ETH zürich Quantum Information Theory Group

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Master's Thesis

Designing experiments with neural networks

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Acknowledgments

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Zurich, April 14, 2020

Eduardo Gonzalez Sanchez

Abstract

(*Mock version, not definitive*) In this work we propose a new model that mixes reinforcement learning and deep learning to create agents able to design strategies for experiments, using as feedback only the quality of the predictions about properties of the physical system made exclusively from the data the agents collect. This is could be summarized as 'agents able to do science'; since science checks its validity by making predictions over the physical world. In the thesis we also put the first building blocks of a theoretical model for the scientific method in machines. This last part is important in the long-term goal of developing a variant of quantum theory that can consistently describe agents who are using the theory. If the science of the future is done by machines, we must ensure consistency in the underlying principles driving automated science.

Keywords: Reinforcement learning, deep learning, automated science, feature representation, experiment design, artificial intelligence

Contents

Chapter 1

Preface

Many of the limitations of humans at doing science come from their biological condition:

- Humans have a limited lifespan: 72.6 years on average [9]. When experienced scientists die their knowledge and expertise die with them.
- From the limited lifespan, humans can dedicate only a fraction to do science. This is inevitable since humans need to eat, sleep and deal with social interactions, among other things. Moreover, humans need decades of study and training to start making contributions to the scientific knowledge.
- Humans are susceptible to suffer from diseases and other limiting biological conditions that hinder their scientific production.
- Humans' understanding of the physical world is tightly linked to their limited sensorial perception and other inherited or acquired factors like the language or the cognitive capacity.

Other limitations are indirectly caused by the need to satisfy their biological necessities. For example, a person who wants to dedicate their life to science needs some type of financial support to satisfy the basic human necessities. This support usually comes from a greater institution like a state, a company or a patron. This financial relationship ties infrangibly science to the economical structure of the society. Profitable discoveries are encouraged while resources for unprofitable science are scarce. It can be argued that any form of scientific research, human or not, will require an investment of energy and resources in a society in which those are limited. This can be true, but a more efficient way of doing science will increase science independence from the economy.

At the same time, scientific discoveries influence drastically modern society and its economical structure. They provide new knowledge that allows humanity to develop new tools and protocols to improve human well being. In the last centuries, science has changed society by setting the theoretical and experimental grounds of a technological transformation. It is of public interest to boost and improve scientific production.

During the last century, the amount of available scientific literature has been growing exponentially [13, 3], with a yearly growth rate of $\sim 9\%$ in the last decade. Scholars read on average almost 240 articles per year [15]. Some authors [1] suggest that science is in the midst of a data crisis. Although the available literature grows exponentially the cognitive capacity of human beings remains constant. This forces scientists to derive hypotheses from an exponentially smaller fraction of the collective knowledge. This will lead to scientists increasingly asking questions that already been answered and reducing further the efficiency of scientific production.

Some areas of science are starting to suffer from a reproducibility crisis [12, 2] in which scientists are generally unable to reproduce their peers' findings. Some voices in the physics community [7] point out that foundational physics has been stagnated during the last decades. However, some authors defend that there isn't such a crisis [6]. Nonetheless, it's clear that to sustain an exponential growth of reliable scientific production with no exponentially increasing human effort is impossible, and the crisis is thus, unavoidable.

However, the lack of efficiency in scientific production is not the only drawback produced by the biological limitations of human beings. Humans' intuition and understanding of the physical world is conditioned by the percepts collected by their sensory system. This limitation becomes evident when trying to intuitively understand physical systems that show behaviors that differ from those susceptible to be collected by the sensory system. This is the case of, for example, quantum theory. Humankind has developed tools to overcome the limitations of the sensorial system to observe new properties of physical systems that are out of reach for our biological receptors. For instance, using infrared cameras to map infrared signals to a representation in the visible spectrum, humans can detect infrared radiation. But these tools don't allow to build an intuitive understanding of the phenomena without analogies to the phenomena perceived by the sensory system. For example, people that are blind from birth have never had any input to their visual cortex, so they have no visual intuition which limits their ability to understand some physical concepts. Similarly, the lack of receptors for other arbitrary physical properties

limits human understanding of the physical world and likely hinders scientific advance.

Modern science requires from agents with complex cognitive abilities. So far humans are the only known material structure able to perform it. It is true that some animals perform scientific behavior, like Crows or monkeys solving puzzles by trial and error. But those anecdotal examples are far from the formalized version of the scientific method employed by humans. However, humans are also the living f of the possibility of agents performing sophisticated science. There is no reason to think that there's anything special in humans that makes them the best possible form of a scientific agent. Rather it is reasonable to think that there is plenty of space for improvement, since the human brain was designed solely by millions of years of random mutations and natural selection.

