ETH zürich Quantum Information Theory Group

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Master's Thesis

Extracting physical parameters from an environment using AI-agents

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Abstract

An important challenge for the automation of science is to minimize the prior human knowledge built into the machine learning systems. A step in this direction was done in Phys. Rev. Lett. 124, 010508 (2020) where the relevant physical parameters were extracted from experimental data without using prior knowledge about the specific physical system. Here, we go one step further in minimizing prior knowledge: We do not consider the experimental data as given but train AI agents that learn to perform the experiments that provide the necessary data to extract the relevant parameters. To do so, we combine in a modular architecture techniques from reinforcement learning and deep learning. We demonstrate the working of our architecture with some toy examples. Reading out the parameters for the given examples is left for future work.

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

Contents

Preface

Many of the limitations of humans at doing science come from their biological condition. 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 [1, 2], with a yearly growth rate of $\sim 9\%$ in the last decade. Scholars read on average almost 240 articles per year [3]. Some authors [4] 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 [5, 6] 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 is not such a crisis [8]. Nonetheless, it is 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. 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 do not allow to build an intuitive understanding of the phenomena without analogies to the phenomena perceived by the sensory system. For example, the 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 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 proof 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.

Scientific agents need to be designed carefully to minimize the inherited biases and limitations from their human creators. In this thesis, we present a new model

architecture that mixes reinforcement learning with deep learning to create agents that are able to design strategies for experiments. Using as feedback only the quality of the predictions about properties of the physical system. The predictions are made exclusively from the data the agents collect from their sensorial receptors.

Chapter 1

Introduction

Towards the automation of science

Arguably, a crucial step towards the goal of creating an artificial scientific agent is to build agents that can generate theoretical models of the environment in which they exist. We want to minimize the influence of prior human assumptions about the physical world in such artificial agents as much as possible.

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 to process data to create new better models [9]. 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 to the authors, the system autonomously discovers experimental techniques which are a well-known building blocks of modern quantum optical experiments. More work on similar directions can be found in [11, 12, 13, 14, 15, 16].

In the work presented in [17], the authors present a model to discover autonomously the relevant parameters of a physical system from some given experimental data. To do so, they use a neural network architecture that constructs a minimal representation of the system. This is done with variational auto-encoders used to make predictions about the system from which the experimental data was obtained. The auto-encoder structure forces the encoder to reduce the experimen-

tal data to the minimal representation needed for the decoder to correctly emit the answer of all the questions that may be asked. This latent representation stores the meaningful physical parameters that contains the relevant information to make assertions about the physical system. However, although the physical parameters are extracted autonomously from the experimental data, the experimental data fed to the auto-encoder is gathered or generated by humans. A critical stride to minimize the influence of prior human assumptions is to construct agents that can gather the experimental data autonomously without human intervention. The only way to autonomously obtain experimental data is through autonomous experimentation. An artificial scientific agent, in order to be independent from human science, needs to be capable of independently designing and running experiments in the physical world.

In this work, we present a modular machine learning architecture inspired by the scientific method. The agent learns to find the optimal use of some given actions and sensorial receptors to gather data from a simulated physical environment. The model optimizes the experimental strategy to minimize the error on the predictions of some specific properties of the physical system. To achieve this, we mix reinforcement learning agents to decide what experiment to make, trained in parallel with a machine learning set-up that uses the collected data to make the predictions. Those predictions are then are compared to the empirical value of the physical property to test its validity and generate the feedback needed for the training. This model can be combined seamlessly with variational auto-encoders to build agents that can autonomously gather data and learn the meaningful physical parameters of a system with almost no prior human assumptions.

A simple scientific process to train agents

An autonomous scientific agent is by definition an agent that applies the scientific method to generate a theoretical model of its environment. The goal of a scientific agent is to obtain an interpretable model of the environment that that allows to make successful predictions. It is then reasonable to inspire the structure of the learning process of such agents in the well established scientific method of knowledge acquisition. Let us outline informally this process and then explain how it should be followed to train an artificial scientific agent.

To define the simple model used in this work for the scientific process we need two elements: a physical environment and an agent capable of following the

process. The physical environment is a set of elements that change. The agent is a subset of the environment that can obtain information about the environment through observation, formulate questions about the environment, and emit predictions about the environment. The process consists informally of the following steps:

1. **Formulation of a question:** The scientific agent formulates a question about the environment.
2. **Observation:** the agent collects some information about the environment through observation.
3. **Hypothesis:** The agent creates a theoretical model or hypothesis of the environment based on the observations.
4. **Prediction:** The agent emits a testable prediction based on the hypothesis, this is, an experimental outcome to check if the hypothesis is correct.
5. **Test:** An observation to check the validity of the prediction.
6. **Analysis and iteration:** The agent uses the result of the test as feedback to validate or falsify the hypothesis. If the validation is strongly supported by the test the question is considered answered. If not, the agent comes back to 2 and uses the feedback to make new observations and modify the hypothesis.

We base our machine learning model on those steps as follows:

1. **Formulation of a question:** We set a question for the agent. This is the main source of human prior knowledge.
2. **Observation:** done by reinforcement learning agents with access to sensorial receptors and actions to interact with the environment.
3. **Hypothesis:** We set a trainable function that takes the data collected in the observation. For example, in the case of using an artificial neural network, the weights would represent the hypothesis. We can set variational autoencoders to obtain an interpretable minimal representation.
4. **Prediction:** The output of the trainable function with the observation as input.
5. **Test:** The prediction is compared with the experimental outcome that answers the set question.

6. **Analysis and iteration:** from the comparison between the prediction and the experimental outcome a signal is generated to modify the agent. For the reinforcement learning part this signal would be a reward that is high when the prediction is accurate and low when is not. For the predictor function a loss value to modify the parameters defining the function. For example, the mean squared error to apply gradient descent in a neural network.

Structure of the thesis

The thesis consists of five chapters including this introduction. In Chapter 2 we present a detailed description of our machine learning architecture, the Experimenter-Analyzer model. There we explain the basic structure of the model and how it can be implemented to solve a very simple example. In Chapter 3 we study a type of experiments that can be formulated as a multi-armed bandit problem. This is an experiment whose actions can be fixed at the start of the experiment. We show with several examples how to use the most simple structure of our architecture to approach efficiently this kind of set-ups. In Chapter 4 we discuss another type of experiments that cannot be expressed as a multi-armed bandit problem. These are experiments that require from active intervention of an agent during the experiment. For example, the weighting process of a mass using calibrated weights and a beam scale. We show how to exploit the modularity of our architecture to use several reinforcement learning agents to approach the task. Then we demonstrate its validity by successfully finding the optimal strategy in a detailed example. This is achieved through the emerging cooperation of several reinforcement learning agents to maximize a reward. In Chapter 5 we draw the conclusions of this project and outline some future steps to expand the current work.

Chapter 2

Experimenter-Analyzer architecture

2.1 Introduction to the architecture

In this section, we are going to present our proposal for a basic model for a machine learning set-up that designs an experiment that captures the necessary information to find the relevant physical parameters of a system. It is a model that mixes reinforcement learning and deep learning to create agents that can design strategies for experiments. Using as feedback only the quality of the predictions about properties of the system made exclusively from the data the agents have collected.

One of the cornerstones of our architecture is the principle of modularity: in order to be applicable to a wide range of set-ups our machine learning model needs to be constituted by simple individual elements that can be combined to build complex learning loops. The agent is composed of two different kinds of sub-agents that complement each other:

- **Experimenters**: this kind of sub-agents are reinforcement learning based agents. Their 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 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. For example, some auxiliary parameters or what actions were taken previously.

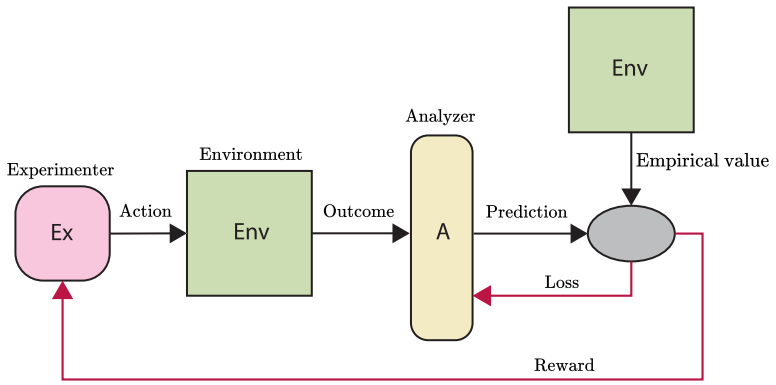


Figure 2.1: Diagram of the simplest combination of elements. The feedback loop consists on the following: 1. The experimenter takes an action. 2. The environment gives back an outcome resulting from the action. 3. The action is taken by the analyzer and used to make a prediction. 4. The prediction about the environment and the empirical value of the environment are compared to generate the loss and the reward to train the analyzer and the experimenter.

