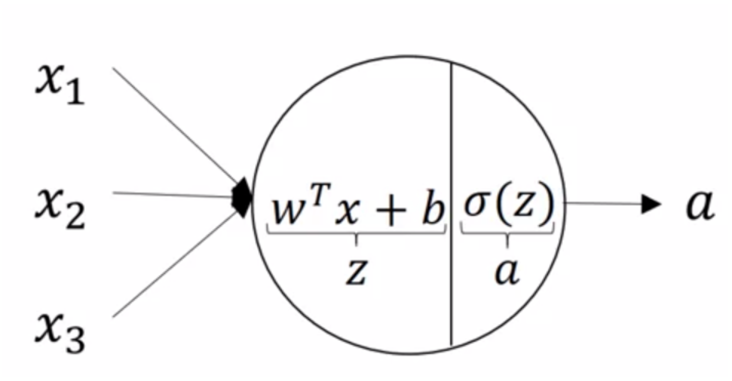


FIGURE 3.3 – Node computation.

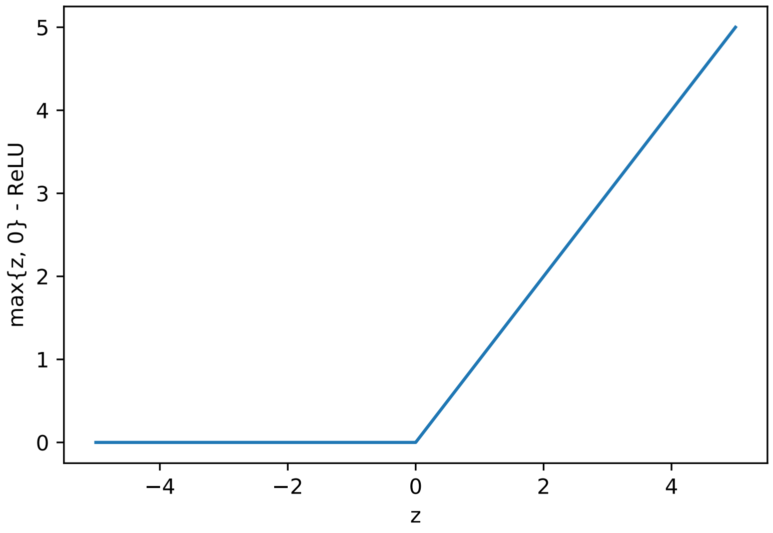


FIGURE 3.4 – Linear rectified unit plot.

A neural network is therefore is a connection of multiple neurons as inputs to other neurons. Let us return our attention to the network from Figure 3.2. We denote $(W, b) = (W^{[1]}, b^{[1]}, W^{[2]}, b^{[2]})$ as the network parameters, where $W^{[l]}$ is the matrix formed by concatenating the individual parameters of the l-th layer such that W_{ij} denotes the parameter associated with the connection between neuron j from the l-th layer and neuron i from layer $l+1$. Similarly, $b^{[l]}$ is the concatenation of the biases b of each neuron of layer $l+1$ and $b_i^{[l]}$ the bias of the i-th neuron of layer $l+1$.

For the network depicted in Figure 3.2, we are now capable of calculating the output y.

For the first layer:

$$z^{[1]} = W^{[1]}x + b^{[1]} \tag{3.5}$$

$$a^{[1]} = \sigma(z^{[1]}) \tag{3.6}$$

And for the second layer:

$$z^{[2]} = W^{[2]}a^{[1]} + b^{[2]} \tag{3.7}$$

$$y = a^{[2]} = \sigma(z^{[2]}) \tag{3.8}$$

We can think of the neural network as a recursive structure where each activation is calculated with the past's layers activation. $a^{[l]}$ can be computed as:

$$z^{[l]} = W^{[l]}a^{[l-1]} + b^{[l]} \tag{3.9}$$

$$a^{[l]} = \sigma(z^{[l]}) \tag{3.10}$$

Note also that $a^{[1]} = x$.

3.2.2 Vectorization

In the previous section, we focused on computing the output of the neural network given a single sample x. In modern days, however, we are normally interested in calculating the output of a neural network for thousands or even millions of samples.

For m samples, we could naively compute the output of the neural network for each example $x^{(i)}$ with Algorithm 1.