Recent advances in artificial intelligence, yet far from achieving an artificial general intelligence, open the door to an automation of science. In the recent years, a vast amount of effort has been dedicated to the development of machine learning techniques to help scientists of the physical sciences to process data to create new better models [4]. However, these machine learning based techniques are just tools to help human scientists to interpret complex data to provide new predictions, and not efforts towards an automation of science. Nonetheless, the potential role that artificial intelligence might play in the process of scientific production has been getting growing awareness. In [10], the authors use a projective simulation model to design complex photonic experiments that produce high-dimensional entangled multiphoton states. According the authors, the system autonomously discovers experimental techniques which are a standard in modern quantum optical experiments. In [8] the authors explore the use of variational autoencoders to extract autonomously physically relevant parameters from physical data without prior assumptions about the physical system. In [11] they expand the work to present an architecture based on communitcating agents that deal with different aspects of a physical system and show that it can be combined with reinforcement learning techniques. More work on similar directions can be found in [citas articulo de Raban II].

However, scientific agents need to be designed carefully to minimize the inherited biases and limitations from their human creators. In this thesis we present a minimal axiomatic model for science and a new model architecture that mixes reinforcement learning with deep learning to create agents capable to design strategies

for experiments. Using as feedback only the quality of the predictions about properties of the physical system made exclusively from the data the agents collect from their sensorial available receptors.

Here I will write a couple of paragraphs explaining the structure of the thesis and pointing out to the repository, where to find the code, etc.

Chapter 2

Minimal model for science

2.1 Introduction

In this section, we introduce a minimal set of definitions and assumptions to define a scientific method. In the goal of achieving an independent automated science protocol, we must ensure consistency in the underlying principles to avoid unwanted biases and preconceptions inherited from humans.

2.1.1 First assumption: Dynamicality

We start with a universe U. Since the goal is to create agents able to decipher the properties of the universe U, we must make the minimal number of assumptions that allow us to set a scientific method. First, we need the universe to be dynamical. If the universe is static, nothing changes and no science is possible. This will give use the first assumption:

A1 (Dynamicality): There exists a dynamical universe U.

We can represent the dynamical nature of the universe by parametrizing it with a real parameter $\tau \in (-\infty, \infty)$, so that the state of the universe is a function of τ. Note that we are not assuming any property of the universe function $U(\tau) \rightarrow S$, where S is the set of possible states of the universe. For example, it may look that by setting the parameter τ unbounded we may be forcing the universe U to have unbounded dynamics. However, we could have $U(\tau)$ so that:

$$U(\tau \leqslant \tau_{\text{initial}}) = s_{\text{initial}}$$
$$U(\tau \geqslant \tau_{\text{terminal}}) = s_{\text{terminal}}$$

where $s_{\text{initial}}, s_{\text{terminal}} \in S$ are the initial and terminal states of the universe U. We aren't making any assumptions about the dynamical bounds on U. Also, we aren't making any assumptions on any other properties of $U(\tau)$ or even on what the elements of S are. We aren't also making any assumption on the continuity of the dynamics, since we could have:

$$U(\tau_i > \tau \geqslant \tau_{i+1}) = s_{\tau_i}, \quad \forall i \in \mathbb{N}$$

where $\{\tau_i\}_{i=0}^{\infty}$ is an arbitrary monotonically increasing sequence of real numbers. We aren't assuming as well anything about the deterministic nature of U, since $U(\tau)$ could be a probabilistic function. The only assumption made by the statement **A1** is that the universe evolves according some rule $U(\tau)$.

Note that the parameter τ doesn't necessarily represent the time as perceived by humans. It's just a parameter defined to convey the dynamical nature of the universe.

Example 2.1.1. In this example we are going to define a universe that satisfies **A1**. The universe U consists of n^2 elements $\{a_{jk}\}_{j,k=0}^{n-1}$. Each element can exist in one of two substates: $\{1, 0\}$. The set of states S is then $\{0, 1\}^{n^2}$. Now we need to equip the universe with a dynamical law $U(\tau)$. Assuming a discrete evolution, it could be, for example, the laws of a deterministic cellular automata. Or a probabilistic law so that each element changes its state with a certain probability in each dynamical step. It could be any rule that associates a state of S with each discrete value τ_i. However, we could also have continuous dynamics. For instance, we can set:

$$P(a_{jk} = 1, \tau) = e^{-\tau^2}, \quad \forall j, k \tag{2.1}$$

where $P(a_{jk} = 1, \tau)$ is the probability of the element a_{jk} being in the state 1 at the *time* [1] τ. With this dynamical law, the evolution of the universe is unbounded, although it has terminal and initial states: all elements in the substate 0. One may ask what it means that the universe is described by a probability function like (2.1). It means that at a given value of τ the state of the universe is choosen randomly according to (2.1).

From the assumption **A1** we can deduce some consequences.

Claim 2.1.2. *Any universe that satisfies **A1** has at least one element that can exist in more than one substate.*

[1] For communicative convenience we use the word time to design the value of τ. However, it doesn't mean that τ represents the time as perceived by humans.

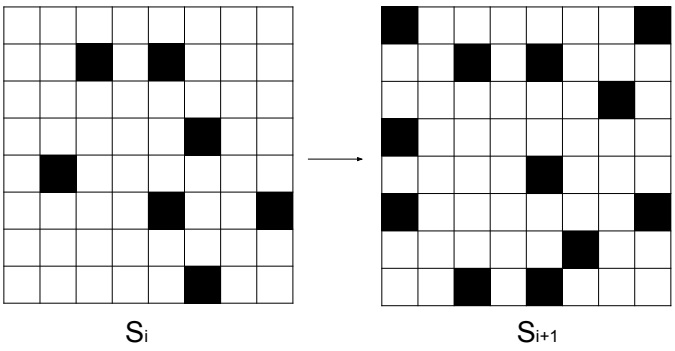


Figure 2.1: Graphical representation of the dynamical change of a universe with $n = 8$.