- **Analyzers**: this kind of sub-agents are learning agents that take the information gathered to make predictions about the environment. Then, based on the accuracy of those predictions compared to the empirical values [1] of the environment a reward is generated to train all the sub-agents.

To get a better understanding of the purpose of each part of the architecture let us take a look to the simplest structure that can be formed with it (Fig. 2.1). To illustrate it let us imagine a simple physical set-up. Suppose we are given 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

[1] One may ask how these empirical values are obtained. Those values could be obtained by measurements made by other experimenters that form part of the learning agent. However, for simplicity in the work presented here we assume that the empirical 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 whose only possible action is to measure the empirical value of the target property.

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 empirical period of the pendulum is observed and compared to the value predicted by the analyzer. Depending on the result of the comparison 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 empirical 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) are generated and the process starts again.

The goal in the set-up depicted in Fig. 2.1 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 experimental strategy and nearly perfect 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 some version of the gradient descent) can exploit those correlations to start the descent to some local or global minimum.

The alert reader may have noted that in 2.1 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 does not know whether the value that it is receiving is the value of M or L. Although it may appear counter intuitive, the optimal analyzer does not care in this particular set-up. The optimal strategy is to treat everything as if it were L since knowing the value of M does not 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 of M and L 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 Experimenter-Analyzer loops can grow very quickly in complexity when several sub-agents are involved. This is why we introduce the 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 placeholder to store information. This placeholder 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 does not provide any easy advantage since to use it we should solve many challenges, for example an increase in the number of features fed 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 does not restart in each iteration.

2.2 General elements and definitions

In this section let us 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 given by a 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 in-

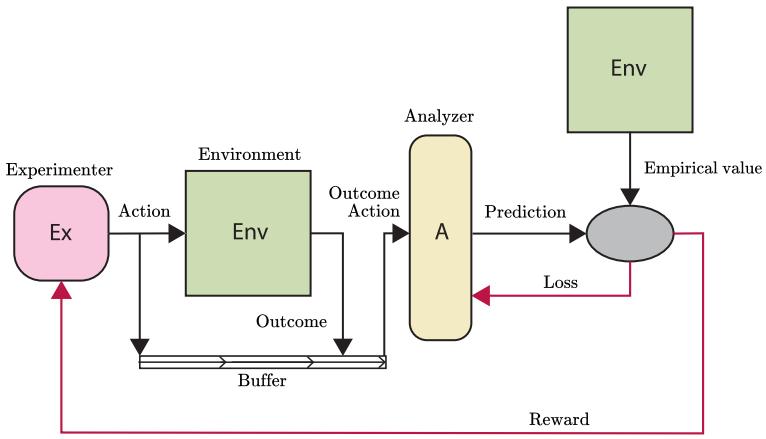


Figure 2.2: Diagram of a simple learning loop with buffer. In this case, the process is identical to the process depicted in Fig. 2.1 with the difference that the values of the action and the outcome are stored in the buffer, and then are passed to the analyzer. In this case the information about which action was taken is available to the analyzer.

fluence 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 $\mathscr{E} : \mathcal{X} \to \mathcal{A}$ 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 usually 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. Mathemati-

[2]Not to be confused with the SPE.

cally it can be represented by a trainable function $\mathscr{A} : \mathcal{M} \to \mathcal{P}$, where $\mathcal{M}$ is the space of measurements and $\mathcal{P}$ is the space of predictions. In the context of minimal representation learning [17], we can use an autoencoder structure to split $\mathscr{A}$ in two parts: $\mathscr{A} : \mathcal{M} \to \mathcal{R} \to \mathcal{P}$, where $\mathcal{R}$ is the representation space.

- **Reward function:** this is a function that compares the empirical value of the target property with the predicted value output by the analyzer. It is used to generate the reward to train the experimenters and it is a function $r : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$
- **Loss function:** this is a function that compares the empirical value of the target property with the predicted value output by the analyzer. It is used to generate the loss to train the analyzer and it is a function $L : \mathcal{P} \times \mathcal{P} \to \mathbb{R}$

Example 2.2.1. Let us complete the example of the pendulum to fully illustrate the architecture. First, we define the SPE. Let us 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:

$$S \equiv \{(m, l) : m \in [0.1, 1], l \in [0.1, 1]\} \tag{2.1}$$

Now, let us 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:

- We define the value function $Q : \mathcal{A} \times \mathcal{X} \to \mathbb{R}$ that associates with each action $a \in \mathcal{A}$ a value $Q(x, a) = q_{x,a}$. If $\mathcal{A}$ and $\mathcal{X}$ are discrete spaces we can associate a value table to Q with elements $Q(x, a)$. In the case where $\mathcal{X}$ is $\varnothing$, the value table is just a vector $\mathbf{Q} = (q_0, q_1, ..., q_k)$, where k is the number of elements in $\mathcal{A}$.
- In 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:

$$q_a \leftarrow q_a + r \tag{2.2}$$

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

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

$$a = \arg\max_{\lambda \epsilon \mathcal{A}} Q(\lambda) \tag{2.3}$$

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

Note that the choice of (2.2) 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 selected afterwards 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 (2.3). The easiest way to achieve this 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 policy given in (2.3) with probability $P_{\text{greedy}} = 1 - \epsilon$ and a random action with a probability $P_{\text{random}} = \epsilon$. 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:

$$\text{if } \epsilon > \epsilon_{\text{min}} \qquad \epsilon \leftarrow \epsilon - \delta_\epsilon \tag{2.4}$$

$$\text{else} \qquad \epsilon \leftarrow \epsilon_{\text{min}} \tag{2.5}$$

For the analyzer, we set a trainable real function $\mathscr{A} : S \rightarrow \mathbb{R}$. 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 gradient descent algorithm and 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:

$$r(T_{\text{pred}} \approx T) \approx 1 \tag{2.6}$$

$$r(T_{\text{pred}} >> T \text{ or } T_{\text{pred}} << T) \approx 0 \tag{2.7}$$

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

$$r(\Delta) = \exp\left(-\frac{1}{2}\left(\frac{\Delta}{\sigma}\right)^2\right) \tag{2.8}$$

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

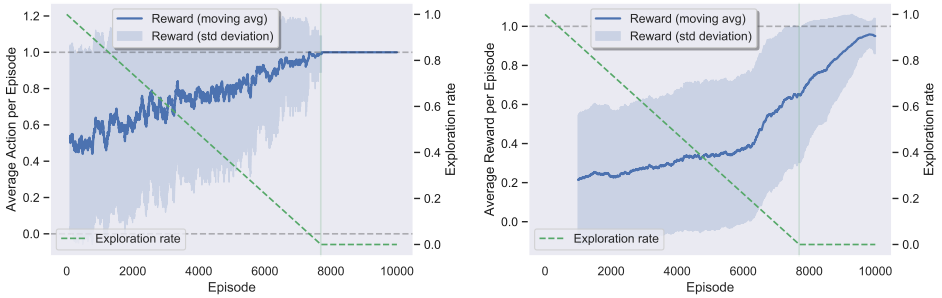
Now we have every element defined. Let us outline the full algorithm in pseudocode:

Algorithm 1 Simple learning loop

```
procedure PENDULUM
count = 0
while count < N_Episodes :
    M, L ← random sample M, L
    T ← T(L)
    pendulum ← [M, L, T]
    action ← arg max Q
    measurement ← pendulum[action]
    prediction ← analyzer(measurement)
    Apply GD to analyzer with data point (measurement, T)
    reward ← reward(prediction, T)
    Q[action] ← Q[action] + reward
    count ← count + 1
```

Let us 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 Fig. 2.3 and Fig. 2.4 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