Algorithm 1: Naive algorithm for computing NN output of m samples.

```
Result: Output of NN for m samples.
for $i$ = 1 to $m$ do
    $a^{[0]} = x^{(i)}$
    for $j$ = 1 to $L$ do
        $z^{[j](i)} = W^{[j]}a^{[j-1](i)} + b^{[j]}$
        $a^{[j](i)} = \sigma(z^{[j](i)})$
    end
    $y^{(i)} = a^{[l](i)}$
end
```

In practice this algorithm runs relatively slow since it computes the output of the network sequentially for each sample and we will apply vectorization to achieve a much faster algorithm.

Firstly, Vectorization is a technique that transforms a set of computations done sequentially in a for loop into matrix operations. We will now vectorize our initial problem.

Let us define the following matrices

- X is a matrix where column i is the i-th sample $x^{(i)}$ and $W^{[l]}$. We can analogously define matrices A and Z. $X = \begin{bmatrix} x^{(1)} & x^{(2)} & \dots & x^{(m)} \end{bmatrix}$.
- $W^{[l]}$ is the weight matrix for the l-layer, as defined in Section 3.2.1.
- $b^{[l]}$ is the bias vector for layer l, as defined in Section 3.2.1.

For the vectorized version of Algorithm 2.

Algorithm 2: Vectorized algorithm for computing NN output of m samples.

```
Result: Output of NN for m samples.
for $j = 1$ to $L$ do
    $Z^{[j]} = W^{[j]}A^{[j-1]} + b^{[j]}$
    $A^{[j]} = \sigma(Z^{[j]})$
end
```

The vectorized version is much better since these matrices operations can be greatly sped up on GPUs or hardware that have support for Streaming SIMD Extensions (SSE). The great majority of popular deep learning libraries use as much vectorization as they can.

3.2.3 Deep Neural Networks

We can extend the architecture we saw on Section 3.2.1 to a higher number of layers called deep neural networks. Figure 3.5 illustrates a neural network with multiple hidden layers.

The activation of layer $l + 1, l > 1$, can be calculated according to Equation 3.9.

3.3 Learning

As described in the previous section, feedforward networks defines a mapping $y = f(x; \theta)$, or, equivalently, serve as general function approximators.

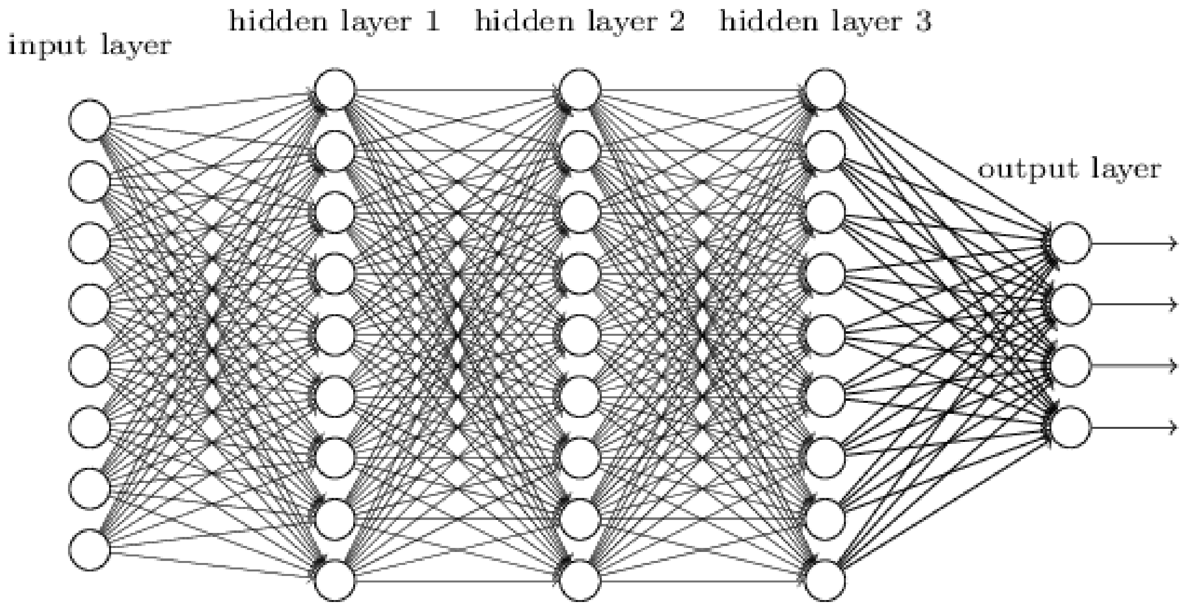


FIGURE 3.5 – Neural network with multiple layer.