The f of this claim is obvious: an empty set cannot change. A set in which all elements can exists in only one substate also cannot change. Therefore, the simplest universe in which **A1** holds is a universe with only one element that can exists in two substates, this is, a bit that changes its value according to a dynamical law.

2.1.2 The scientific method

Now we need to define what is science in this minimal context. First, let's define what an agent is.

Definition 2.1.3. An agent A is defined as a subset of the universe U. $A(\tau)$ is the composition of A at the dynamical value τ. The dynamical evolution of A is determined by the dynamical evolution of U.

This is a very broad definition of an agent, since we define them just as subsets of the universe, so anything can be an agent. We can safely make this assumption since humans and computers are subsets of the universe. The definition implies that agents obey the same physical laws than the universe. Some philosophers would call this implication a materialistic assumption.

Another definition required for science is the definition of measurement or observation. This definition is particularly delicate in the context of quantum theory, so we have to be very careful in its definition.

Definition 2.1.4. An observation $\hat{O}_A$ is defined as the dynamical process in which the state of any subset of an agent A gets correlated to the state of another subset of U, the object O, that may or not be disjoint to A.

This definition is also very broad, so let's explain it. When we talk about observations in the context of humans, we usually understand them as information from an object acquired by our sensorial system, for example by observing with our visual system a bunch of photons emitted from a source of light. However, these terms mean nothing in our minimal model so we need to be more specific. When we see an object, the process, as far as we know, happens because a photon coming from the object hits some receptors in our retina producing a chain reaction that triggers an specific state in some part of the brain. In other words, an specific part of us (the agent A) gets correlated to the state of the object (a subset of O the universe) as a result of the dynamical evolution of the universe. The dynamical process that gets both states correlated is an observation.

Example 2.1.5. In this example we are going to see how an observation translate to our simple model of universe. With the same universe than in 2.1.1, we can define a new dynamical law that consists on a 1 doing a random walk in a bidimensional grid of zeros. Each time an element a_{jk} switches to 1, it gets correlated to the rest of the elements of the universe since all of them must be zero. In this case, the agent A is the subset of U containing only a_{jk} while the object O can be any subset of U. We say then that A has made an observation $\hat{O}_A$.

We need one more definition to define the scientific method. Science is about making predictions about the physical world, so we need to define what a prediction is in our minimal context.

Definition 2.1.6. A prediction is... *(I haven't come yet with a successful definition for a prediction. I'm trying to formulate it with different agents trying to communicate correlations about the "future" of some subsystem of U)*

2.1.3 Second assumption: Emergency

I want to have a formal definition of predictions and the scientific method before writing this subsection. But it's just a corollary of the anthropic principle: if we are able to do science, then the dynamical law of the universe must allow for scientific agents to be generated. For example, a simple cellular automaton that converges to a stable state wouldn't fulfill this assumption.

Chapter 3

Machine Learning theory

TO BE WRITTEN.

Chapter 4

Experimenter-Analyzer model

In this section, we are going to present our proposal for a basic model for a machine learning set-up that designs an experiment applying the scientific method. It is a model that mixes reinforcement learning and and deep learning to create agents able to design strategies for experiments, using as feedback only the quality of the predictions about properties of the physical system made exclusively from the data the agents collect.

One of the cornerstones of our model is the principle of modularity: in order to be applicable to a wide range of set-ups it needs to be constituted by simple individual elements that can be combined to build complex learning loops. The agent that will learn to design experiments and make predictions with them is composed by two different kinds of sub-agents that complement each other:

- **Experimenters**: this kind of sub-agents are reinforcement learning based agents. Its goal is to take decisions about influencing the dynamics of the physical system (e.g by modifying a parameter of a controlled experiment) or about what measurements to make (eg. by choosing what property of the physical system to measure). It could be that the choice of measurement modifies as well the dynamics of the physical system (eg. by choosing which slit to "look at" in the double slit experiment). To choose what actions to take they can consider previous observations and other kind of information.
- **Analyzers**: this kind of sub-agents are learning agents that take the information gathered by the Experimenters to make predictions about the environment. Then, based on the accuracy of those predictions compared to the real values [1] of the environment a reward is generated to train all the sub-agents.