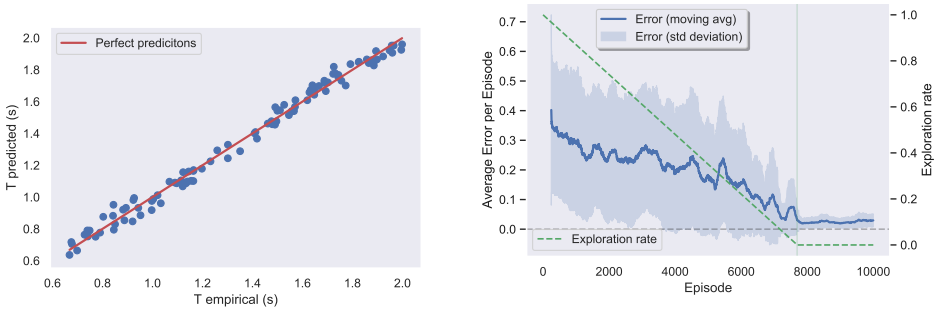


(a) Moving average of the actions

(b) Moving average of the reward

Figure 2.3: (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. Chosen parameters for the training: $\sigma = 0.05$, $N = 10000$, $\text{lr}_{\text{analyzer}} = 0.01$

fitting a continuous single variable function. A task that can be solved optimally by a single layered sigmoidal neural network consisting of enough neurons [18]. This pendulum example, although trivial, is useful to demonstrate 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) Empirical T vs Predicted T

(b) Moving average of the error

Figure 2.4: (a) A sample of the predictions made by the trained agent. We can see how the predictions are very accurate, 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. Chosen parameters for the training: $\sigma = 0.05$, $N = 10000$, $\text{lr}_{\text{analyzer}} = 0.01$

Chapter 3

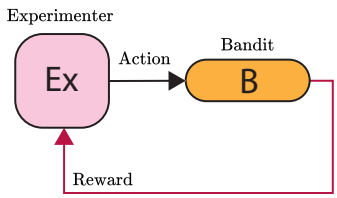
Experimenter-Analyzer for multi-armed bandits

In this chapter, we are going to apply the Experimenter-Analyzer architecture to a modified version of the classical multi-armed bandit problem, a classical problem of reinforcement learning and probability theory. Every experiment whose actions can be decided at the start of the experiment without further intervention, can be expressed mathematically as a multi-armed bandit. Let us start by introducing the general multi-armed bandit problem.

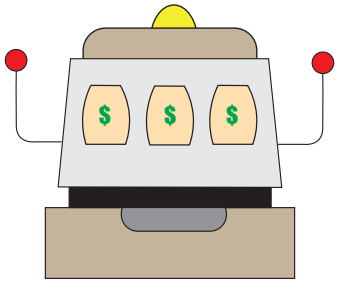
3.1 General multi-armed bandit problem

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. The agent does not 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 $\mathscr{E} : \mathcal{X} \to \mathcal{A}$, 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: 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. Often authors make assumptions on R. For example, R being Markovian if it depends only on



(a) Simple diagram portraying the multi-armed bandit problem.



(b) Draw of a two armed bandit.

Figure 3.1: Multi-armed bandit problem.

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

We define the value $Q_t^*(a)$ of an action $a \in \mathcal{A}$ in the t^{th} episode as the true expected or mean reward associated to the action for that episode. We denote by a_t the action taken and r_t the reward obtained. This is:

$$Q_t^*(a) = \mathbb{E}[r_t | a_t = a] \tag{3.1}$$

In general, how Q_t^* changes between episodes can depend on any of the subsets of the domain of R. The optimal strategy for the k-armed bandit problem is to always choose $a_t^* = \arg\max_{\lambda \in \mathcal{A}} Q_t^*(\lambda)$.

Most reinforcement learning approaches to this problem look for an estimate of $Q_t^*(a)$, $Q_t(a)$, and base their choice on $a_t = \arg\max_{\lambda \in \mathcal{A}} Q_t(\lambda)$. 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 [19]. We are not going to discuss here many of the approaches to solve the multi-armed bandit problem. However, let us outline a very simple algorithm that works particularly well for non-stationary bandits.

3.1.1 Simple reinforcement learning algorithm for non-stationary multi-armed bandits

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 [19],

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 [1]:

$$Q(a) \leftarrow Q(a) + \alpha\,(r - Q(a)) \tag{3.2}$$

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 $q_{a,n}$ the estimate of $Q^*(a)$ for an arbitrary action a at the n^{th} time the action a was taken, then due to (3.2) we have that:

$$\begin{aligned}
q_{a,n+1} &= q_{a,n} + \alpha\,(r_n - q_{a,n}) && (3.3)\\
&= \alpha r_n + (1-\alpha) q_{a,n} && (3.4)\\
&= \alpha r_n + (1-\alpha)\left[\alpha r_{n-1} + (1-\alpha) q_{a,n-1}\right] && (3.5)\\
&= \alpha r_n + (1-\alpha)\alpha r_{n-1} + (1-\alpha)^2 q_{a,n-1} && (3.6)\\
&= (1-\alpha)^n q_{a,1} + \sum_{i=1}^{n} \alpha(1-\alpha)^{n-i} r_i && (3.7)
\end{aligned}$$

The last equation, (3.7), 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 it is known as the *exponential recency-weighted average*. If α is constant on n, the exponential recency-weighted average is also a convex sum of the rewards obtained.

Let us outline with pseudo-code how this agent would work:

Algorithm 2

```
procedure NON-STATIONARY MULIT-ARMED BANDIT AGENT
count = 0
while count < N :
    action ← arg max Q
    reward ← bandit(action)
    Q[action] ← Q[action] + α (reward - Q[action])
    count ← count + 1
```

[1] Note that for the sake of readability we have introduced an slight change in the notation and we omit the subindex t designing the episode. This is implicit since the function Q updates each iteration.

If we pay attention to the pseudo-code, we see that to take the first action we need an initial estimate $q_{a,1}$ for each action. These initial estimates are not irrelevant. They play an important role on the convergence of the algorithm. For example, if we set $q_{a,1} = 0 \ \ \forall a \in \mathcal{A}$, the $\arg\max Q_1$ will output a random action. Therefore, the training can be biased towards that random action depending on the initial reward. Sometimes a good strategy is to set high values of $q_{a,1}$ 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.

3.2 Modified multi-armed bandit problem

If we come back to the pendulum example of Chapter 2, we can map the physical set up to a 2-armed bandit problem. We just need to assign the action of measuring L to one of the arms and measuring M to the other. Then we set the function R of the bandit to be $R : \mathcal{A} \times S \to \mathbb{R}$ as a composition of Gaussian reward function r with the analyzer predicting the period from the outcome. Basically, we assume that the bandit is the result of the interaction between the environment, the analyzer and the Gaussian comparator (Fig. 3.2).

Note that this multi-armed bandit problem is quite difficult: it is non-stationary since the analyzer and the environment change each episode and it is non-Markovian since the performance of the analyzer depends on the training over all the previous episodes. However, as we have seen, even very simple agents perform surprisingly well for this simple case.

If we can map the simple pendulum example to a multi-armed bandit, it is evident that many other physical set-ups can also be mapped to this problem. So instead of transforming physical examples to a multi-armed bandit problem, we can design a customizable multi-armed bandit to represent an infinite variety of physical situations. However, this bandit is only useful to represent those situations in which a discrete set of actions is chosen at the beginning of the experiment without further intervention until the end of the experiment.

In this kind of set up we only have a single experimenter at the beginning of the learning loop. This means that the state space $\mathcal{X}$ of the experimenter's environment is again the empty set $\varnothing$. The action space $\mathcal{A}$ is finite and discrete with $k \in \mathbb{N}$ possible actions. The SPE, in the state $s \in S$, after the action a of the experimenter, generates an outcome $\mathbf{O}(a, s) \in \mathbb{R}^m$, and the value of the target physical property $\mathbf{f}(s') \in \mathbb{R}^l$, where $s' \in S$ is the state of the SPE after the action a. Then, the

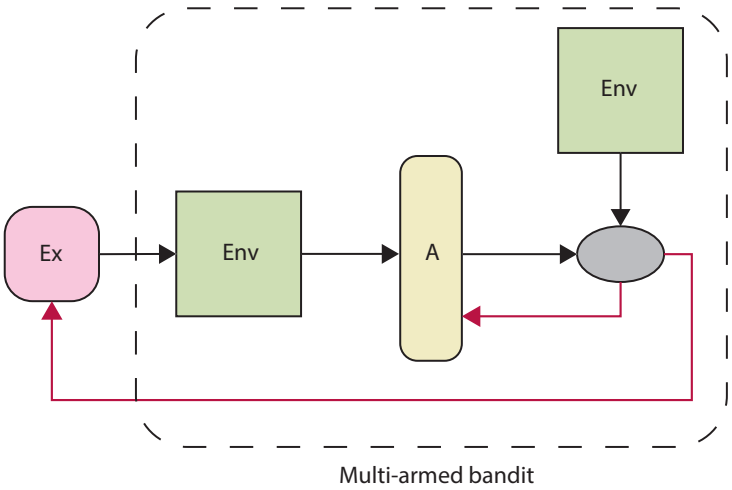


Figure 3.2: Diagram of how the simplest combination for the E-A architecture (2.1) can be modelled as a multi-armed bandit.

analyzer $\mathscr{A}$ is asked to guess $\mathbf{f}(s')$ using the value of $\mathbf{O}(a, s)$ and potentially the action a and some additional auxiliary information $I \in \mathbb{R}^p$. The prediction $\mathbf{P} \in \mathbb{R}^l$ of the analyzer is compared to the actual value of the physical property $\mathbf{f}(s')$ by means of a reward generating function $r : \mathbb{R}^l \times \mathbb{R}^l \to \mathbb{R}$. The output of $r(\mathbf{f}(s'), \mathbf{P})$ is the output reward of the bandit.