This section describes deep learning algorithms that learn the value of the parameters θ that best approximates f.

Most deep learning algorithms need to describe a cost function and optimization algorithm.

3.3.1 Cost Function

The cost function $J(\theta)$ is a metric of how good our estimator is to our dataset: the lower the cost function, the less error the model has when predicting y. It describes the function that we wish to minimize and normally it envolves an average of the errors between the the target value of a sample and the predicted value of the estimator for the sample.

For example, for the problem of linear regression where X are the sample values and y are the target values for our dataset, we wish to learn the parameters θ from our function approximator f. The most used cost function for this problem is

$$J(\theta) = \frac{1}{m}\sum_{i=1}^{m}(y_i - f(x_i,\theta))^2 \tag{3.11}$$

Another example is the logistic regression problem. The most common cost function for this problem is

$$J(\theta) = -\frac{1}{m}\sum_{i=1}^{m}[y_i \log f(x_i, \theta + (1 - y_i) \log 1 - f(x_i, \theta)] \tag{3.12}$$

Choosing a good cost function greatly impacts how good the design of the deep neural network is.

3.3.2 Optimization Algorithms

After defining a cost function, finding the parameters that effectively minimize the cost function is not trivial. The non linearity of NN causes most cost functions to be non-convex and therefore, neural networks are usually trained by iterative, gradient-based optimizers. In practice, however, this is very unlikely (SWIRSZCZ *et al.*, 2017; GOODFELLOW *et al.*, 2014; LIN *et al.*, 2017).

Section 3.4 describes how neural networks gradients can be calculated.

3.3.2.1 Gradient Descent

One of the most common optimization algorithm is Gradient Descent. It is an iterative first-order method that tries to find a local minimum for a function f by moving in the negative direction of its gradient. Specifically for neural networks, our goal is to minimize the cost function $J(\theta)$. The algorithm's update step is Equation (3.13) done for each θ_i

$$\theta_i = \theta_i - \alpha\frac{\partial J}{\partial \theta_i} \tag{3.13}$$

The learning rate, α measures how big the update step in the direction of the gradient will be.

For example, let $g : \mathbb{R}^2 \to \mathbb{R}$ given by $g(x, y) = y \sin(x) - x \cos(y)$. Figure 3.6 illustrates 5 steps of the gradient descent algorithm. Notice how the red circle is the starting point and after the last iteration, the algorithm arrives approximately at a local minimum.

3.3.2.2 Stochastic Gradient Descent

Another popular algorithm is Stochastic Gradient Descent (SGD) that is a stochastic approximation of Gradient Descent. Instead of calculating $J(\theta)$ as an average between all the samples, the gradient update step is done once per sample. It calculates an approximation of the gradient and updates the parameters θ_i with every sample. Algorithm 3