[1] One may ask how these real values are obtained. Those values could be obtained by measure-

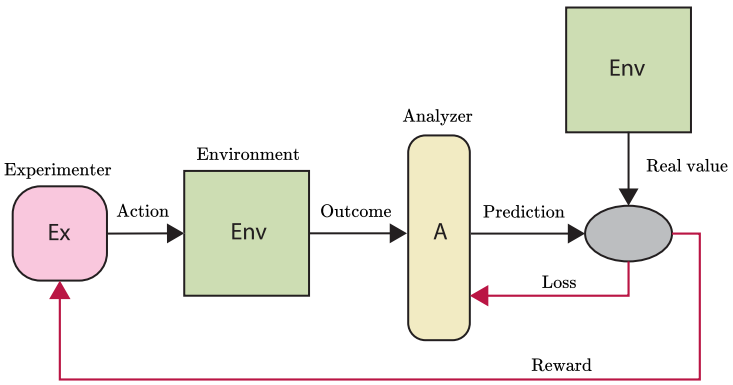


Figure 4.1: Diagram of the simplest combination of elements. The feedback loop consists on the following: 1. The Experimenter takes an action. 2. The environment gives back an outcome resulting from the action. 3. The action is taken by the analyzer and used to make a prediction. 4. The prediction about the environment and the real value of the environment are compared to generate the loss and the reward to train the Analyzer and the Experimenter.

To get a better understanding of the purpose of each part of the model let's take a look to the simplest structure that can be formed with the model (Fig. 4.1). To illustrate it let's imagine a simple physical set-up. Suppose we have a simple gravity pendulum of length L and mass M and the goal is to find the oscillation period on Earth's surface. We know the period is a function only of the length L and the value of the Earth's gravity (which we assume to be constant): $T \approx 2\pi\sqrt{\frac{L}{g}}$, so the value of the mass M is irrelevant for the purpose, but in principle this is unknown to the agent. In this set-up we give the Experimenter two possible actions to take (but only one try): either measuring the mass M (eg. by using a calibrated spring) or measuring the length L of the string (e.g by using a calibrated ruler). When the Experimenter takes an action over the Environment, it produces an outcome (either the mass M or the length L). This outcome is passed to the Analyzer which tries to make a guess of the period based on the value of the outcome of Experimenter's action. Then the real period of the pendulum is observed and compared to the value predicted by the Analyzer. Depending on the result of the comparison

ments made by other Experimenters that form part of the learning agent. However, for simplicity in the work presented here we assume that the real values needed to check the validity of the prediction are always accessible with unlimited accuracy to the agent. In the context of this modular framework we could assume that we have an Experimenter that its only possible action is to measure the real value of the target property.

a loss and a reward are generated to train the Experimenter and the Analyzer. In general: the closer the value of the prediction to the actual value the smaller the loss and the higher the reward. After the iteration is completed, a new pendulum with new values of M and L (ideally generated uniformly at random under the i.i.d. assumption) is generated and the process starts again.

The goal in the set-up depicted in Fig. 4.1 is to form a feedback loop between the Experimenter and the Analyzer from the, at first unknown, correlations between the outcomes and the values to be predicted. The better the Experimenter gets, the better the data available for the Analyzer to make better predictions that will generate better rewards for the Experimenter. Hopefully, this feedback loop will converge to an optimal experiment strategy and an optimal model for the predictions. At the beginning both sub-agents will start by giving random outputs since they are not trained. This is what we call the *exploration phase* and it is of fundamental importance for the feedback loop to start. It can be artificially enforced, for example with ϵ-greedy algorithms that we will discuss later in this work. If there exists any correlation between the choices of the Experimenter and the target value to be predicted, the Analyzer's training algorithm (usually Stochastic Gradient Descent) can exploit those correlations to start the descent to some local or global minimum. This working principle is somehow similar to the use of artificial neural networks for feature selection in classical machine learning theory.

The alert reader may have noted that in 4.1 the Analyzer has no apparent way of telling which action the Experimenter took, since it only receives the outcome of the experiment. Therefore the Analyzer doesn't know if what is receiving is the value of M or L. Although it may appear counter intuitive, the Analyzer doesn't care in this particular set-up. The optimal strategy is to treat everything as if it were L since knowing the value of M doesn't provide any information about T. However, it may make sense for the Analyzer to know when M is provided if the objective is to minimize the loss function (e.g. if the Analyzer knew that the value corresponds to M the optimal prediction would be the random guess that minimizes the loss). In practice, unless the distributions where M and L are generated from are the same, the Analyzer learns to differentiate them with high confidence just by value of the outcome. However, in other set-ups this may not be the case and the information about what actions were taken is useful for the Analyzer to make the predictions. In this case, we should also feed the actions as inputs to the Analyzer. As we will see, these Experiment-Analyzer loops can grow very quickly in complexity when several sub-agents are involved. This is why we introduce the

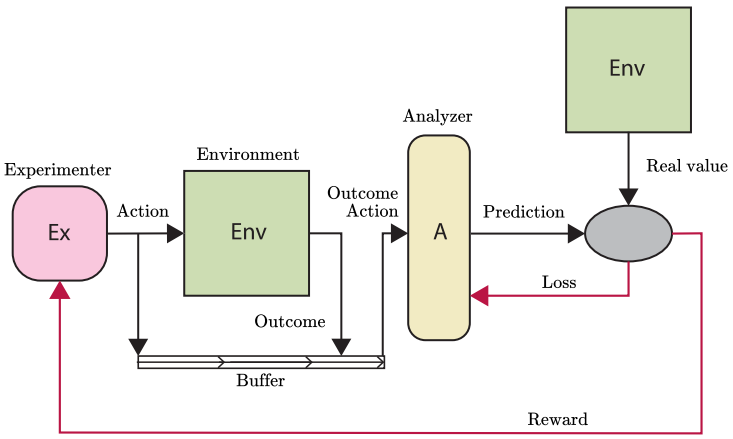


Figure 4.2: Diagram of a simple learning loop with buffer. In this case, the process is identical to the process depicted in Fig. 4.1 with the difference that the values of the action and the outcome are stored in the buffer, and then passed to the analyzer. In this case the information about which action was taken is available to the Analyzer.

concept of *buffer*.