Example 3.2.1. We can illustrate again what each element of the bandit is with the familiar pendulum example. In the pendulum example:

- $k = 2$, since there are only two possible actions.
- $s' = s$ since the actions do not change the state of the pendulum represented by the tuple (M, L).
- $f(s') = T(L) = 2\pi\sqrt{L/g}$ and therefore $l = 1$.
- $O(a = 0, s = (L, M)) = M$ and $O(a = 1, s = (L, M)) = L$. Therefore $m = 1$, since the outcome is just a real number.
- r is defined by (2.8).
- There's no auxiliary information I.

Now let us explore different versions of this modified multi-armed bandit.

3.3 Modified multi-armed bandit: single parameter per lever

In this example, the multi-armed bandit is going to be very simple. There are k arms. One of them, the arm t (target) is special. This arm is generally selected at random in the first episode. At the beginning of each episode, the state of the SPE is generated by associating to each arm a real number v_k. Each value v_k is sampled from the same uniform distribution $\mathcal{U}(v_{min}, v_{max})$. Formally, the SPE state space is:

$$S \equiv \{s = (v_0, v_1, ..., v_k) \in \mathbb{R}^k : \tag{3.8}$$

$$\forall i \;\; v_i \sim \mathcal{U}(v_{min}, v_{max})\} \tag{3.9}$$

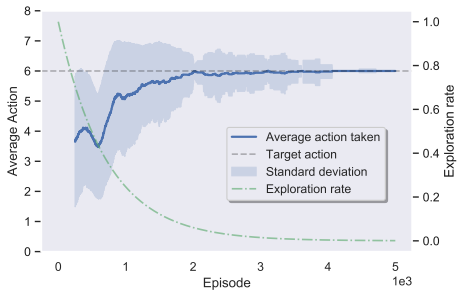
Each time a lever a is pulled, the outcome $O(a, s)$ is just the the value v_a associated to the arm a. We choose the function $f(s)$ to be any real function of only the value of the target arm. For instance, $f(v_t) = v_t^2$. Then the analyzer is fed the outcome $O(a, s) = v_a$ to try to predict $f(v_t)$. It produces a prediction $\mathscr{A}(v_a) = p$ that is used to generate a reward $r(p, f(v_t))$ according to (2.8). Then the analyzer and the experimenters are trained with their respective algorithms.

It is clear that the analyzer would be able to make a prediction of $f(s)$ better than random guessing only if the experimenter chooses the target arm t. Note also that the pendulum example is just a particular case of this example. We just need to set t as the arm that outputs L, and $f(v_t) = T(L)$.

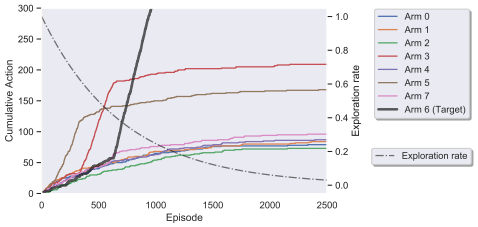
Let's run a few different cases to see it performs with different configurations.

Example 3.3.1. In this example, let us set:

- The number of arms to $k = 8$.
- The function $f(v_t)$ to be the identity $f(v_t) = v_t$
- The experimenter is based on the algorithm described in 3.1.1, equipped with an ϵ-greedy exploration phase with exponential decrease of the exploration rate.
- The analyzer is a feed-forward neural network with two fully connected layers, and each layer consisting of 16 neurons activated with the ReLU function. The optimizer is just the gradient descent algorithm. This analyzer is of unnecessary complexity for this task, but it will be useful later for more complex functions $f(v_t)$.



(a) Moving average of the actions



(b) Cumulative number of actions taken by the experimenter

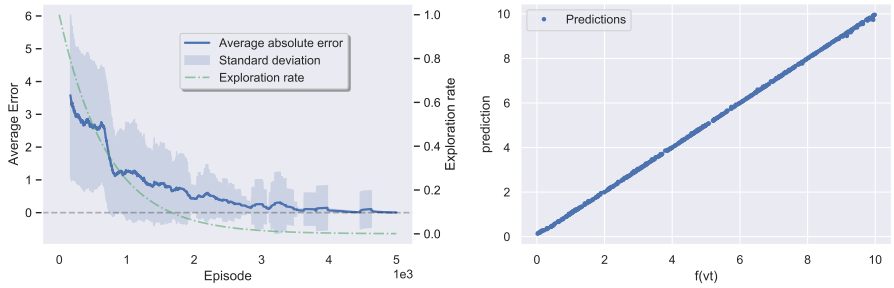
Figure 3.3: Training process of the scenario from Example 3.3.1. These two figures shows us how the agent realizes that in order to get a reward it needs to take the target action (the lever 6 in this case). In (a), we can see the average value of the action taken in each episode how it converges to the target lever. In (b), we can see the cumulative number of actions taken by the agent and how around the 600^{th} episode the agent finds the target arm and chooses it whenever a greedy action is taken. Chosen parameters for the training: $N = 5000$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$

- The reward generating function r is defined as in eq. (2.8).

Running a few tries we find that by setting the number of episodes to $N = 5000$ the agent always finds the target lever and correctly learns the identity function. In Fig. 3.3b we can observe how the agent discovers the target lever around the episode 600, and once the lever is found, as it is expected, the analyzer converges very quickly to the identity function (Fig. 3.3a). Although this example might look trivial, is not evident that it should work. Note that at the beginning, neither the experimenter or the analyzer have any information about the target lever or the function $f(s')$. In the exploration phase, the experimenter chooses random levers and the analyzer tries to fit the function with most of the times useless inputs but $1/8^{\text{th}}$ of the times a useful value. Then the gradient descent algorithm is applied and results to be surprisingly robust against the noise produced by the useless inputs.

Example 3.3.2. In this example, we consider the same configuration as in the previous example but changing only the function $f(s')$. Instead of the identity we are going to ask for a complicated function and test if the agent finds the lever. The chosen function is:

$$f(s') = f(v_t) = e^{\sin(v_t)} \tag{3.10}$$



(a) Average error per episode (b) Predicted value vs. Target value

Figure 3.4: Performance of the example 3.3.1. These two figures shows us how the agent performs the identity function. In (a), we can see the average value of the error drops quickly to zero as the agent identify the correct lever and the exploration rate vanishes. In (b), we can see the predictions of the agent after 5000 episodes and how it fits nearly perfectly the identity function. Chosen parameters for the training: $N = 5000$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$

Keeping the same hyper-parameters we observe that 5,000 episodes are not enough for the agent to succeed. However, trying with 50,000 episodes we observe that the agent finds the correct lever (Fig. 3.6a) and successfully learns the function $f(v_t)$ (Fig. 3.5). This reveals that non-trivial correlations can proportionate enough bias to initiate the feedback loop, although the duration of the exploration phase for it to start increases with the complexity of the correlation.

Example 3.3.3. In this example, we are going to see what happens if instead of a small number of arms, we have a large number of arms in which only one gives the relevant value. If we set $k = 100$ and choose a simple, but not trivial polynomial function $f(v_t) = v_t^2 - v_t$, we find that the agent finds the correct lever also in less than 50,000 episodes (Fig. 3.8a). The predictions of the analyzer after the training are nearly perfect due to the simplicity of the function and the high number of training steps.

These last two simple examples show us that the agent performs well for both, complex functions and large action spaces. As we will see in another example later, even with a more complex configuration and 2,000 different levers the agent is able to find the correct lever (although the training took around 5h in an average laptop processor).