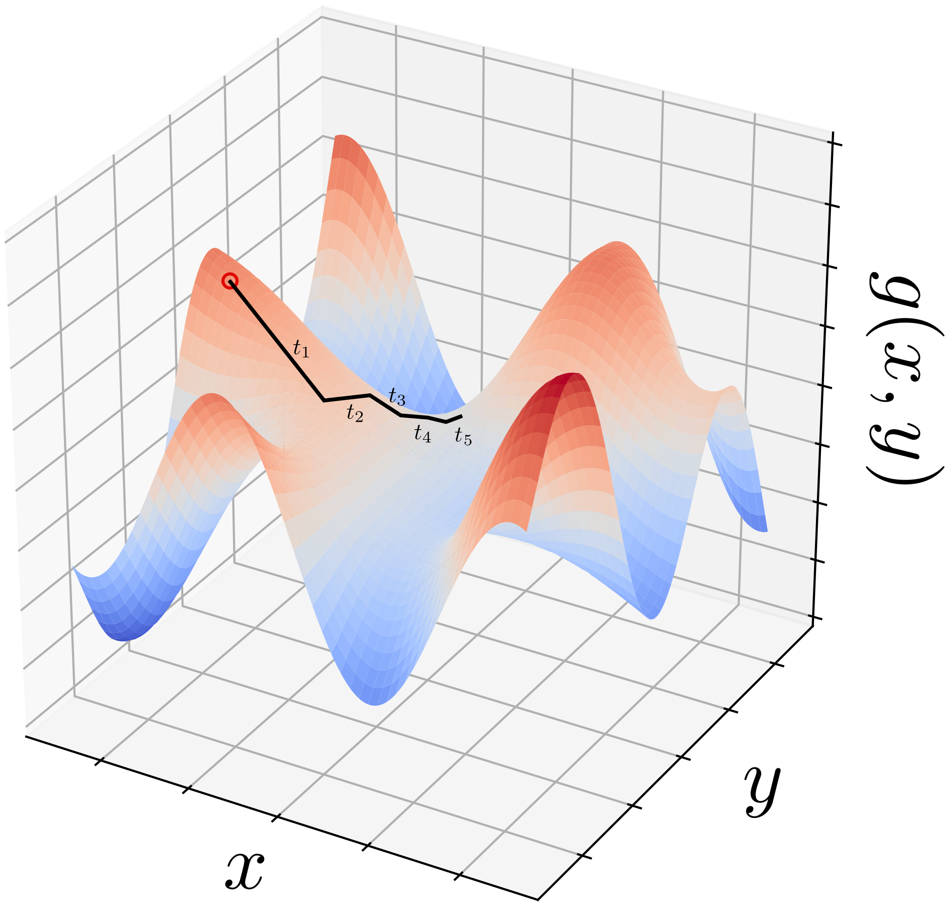


FIGURE 3.6 – Gradient descent on function g.

describes SGD

Algorithm 3: SGD algorithm.

```
Result: Function minimum
while An approximate minimum is not obtained do
    Randomly shuffle examples in the training set
    for i = 1,2,..., m do
        $\theta_i = \theta_i - \alpha \nabla J_i(\theta)$
    end
end
```

The gradient approximation for SGD is much faster to compute, however, since it is a noisy estimate of the gradient, SGD may need more steps to converge to a local minimum.

3.3.2.3 Mini-Batch Gradient Descent

Finally, Mini-Batch Gradient Descent combines the idea from Gradient Descent and SGD. It computes the gradient using more than one training example, called a *mini-batch*, at each step. It may result in smoother convergence and the code can be accelerated by making use of vectorization.

3.4 Back Propagation

We have seen how a few gradient-based optimization algorithms work. To minimize the cost function we need to compute the partial derivatives of the cost function w.r.t. to each weight of the neural network. Calculating these partial derivatives manually would be computacionally infeasible for large networks. In deep neural networks, by using the chain rule, we can calculate the partial derivatives in an efficient and compact way.

Backpropagation is an algorithm that computes the gradients of the loss function w.r.t. each input from the network.

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Appendix A - Tï¿½picos de Dilema Linear

A.1 Uma Primeira Seção para o Apêndice

A matriz de Dilema Linear M e o vetor de torques inerciais b, utilizados na simulação são calculados segundo a formulação abaixo:

$$M = \begin{bmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{bmatrix} \tag{A.1}$$

FIGURE A.1 – Uma figura que está no apêndice

Annex A - Exemplo de um Primeiro Anexo

A.1 Uma Seção do Primeiro Anexo

Algum texto na primeira seção do primeiro anexo.

FOLHA DE REGISTRO DO DOCUMENTO

1. CLASSIFICAÇÃO/TIPO TC	2. DATA 4 de marï¿½o de 2015	3. DOCUMENTO Nº DCTA/ITA/DM-018/2015	4. Nº DE PÁGINAS 42

5. TÍTULO E SUBTÍTULO:
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6. AUTOR(ES):
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8. PALAVRAS-CHAVE SUGERIDAS PELO AUTOR:
Cupim; Cimento; Estruturas

9. PALAVRAS-CHAVE RESULTANTES DE INDEXAÇÃO:
Cupim; Dilema; Construï¿½ï¿½o

10. APRESENTAÇÃO: (**X**) **Nacional** ( ) **Internacional**
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11. RESUMO:

12. GRAU DE SIGILO:
(X) **OSTENSIVO** ( ) **RESERVADO** ( ) **SECRETO**