In our model we can use a buffer to store everything that we might want to feed to the agents. Usually this will be the actions taken and the outcomes obtained in every observation of the environment, although we have the freedom to add whatever we might need. It is just a variable to store information. This variable is not strictly needed, since we could establish directly the connections between the different subagents and environment outcomes. However, when we have a few sub-agents with several outcomes it becomes very difficult to keep track of each connection and to represent them. In these cases, the concept of buffer becomes highly useful from an illustrative point of view. Usually, the buffer is emptied at the end of each episode or iteration of the learning loop. We could not do so, but in practice, keeping the data in the buffer doesn't provide any easy advantage since to use it we should solve many challenges, for example an increase on the number of features feeded to the agents each episode. We won't refer the buffer as *memory* in this work, since the word *memory* is reserved for an element of some versions of sub-agents that doesn't restart in each iteration.

4.1 General elements and definitions

In this section let's define more formally some of the elements and concepts of our model.

- **Simulated physical environment (SPE):** it represents the physical world that determines the outcomes of all the measurements realized by the agent. It is completely represented by a state $s \in S$, where S is the set of all possible states in which the SPE can be. For this particular model we assume that the evolution of the system is assumed to be given by a Markovian function $f : S \to S$ such that $f(s_\tau) = s_{\tau+1}$. This function maybe deterministic or not.

- **Agent:** the agent is formed by the composition of two kind of different sub-agents:

  - **Experimenter:** this part has the task of making decisions that will have an effect on the observations. This effect could be due to the influence of the decisions in the evolution of the system (for example, if the agent decides to shoot a bullet to a box with a certain velocity) or due to the fact that the decisions themselves could be what observations to make (for example, choosing to measure the position of a box within a spatial range). This agent will be implemented using reinforcement learning techniques. Mathematically it can be represented by a trainable function $E : \mathcal{X} \to \mathcal{A}$ where $\mathcal{A}$ represents the space of possible actions and $\mathcal{X}$ is an arbitrary space that can represent any accessible information that might be useful to make a choice of action. In the context of reinforcement learning, $\mathcal{X}$ is the set of states of the sub-agent's environment[2].

  - **Analyzer:** the goal of this part of the agent is to process the data collected in the observations after the action of the Experimenter to predict a physical property of the SPE. This property could be a physical parameter of the system or a prediction of the dynamics of the environment. It will usally consist of a regular regression neural network or an autoencoder, depending on the specific set-up. But we could use any trainable function like SVMs or any kind of regression. Mathemat-

[2] Not to be confused with the SPE.

ically it can be represented by a trainable function $A : \mathcal{M} \to \mathcal{P}$, where $\mathcal{M}$ is the space of measurements and $\mathcal{P}$ is the space of predictions.

- **Orchestration:** when coding we will call Orchestration everything that connects the different parts to complete a feedback loop. For example, one of the tasks of the Orchestration is to transform the state of the SPE into the measurements received by the Analyzer. The Orchestration is needed when we simulate fictitious physical situations in a computer to test our models. It represents somehow something analogous to the sensors and wires that connect the external environment to the processor of an autonomous robot.

Example 4.1.1. Let's complete the example of the pendulum to fully illustrate the architecture. First, we define the SPE. Let's assume that the mass of the pendulum and the length of the string are sampled uniformly at random from the intervals $0.1 \text{ kg} < M < 1 \text{ kg}$ and $0.1 \text{ m} < L < 1 \text{ m}$. The space of states of the SPE is then:

$$S \equiv \{(m, l) : m \in [0.1, 1], l \in [0.1, 1]\} \tag{4.1}$$

Now, let's define an Experimenter. In this case, the Experimenter's environment space $\mathcal{X}$ is the empty set $\varnothing$, since there is no input. This means that the agent takes the action based solely on the rewards obtained. The action space $\mathcal{A}$ is just $\{0, 1\}$, with 0 representing the action of measuring the mass and 1 the action of measuring the length.

We can therefore set a very basic decision rule for our Experimenter agent:

- Let $\mathbf{Q} = (q_0, q_1)$ be the value table, where q_0 and q_1 are the values associated with the actions 0 and 1 respectively. Q can be also understood as a trainable function $Q : \mathcal{X} \times \mathcal{A} \to \mathbb{R}$. Initially $Q(a) = 0 \ \forall a \in \mathcal{A}$.

- Every episode, the agent takes an action a and receives a reward r after taking the action. The update rule for $\mathbf{Q}$ is the following:

$$q_a \leftarrow q_a + r \tag{4.2}$$

  This is, the value q_a is just the cumulative reward obtained by the action a.