In the next examples we will try different configurations in which the outcomes

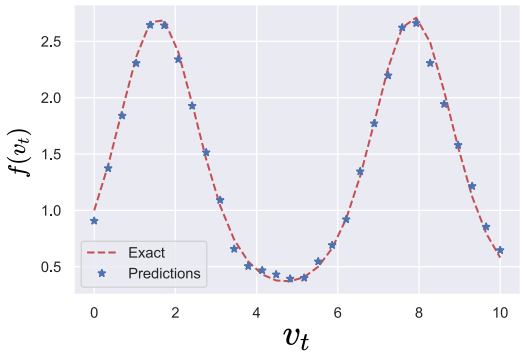
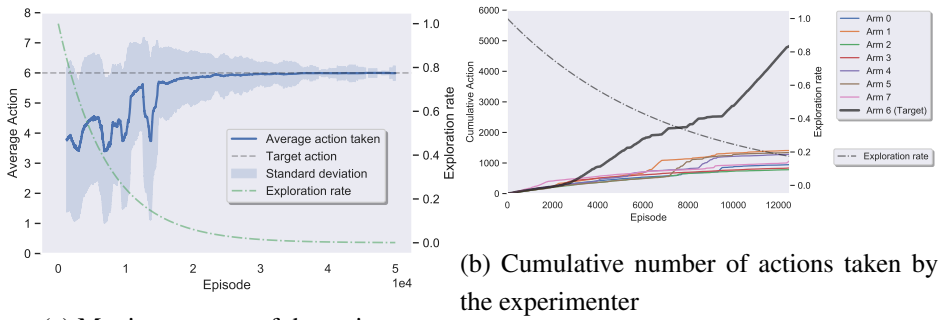


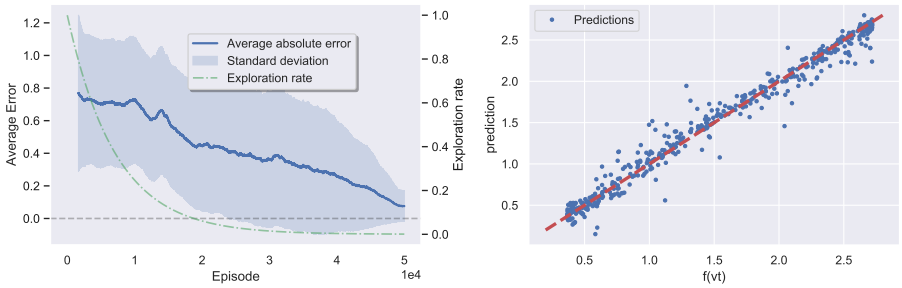
Figure 3.5: Graphical representation of the predictions made by the analyzer after the training compared to the exact value $\mathscr{E}^{\sin(v_t)}$ for the interval $[v_{min} = 0, v_{max} = 10]$ after 50,000 episodes of training.



(a) Moving average of the actions

(b) Cumulative number of actions taken by the experimenter

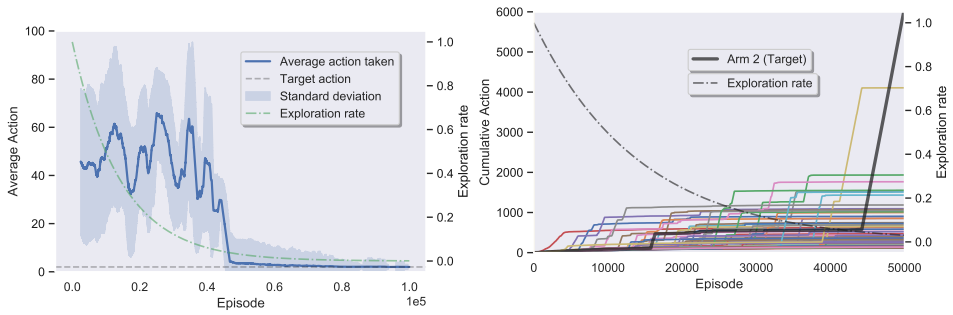
Figure 3.6: Training process for the scenario from Example 3.3.2. These two figures shows us how the agent realizes that in order to get reward it needs to take the target action (the lever 6 in this case). In (a) we can see the average value of the action taken in each episode and how it converges to the target lever. In (b), we can see the cumulative number of actions taken by the agent and how around the 2000^{th} episode the agent finds the target arm and chooses it whenever a greedy action is taken. Chosen parameters for the training: $N = 50,000$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$



(a) Average error per episode

(b) Empirical value vs. Predicted value

Figure 3.7: Performance for the scenario of Example 3.3.2. These two figures shows us how the agent learns to perform the correct function. In (a), we can see the average value of the error drops to zero as the agent identify the correct lever and the exploration rate vanishes. In (b), we can see the predictions of the agent after 50,000 episodes and how it fits with acceptable accuracy the target function. Chosen parameters for the training: $N = 50,000$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$



(a) Moving average of the actions

(b) Cumulative number of actions taken by the experimenter

Figure 3.8: Training process of the scenario from Example 3.3.3 . These two figures shows us how the agent realizes that in order to get a reward it needs to take the target action (the lever 2 in this case). In (a), we can see the average value of the action taken in each episode and how it converges to the target lever, despite of the large number of levers. In (b), we can see the cumulative number of actions taken by the agent and how around the $40,000^{\text{th}}$ episode the agent finds the target arm and chooses it whenever a greedy action is taken. Chosen parameters for the training: $N = 10^5$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$

are multidimensional. We will also introduce the concept of auxiliary parameters, which will turn out to be very useful for more complex configurations of the E-A architecture.

3.3.1 Modified multi-armed bandit: multiple parameters per lever

In this example, we are going to set $k = 8$ again. In this case, each lever is going to have three values associated instead of only one. But we keep only a valid target lever t and the rest outputs useless values. At the beginning of each episode, the state of the SPE is generated by associating to each arm three real numbers $\{x_a, y_a, z_a\}$. The values ares sampled from the uniform distributions $\{\mathcal{U}(v_{min}, v_{max})\}_{v=x,y,z}$. Formally, the SPE state space is:

$$S \equiv \{s = (x_0, y_0, z_0, ..., x_k, y_k, z_k) \in \mathbb{R}^{3k} : \tag{3.11}$$

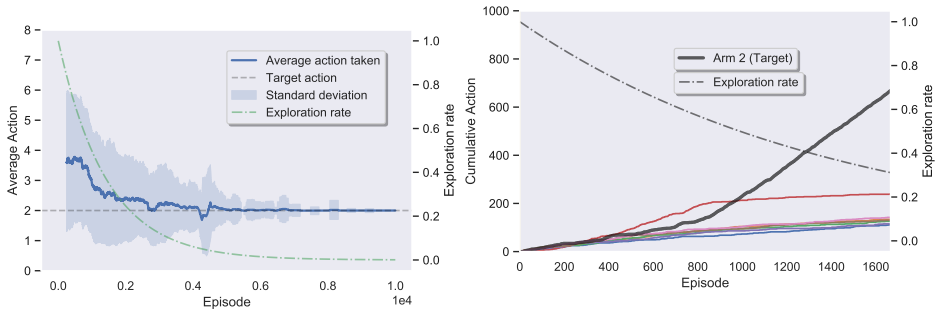
$$\forall v, i \;\; v_i \sim \mathcal{U}(v_{min}, v_{max})\} \tag{3.12}$$

Now we can set $f(s')$ to be 3-variable function, for example:

$$f(x_t, y_t, z_t) = x_t y_t z_t \tag{3.13}$$

Note that in this case at the input of the analyzer we will feed three parameters instead of one, maintaining the same hidden layers. Keeping the rest of the agent settings like in the previous examples we find that it discovers the correct action and learns to predict $f(s')$ in less than 10,000 episodes. This behavior is almost as good as for the single variable case (Fig. 3.9a). This means that adding more elements to the outcomes does not affect the performance of the algorithm. This was to be expected, since the addition of more parameters adds more tools to recognize the correlations at the expense of a maybe more complicated computation of the function. However, the used analyzer has enough flexibility to fit to those kind of functions.