- The agent's policy $E : \varnothing \to \mathcal{A}$ or decision rule is:

$$a = \arg\max_{x \in \mathcal{A}} Q(x) \tag{4.3}$$

  This is, the Experimenter takes the action a with the highest q_a, and E is trained by updating $\mathbf{Q}$ each episode.

Note that the choice of (4.2) is just to illustrate that we can build Reinforcement Learning agents with very simple rules. We could have chosen instead of the cumulative reward the average reward obtained with the action, but the working principle would be identical.

However, our policy is still flawed, since the first action that gets a reward would always be elected afterward independently of its optimality. To solve this we can force the agent to initially explore different options ignoring the decision rule, and slowly, when the values q_a are more reliable, let the agent choose according to (4.3). The easiest way to achieve that is with an ϵ-greedy decision algorithm: we set an exploration rate ϵ that decreases in each episode until it reaches a minimum value $\epsilon_{\text{min}} \geqslant 0$. The Experimenter is set to take the (4.3) policy with probability of $P_{\text{greedy}} = 1 - \epsilon$ and a random action with a probability of $P_{\text{random}} = \epsilon$. We have the freedom to choose how to decrease the value of ϵ, and it may have a crucial impact on the training. A very popular rule is to decrease the value constantly by subtracting $\delta_\epsilon = 1/N$, where N is the number iterations of the training. So in each episode:

$$\text{if } \epsilon > \epsilon_{\text{min}} \qquad \epsilon \leftarrow \epsilon - \delta_\epsilon \tag{4.4}$$

$$\text{else} \qquad \epsilon \leftarrow \epsilon_{\text{min}} \tag{4.5}$$

For the Analyzer, we set a trainable real function $A : S \rightarrow \mathbb{R}$. We can use any trainable function, but to keep it simple let's use a regular feed-forward neural network with one hidden layer of two neurons, trained with the Stochastic Gradient Descent (SGD) algorithm and a the Mean Squared Error (MSE) loss.

We need now to define how to calculate the reward. In our case we want the reward function to be high when the Analyzer predicts a period T_{pred} close to the real period of the pendulum and low when the period prediction is far. So, ideally we would like a function that:

$$r(T_{\text{pred}} \approx T) \approx 1 \tag{4.6}$$

$$r(T_{\text{pred}} >> T \text{ or } T_{\text{pred}} << T) \approx 0 \tag{4.7}$$

One natural way to achieve this is using a Gaussian distribution over the relative error $\Delta = (T - T_{\text{pred}})/T$. This is:

$$r(\Delta) = \exp\left(-\frac{1}{2}\left(\frac{\Delta}{\sigma}\right)^2\right) \tag{4.8}$$

and σ allows us to modify the precision we want in order to achieve a reward.

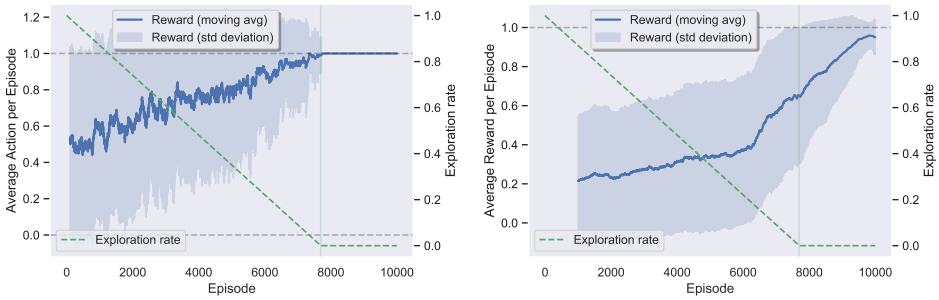
Now we have every element defined. Let's outline the full algorithm in pseudocode:

Algorithm 1 Simple learning loop

procedure PENDULUM
count = 0
while count $< N$:
    $M, L \leftarrow$ random sample M, L
    $T \leftarrow T(L)$
    pendulum $\leftarrow [M, L, T]$
    action $\leftarrow \arg\max Q$
    measurement $\leftarrow$ pendulum[action]
    prediction $\leftarrow$ analyzer(measurement)
    Apply SGD to Analyzer with data point $(\text{measurement}, T)$
    reward $\leftarrow$ reward$(\text{prediction}, T)$
    $Q[\text{action}] \leftarrow Q[\text{action}] + \text{reward}$
    count $\leftarrow$ count $+ 1$

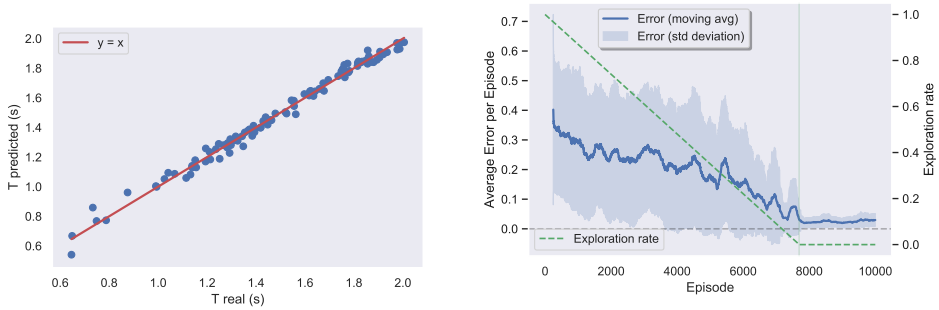
Let's see how this simple algorithm performs in the task. Ideally, the Experimenter would find the optimal policy which consists in choosing always to measure the length and the Analyzer would learn to estimate accurately T from the data obtained by the Experimenter. In our experiments, with this simple structure of only two neurons and the very naive reinforcement learning policy the agent consistently finds the optimal action (to measure L). It also accurately predicts the value of T in less than 10,000 episodes. With less episodes it is less consistent in finding the optimal policy.

In the figures Fig. 4.3 and Fig. 4.4 we can observe the evolution of different parameters during the training. All the parameters show successful learning of both, the optimal policy and the prediction of the period. More complex neural network structures and longer trainings can achieve much lower errors. However, this is not a surprise since once the optimal policy is obtained the process just consists on fitting a continuous single variable function. A task that can be solved optimally by a single layered sigmoidal neural network [5]. This pendulum example, although trivial, is useful to appreciate the working principle behind the Experimenter-Analyzer architecture and how the feedback loop is formed. In the next section we are going to explore less trivial examples with more complex learning loops.



(a) Moving average of the actions (b) Moving average of the reward

Figure 4.3: (a) The moving average of the actions taken in each episode. We can see how it starts taking both actions evenly with an average of 0.5. This is expected since at the beginning $\epsilon \approx 1$. As ϵ decreases the Experimenter starts to take more greedy actions and gets biased towards the action 1 (measure L). This bias appears as a result of the existing correlation between L and T, but not between M and T. This correlation is exploited by the SGD algorithm for the neural network of the Analyzer. (b) The moving average of the reward obtained in each episode. At the beginning the reward obtained is low and similar to those obtained with random guesses. However, it increases slowly, apparently because the Analyzer starts to exploit slightly the correlation between L and T. This slight improvement over the prediction for the outcomes of Action 1, creates the bias that starts the feedback loop. Values: $\sigma = 0.05$, $N = 10000$, $\text{lr}_{\text{Analyzer}} = 0.01$, Optimizer = Adam



(a) Real T vs Predicted T (b) Moving average of the error

Figure 4.4: (a) A sample of the predictions made by trained agent. We can see how it fits the $y = x$ line, showing that it learned the relation between L an T. (b) In this figure we can see how the error decreases to almost zero with very low deviation.Values: $\sigma = 0.05$, $N = 10000$, $\text{lr}_{\text{Analyzer}} = 0.01$, Optimizer = Adam

Chapter 5

E-A architecture in different scenarios

5.1 Scenario 1: Modified multi-armed bandit

In the first section of this chapter we are going to study a modified version of the classical Multi-armed bandit problem, a classical problem of Reinforcement Learning and Probablity Theory. We will show that we can map any experiment consisting of a non-interactive discrete choice measurements to our modified multi-armed bandit.

5.1.1 General multi-armed bandit problem

Suppose that we have an agent that has access to a k-armed bandit. Each time the agent pulls one of the k levers the bandit produces a reward. The objective of the agent is to maximize the obtained reward in a determined number of trials or episodes N, but the agent doesn't know how the bandit produces the rewards. Its only way of getting information about the reward system is by trial and error by pulling the levers and obtaining rewards.

Mathematically we can model our agent as an Experimenter $E : \mathcal{X} \to \mathcal{A}$, where the action space is $\mathcal{A} = \{0, 1, ..., k\}$ and the state space $\mathcal{X}$ is again the empty set $\varnothing$. The bandit can be modelled as a probabilistic function $R : A \times ... \to \mathbb{R}$, with "..." meaning that in principle the generated reward can depend on anything, for example, the previous actions, the previous rewards, the number of trials, the number of times a lever has been pulled, etc. This is an extremely general problem, so often authors make assumptions on R. For example, R being

Markovian if depends only on the last rewards and/or actions. Or stationary if R can be modeled as a set of immutable distributions $R = \{R_1, ..., R_k\}$, each distribution being associated with the rewards delivered by each of the arms of the bandit.

We define the value $Q^*(a) = q_a^*$ of an action $a \in \mathcal{A}$ as the true expected or mean reward associated to the action. We denote by a_n the action taken in the n^{th} episode, and r_n the reward obtained. This is:

$$Q^*(a) = \mathbb{E}[r_n | a_n = a] \tag{5.1}$$

Note that, although we don't write it explicitly, $Q^*(a)$ can also depend on any of the subsets of the domain of R. The optimal strategy for the k-armed bandit problem is to always choose $a* = \arg\max Q^*(x)$.