A question that one may ask is: "What if the agent is allowed to pull more than one lever per episode, for example, n levers, to then be asked for a prediction that involves the parameters of $l \leqslant n$ levers?" In such a case the problem can be mapped to a single-lever bandit like the ones we have seen by associating a lever to each one of the possible combinations of pulls. This is, for a bandit with k levers and n pulls each episode, the number of possible combinations is just $\binom{k}{n}$. And each new bandit would output the n parameters that would result from all the pulls of the associated combination. We could also tackle the problem by using the original



(a) Moving average of the actions

(b) Cumulative number of actions taken by the experimenter

Figure 3.9: Training process of the scenario from the 3-variable example. These two figures shows us how the agent realizes that in order to get a reward it needs to take the target action (the lever 2 in this case). In (a), we can see the average value of the action taken in each episode and how it converges to the target lever. In (b) we can see the cumulative number of actions taken by the agent and how around the $10,000^{\text{th}}$ episode the agent finds the target arm and chooses it whenever a greedy action is taken. Chosen parameters for the training: $N = 10^4$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$

bandit and train n experimenters in parallel. A more interesting, but also more difficult problem, is to create an agent that also optimizes in the number of pulls per episode, to find the minimum number l of pulls needed to maximize the precision of the predictions. This kind of agent would be very interesting in the context of minimal representation learning. The main challenge here is that changing the number of pulls changes also the number of features fed to the analyzer. A possible solution would be to add a penalization to the reward proportional to the number of pulls performed per episode and solving the issue of the number of features by using placeholders to keep the neural network architecture working. However, the design of this architecture is beyond the scope of this work and it is let for future investigations.

3.3.2 Modified multi-armed bandit with auxiliary parameters

In this version of the multi-armed bandit we are going to introduce a slight change in the architecture of the bandit. This consists in adding to the input of the analyzer some auxiliary information needed to make the prediction. In addition to the outcome $\mathbf{O}(a, s)$ and potentially the action a, we can also feed more parameters that

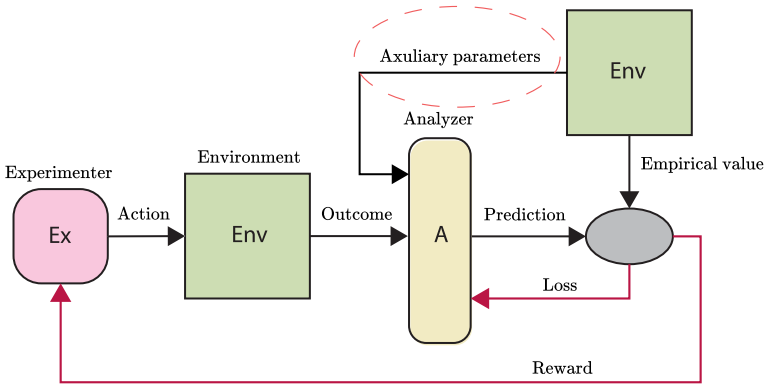
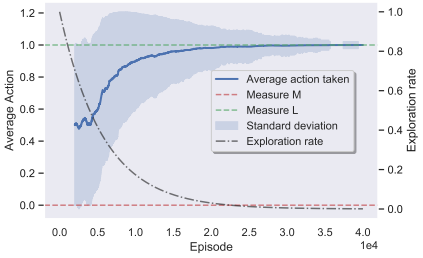


Figure 3.10: To add the auxiliary parameters to the learning loop we just need to make a small modification to the structure.

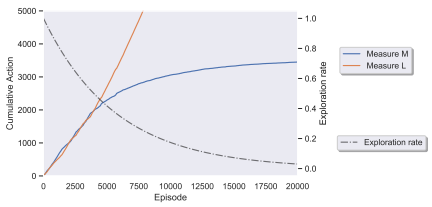
might be relevant to make the prediction or even to ask for an specific prediction. This is similar to what authors call *question input* in the SciNet architecture presented in [17]. Let us illustrate again this concept by using the pendulum example.

Suppose that, instead of directly asking the analyzer for the period T of the gravity pendulum, what we want the analyzer to predict is the angle $\theta(\tau)$ of the pendulum at a given time τ. The accuracy of the analyzer predicting the angle would determine the reward. However, the dynamics are determined by a second order differential equation. In order to predict the angle $\theta(\tau)$ correctly, the analyzer needs at least three extra parameters. The time τ and the values $\theta(0)$ and $\dot{\theta}(0)$. It is, in general, a good practice to sample the extra features of the analyzer uniformly at random from a selected interval. This would force the analyzer to learn without bias within the given interval. We can see how the learning loop is modified with the new addition (Fig. 3.10). We should not expect any drastic change in the performance compared to the multi-parameter case. We are just adding parameters, the only difference is that they are not determined by the action of the experimenter. This means that the analyzer has some degree of information even if the experimenter takes wrong choices. We can expect the analyzer performing better than random guessing regardless the performance of the experimenter.

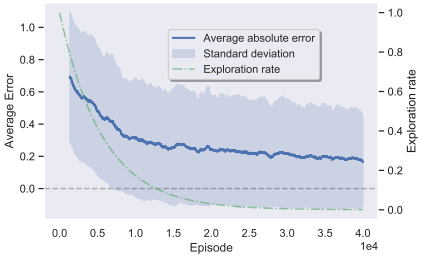
Example 3.3.4. This example will complete the pendulum example. Instead of asking the analyzer to predict the value of the period T, we are going to ask for the angle $\theta(\tau)$ of the pendulum. To do it we are also going to feed to the analyzer the instant τ and the initial values $\theta(0)$ and $\dot{\theta}(0)$. All these values are generated from a uniform distribution randomly each episode. We assume that the pendulum



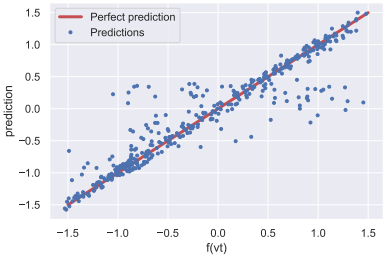
(a) Actions moving average



(b) Cumulative actions taken



(c) Absolute error moving average



(d) Empirical value vs. Predicted value

Figure 3.11: Summary of the training for the example 3.3.4. We observe that the actions converge like in previous examples. The analyzer does not completely fit the function, although shows clear signs of learning. This could be due to an inadequate Neural Network architecture or insufficient training. Chosen parameters for the training: $N = 40,000$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$

behaves like an simple harmonic oscillator and therefore:

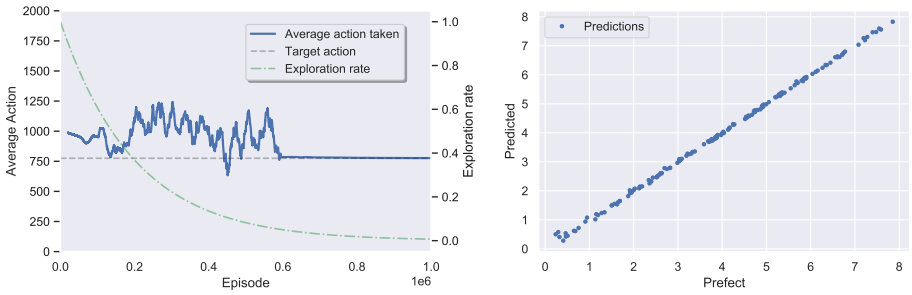
$$f(L, \tau, \theta(0), \dot{\theta}(0)) = \theta(\tau) = \theta(0)\cos(\omega\tau) + \dot{\theta}(0)\sin(\omega\tau) \tag{3.14}$$

where $\omega = \sqrt{g/L}$. The results are shown in Fig. 3.11.

Example 3.3.5. In this short example let us see how our agent can solve a multi-armed bandit problem with $k = 2000$, with an auxiliary parameter and a non-trivial function to predict. There is only a target lever t that outputs the value v_t. Let u be an auxiliary parameter sampled form a uniform distribution and fed to the analyzer. The function asked to predict is:

$$f(u, v_t) = \sqrt{u v_t \sin(v_t)} \tag{3.15}$$

We ran it for $N = 2 \times 10^6$ and we found that the agent successfully discovered the correct lever in around 6×10^5 episodes (Fig. 3.12a).



(a) Moving average of the actions taken (b) Empirical value vs. Predicted value

Figure 3.12: Summary of the training example (3.3.5) Chosen parameters for the training: $N = 2 \times 10^6$, $\alpha_{\text{experimenter}} = 0.01$, $\text{lr}_{\text{analyzer}} = 0.01$, $Q_1 = 0$, $\sigma = 0.05$

3.3.3 Summary of the multi-armed bandit

In this section we showed how the E-A architecture successfully finds the correct strategies for multi-armed bandit like experiments in every tested case. However, the computation time scales poorly to large action spaces. Although these type of problems are from limited interest, they are useful to show the ability of the E-A architecture to find unknown correlations solely by empirical validation.

Chapter 4

Experimenter-Analyzer for sequential experiments

In the previous section we showed how the simplest version of the E-A architecture can find the optimal strategy for experiments that can be expressed as a multi-armed bandit problem. This is: experiments with a discrete number of actions that can be predetermined before the experiment is started. However, it is not possible in general to express every experiment as a multi-armed bandit problem. For example, if the action space is continuous (e.g. selecting the position of a detector) or if the experiment requires a dynamical intervention. For example, if in an experiment consisting of sequential actions the result of the preceding actions is required to choose the optimal action in the current step. In this section we are going to show how one can tackle these latter experiments using the E-A architecture.

4.1 Sequential experiments

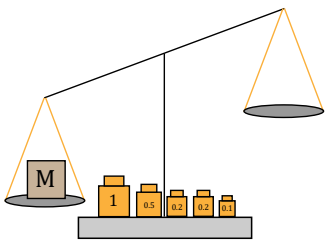
So far, all the E-A models we have used consists of an experimenter $\mathscr{E} : \varnothing \to \mathcal{A}$ whose action a over the environment in the state s produce some outcome $\mathbf{O}(a, s)$. Then the outcome and maybe some additional information are fed to the analyzer $\mathscr{A} : \mathcal{M} \to \mathcal{P}$ to output a prediction about a physical property of the system. Then such a property is observed (or in our case, simulated) and compared to the prediction to generate a reward and a loss, to train both both, the experimenter and the analyzer. This simple structure is enough for experiments in which we can group all actions and measurements to be taken in a single action at the beginning of the experiment. For example, if the experiment consists of measuring different

parameters of an electric circuit to know the power consumed by a section of the circuit. We can group all those choices of measurements, e.g. measuring the intensity at node A and the voltage at node B, in a single action taken at the beginning of an episode. This is because the outcomes of the measurements do not influence each other. However, in other experiments the outcomes of previous actions may influence the actions to be taken in order to get the correct parameters for a prediction. We will call this experiments *sequential*, since a number of actions need to be taken sequentially. Let us illustrate the concept with an example of a sequential experiment:

Example 4.1.1. Imagine an experiment that has the objective of determining the mass M of an object with the following tools:

- A beam balance with two plates that leans to the side of the heavier plate.
- A set of calibrated weights consisting of:
  - A mass of 100 g
  - Two masses of 200 g
  - A mass of 500 g
  - A mass of 1 kg

If the mass M to be weighted is less than 2 kg we can find value of the mass M, with an uncertainty of 100 g or less, in only five uses of the scale. For example, if the mass is 1.3 kg a procedure would be the following:



1. M vs 2 kg → right
2. M vs 1 kg → left
3. M vs 1.5 kg → right
4. M vs 1.2 kg → left
5. M vs 1.4 kg → right
6. We know that the mass is:
   1.3 kg $\pm$100 g

However, in order to find the value of M in five uses of the scale or less we cannot have a prefixed strategy at the start of the experiment. We need to observe

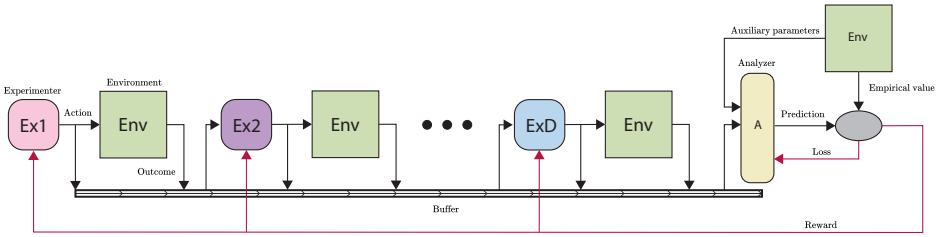


Figure 4.1: Diagram of the learning loop for a E-A architecture for a sequential experiment with D steps. The structure is the same as for the simple case but concatenating D experimenters instead of a single one.

the outcomes of each measurement individually and respond accordingly. We can not express then this experiment as a multi-armed bandit decision problem and therefore it is a sequential experiment.

4.2 E-A for sequential experiments

In this section we are going to explain how to use the E-A architecture to tackle sequential experiments. The basic idea behind this approach is to concatenate as many experimenters as sequential actions are needed. Each experimenter is fed with the information gathered by the actions of the preceding experimenters.

Suppose we have a sequential experiment that consists of D sequential actions. Then we would have D different experimenters $\mathscr{E}_n : \mathcal{X}_n \to \mathcal{A}_n$ with $\mathcal{X}_0 \equiv \varnothing$. Each $\mathcal{A}_n$ can be different depending on the nature of the experiment, since the experimenters $\mathscr{E}_n$ could be different reinforcement learning agents with different architectures. The experimenters' environments $\mathcal{X}_n$ can consist of any information stored in the buffer at the moment they are fed to $\mathscr{E}_n$. The SPE is in the state $s_n \in S$ when the action $a_n \in \mathcal{A}_n$ is taken and it produces the outcome $\mathbf{O}_n(a_n, s_n) \in \mathbb{R}^{d_n}$ where d_n is the number of parameters that are outputted after the action a_n. Then, as in the single experimenter version, all the information in the buffer together with auxiliary parameters can be stored into $m \in \mathcal{M}$ to fed the analyzer $\mathscr{A} : \mathcal{M} \to \mathcal{P}$. Then the prediction is compared with the empirical value of the property to be predicted with a reward generation function r_n. The reward could be different for each experimenter depending on the nature of the architecture. However, in this work we only explored the architecture with a single reward generation function r for all experimenters.

One of the main limitations of this approach is that we need to fix the number

D of actions beforehand. In some experiments this may not be relevant since the number D is fixed by the experiment itself. However, in others this fact might be important. For example, in the context of the example 4.1.1, we may ignore what the minimum number of actions needed to determine the mass with an uncertainty of less than 100 g is. The agent will only search for the best strategy for the given D actions, which may not be optimal.

4.3 Example

In this section we consider an example of a sequential experiment in which the A-E architecture finds the optimal strategy.

4.3.1 The experiment

We have a box of mass M on an infinite horizontal surface with friction coefficient μ respect to the mass M. The SPE is programmed so that a cannon shoots a bullet of mass m with velocity v that collides inelastically with M when an episode is started. The mass M is the only parameter that is reset at each episode by sampling uniformly at random from the interval $[M_{min}, M_{max}]$. We can calculate the distance traveled by the box using the conservation of momentum. The moment of the bullet is $p_b = mv$. Applying the conservation of momentum we can obtain the velocity of the box after the impact:

$$v' = \frac{p_b}{M'} = \frac{m}{M+m}v \tag{4.1}$$

where $M' = m + M$ is the mass of the moving block formed by the bullet and the box. We know that the friction force is $F = \mu N = \mu(m + M)g$. When the box stops, due to the conservation of energy, the work realized by the friction force must be the kinetic energy K of the mass M' of the block after the impact of the bullet. Since the friction force is assumed to be constant, the work done is $W = Fx = \mu(m+M)gx$, where x is the distance traveled until it stops. Equating this term to the kinetic energy we obtain:

$$x = \frac{1}{2g\mu}\left(\frac{vm}{M+m}\right)^2 \tag{4.2}$$

We give the agent access to two sensors to measure the position of the box:

- **A low precision but wide range (LPWR) position sensor**: it works as follows: the landing zone is divided into four regions or zones of equal size.

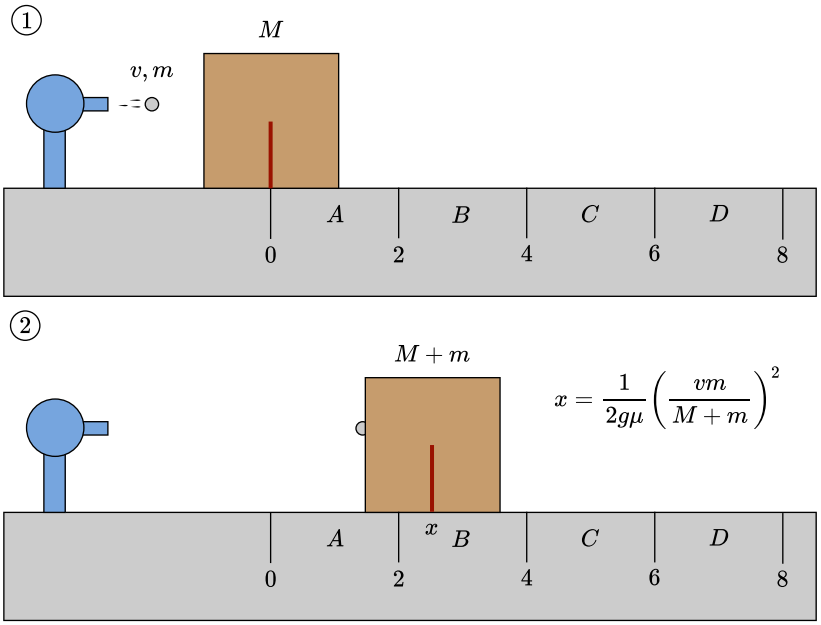


Figure 4.2: Diagram explaining the physical environment. The cannon shoots a bullet of mass m with velocity v. When it collides inelastically with the box of mass M, the box displaces. Due to the friction force it stops in one of the four zones A, B, C or D.