Most reinforcement learning approaches to this problem look for an estimate of $Q^*(a)$, $Q(a)$, and base their choice on $a = \arg\max Q(x)$. In general, the best algorithm depends deeply on the characteristics of R, e.g., an algorithm that works well for stationary bandits can perform very poorly on non-stationary bandits. The interested reader can read a gentle introduction to the multi armed bandit problem in the Chapter 2 of [14]. We are not going to discuss here many of the approaches to solve the mult-armed bandit problem. However, let us outline a very simple algorithm that works particularly well for non-stationary bandits.

5.1.2 Simple Reinforcement Learning algorithm for nonstationary multi-armed bandit

Let us outline a simple algorithm that we will use later in this section. This algorithm can be understood as a particular case of the Q-Learning algorithm, where the state space of the experimenter $\mathcal{X}$ is the empty set $\varnothing$ and the discount factor γ is set to zero. The update rule for the estimate $Q(a)$ each time the action a is taken is:

$$Q(a) \leftarrow Q(a) + \alpha\,(r - Q(a)) \tag{5.2}$$

where $\alpha \in (0, 1]$ is the called the learning rate, Q_a is the estimate value for the action a and r is the reward obtained after taking the action a.

If we name by Q_n the estimate of $Q^*(a)$ for an arbitrary action a at the $(n)^{\text{th}}$ time the action a was taken, then due to (5.2) we have that:

$$
\begin{aligned}
Q_{n+1} &= Q_n + \alpha\,(r_n - Q_n) && (5.3)\\
&= \alpha r_n + (1-\alpha)Q_n && (5.4)\\
&= \alpha r_n + (1-\alpha)\left[\alpha r_{n-1} + (1-\alpha)Q_{n-1}\right] && (5.5)\\
&= \alpha r_n + (1-\alpha)\alpha r_{n-1} + (1-\alpha)^2 Q_{n-1} && (5.6)\\
&= (1-\alpha)^n Q_1 + \sum_{i=1}^{n} \alpha(1-\alpha)^{n-i} r_i && (5.7)
\end{aligned}
$$

The last equation, (5.7), is just a weighted average of the rewards obtained, where the weights give exponentially less importance to rewards coming from distant actions in the past. Sometimes is known as *exponential recency-weighted average*.

Claim 5.1.1. *If α is constant on n, the exponential recency-weighted average is also a convex sum of the rewards obtained.*

f: Since $\alpha \in (0, 1]$ all the coefficients are no greater than 1. We just need to prove that $\forall n$ they sum to one. If we write the sum S_n of the coefficients at the time n:

$$S_n = (1-\alpha)^n + \sum_{i=1}^{n} \alpha(1-\alpha)^{n-i} \tag{5.8}$$

We also have that:

$$
\begin{aligned}
(1-\alpha)^n &= (1-\alpha)(1-\alpha)^{n-1} && (5.9)\\
&= (1-\alpha)^{n-1} - \alpha(1-\alpha)^{n-1} && (5.10)
\end{aligned}
$$

Inserting (5.10) in (5.8) we get:

$$
\begin{aligned}
S_n &= (1-\alpha)^{n-1} - \alpha(1-\alpha)^{n-1} + \sum_{i=1}^{n} \alpha(1-\alpha)^{n-i} && (5.11)\\
&= (1-\alpha)^{n-1} + \alpha \sum_{i=1}^{n-1} \alpha(1-\alpha)^{n-1-i} && (5.12)
\end{aligned}
$$

If we call $l = n - 1$ we obtain exactly (5.8) but with l instead of n. We can repeat this process until the new index happens to be 1. Then we have:

$$S_n = (1-\alpha) + \alpha = 1 \quad \square \tag{5.13}$$

Lets outline with pseudo-code how this agent would work:

Algorithm 2

1: **procedure** NON-STATIONARY MULTIARMED-BANDIT AGENT
2: count = 0
3: **while** count $< N$:
4: action $\leftarrow \arg\max Q$
5: reward $\leftarrow$ bandit(action)
6: Q[action] $\leftarrow$ Q[action] + α (reward - Q[action])
7: count $\leftarrow$ count + 1

If we pay attention to the pseudo-code we see that for taking the first action we must have an initial estimate Q_1 for each action. These initial estimates aren't irrelevant. They play an important role in the convergence of the algorithm. For example, if we set $Q_1 = 0 \ \ \forall a \in \mathcal{A}$, the $\arg\max Q_1$ will output a random action. Therefore, the training can be biased towards that action depending on the initial reward. Sometimes a good strategy is to set high values of Q_1 for all actions. This will make the agent overoptimistic in the estimate, forcing it to explore all options until getting a more realistic estimate of the reward.

It can be shown that choosing the following learning rate give us an exponential recency-weighted average without initial bias:

$$\alpha_n = \beta / o_n \tag{5.14}$$

where β is a constant parameter and o_n is a constant step size updating parameter so that:

$$o \leftarrow o + \beta(1 - o) \tag{5.15}$$

with an initial value of $o_1 = 0$ for all actions.

5.2 Scenario 2: Spring-Shooting experiment

5.3 Scenario 3: Shooting with two position sensors

So far we have used always the same architecture with a Q-table that chooses a predefined experimenter to optimize the reward obtained by the Analyzers prediction. However, it may be the case in which we have experiments with several measurements or actions that depends on the outcomes of the previous observations.

Appendix A

Appendix ?

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