This sensor outcomes the middle point of the zone in which the box has landed. For example, in the situation depicted in Fig. 4.2 this sensor would produce the outcome: 3, since it is the middle point of the zone B. This allows to know roughly where the box landed, but with low accuracy.

- **A high precision but narrow range (HPNR) position sensor**: It works as follows: to activate it you need also to specify a region and if the box landed on the specified region the outcome of the sensor is the exact position of the box. Otherwise it outputs a constant negative value (set to -1) representing a failed measurement. For example, in the situation depicted in Fig. 4.2 if this sensor is placed in the zone B it will output the value of x. If placed in any other zone it outputs -1.

The goal of the agent is to predict the position in which the box will land for a shooting with velocity v_{test} and bullet mass m, but only with **two uses of the sensors**. The velocity v_{test} is selected randomly each episode from a uniform distribution for the interval $(\frac{v}{2}, v + \frac{v}{2})$. This velocity v_{test} would be the auxiliary parameter fed

to the analyzer. Note that the choice of the interval is made to keep a similar order of magnitude between the test shooting and the experiment shooting. We could have chosen any other interval. Using the same procedure that we did for the first shooting, we can find that the new displacement d of the box after the shooting is:

$$d = \frac{1}{2g\mu}\left(\frac{v_{test}m}{M+2m}\right)^2 \tag{4.3}$$

Since d depends on the mass M, and M can be inferred from the first displacement x using (4.2), the agent has enough information to predict the displacement of the test shooting if it detects correctly the position x of the box.

This experiment is sequential because to always obtain the exact position of the box, the agent needs to use sequentially the sensors in a specific way. This strategy consists of choosing in the first try the LPWR sensor, to detect in which zone the box landed, and in the second use of the sensors to choose the HPNR sensor and place it in the zone inferred from the first outcome.

4.3.2 Mathematical characterization of the experiment

Let us contextualize each element of the training using the mathematical formulation used in the text.

- The state of the SPE is determined by the tuple $s = (M, v_{test})$.
- The E-A agent has two experimenters: $\mathscr{E}_1 : \mathcal{X}_1 \to \mathcal{A}$ and $\mathscr{E}_2 : \mathcal{X}_2 \to \mathcal{A}$ where $\mathcal{X}_1 = \varnothing$ and $\mathcal{X}_2 = \mathcal{A} \times \mathbb{R}$, since we feed the second experimenter the action a_1 of $\mathscr{E}_1$ and the outcome $O(a_1)$ of its action.
- The action space for both experimenters is $\mathcal{A} = \{0, 1, 2, 3, 4\}$, with the action 0 representing the action of using the LPWR sensor, and the actions $\{1, 2, 3, 4\}$ represent the actions of using the HPNR and placing it in the zones A, B, C and D respectively.
- The analyzer is $\mathscr{A} : \mathcal{M} \to \mathbb{R}$, where each element of $\mathcal{M}$ is a tuple $(a_1, O(a_1, s), a_2, O(a_2), v_{test})$.
- The quantity to be predicted is $f(s) = d = \frac{1}{2g\mu}\left(\frac{v_{test}m}{M+2m}\right)^2$
- The reward function is $r(\Delta) = \exp\left(-\frac{1}{2}\left(\frac{\Delta}{\sigma}\right)^2\right)$, where $\Delta = \frac{f(s)-p}{p}$ and p is the output of the analyzer.
- The loss function for the analyzer is $L(f(s), p) = (f(s) - p)^2$.

4.3.3 Technical details of the agents

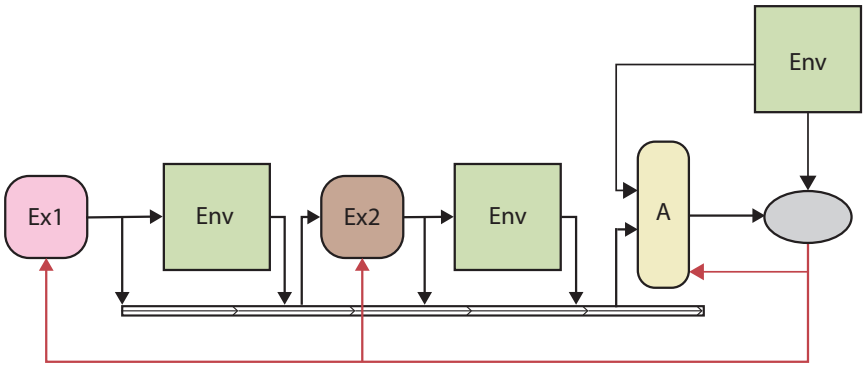


Figure 4.3: Diagram of the learning loop for the experiment.

Experimenter 1

$\mathscr{E}_1$ is the same kind of experimenter that we used in the previous examples (2), since for $\mathscr{E}_1$ everything looks like a multi-armed bandit. The agent was subjected to an ϵ-greedy exploration phase with linear decrease of the exploration rate.

Experimenter 2

For the experimenter 2, now we have inputs, so the reinforcement learning algorithm of $\mathscr{E}_1$ is not valid. Since some of the inputs are real numbers, we opted to use a standard Deep Q Network [19] algorithm with online training. We also tried a modified version of the Deep Q Network (DQN) algorithm equipped with a memory and two neural networks [20] to improve the performance. We could have opted for a normal Q-learning algorithm as well, but would have required some amount of hardcoding, which is undesirable in our purpose of finding agents as independent as possible.

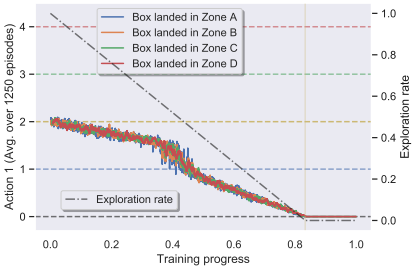
The structure of the neural network for this agent is a tw fully connected hidden layers (16x16) of sigmoidal neurons for both versions. We ignore if this is an appropriate structure since we haven't performed an optimization of the hyperparameters.

The agent was subjected parelly to the same ϵ-greedy exploration phase than $\mathscr{E}_1$.

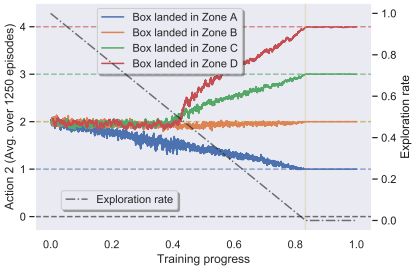
Analyzer

The analyzer in this case is a feed-forward neural network with 3 fully connected hidden layers (20x10x2) of ReLU neurons.

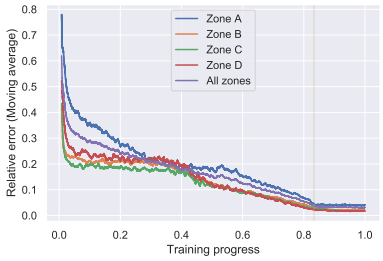
4.3.4 Results and discussion



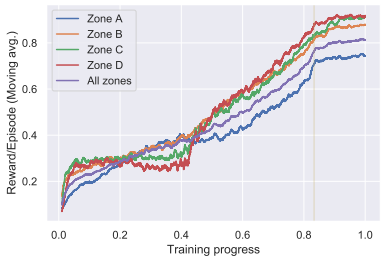
(a) Action 1 by zone (moving average)



(b) Action 2 by zone (moving average)



(c) Relative error (moving average)



(d) Reward per episode (moving average)

Figure 4.4: Summary of the training for the simple DQN agent. In (a), we can see how the first experimenter learns to take the action 0, this is, using the LPWR sensor always. In (b) we see how the second experimenter learns the optimal strategy converging to the correct action for every zone. This implies the agent learns to interpret correctly the outcome obtained by $\mathscr{E}_1$ and places the HPNR sensor in the corresponding zone. In (c), we observe the decrease on the relative error, that goes to nearly zero for every zone, meaning that the analyzer learns to interpret correctly the outcomes. In (d), we see the reward obtained by the agent per episode. It gets close to the maximum of one at the end of the training for all zones. Number of episodes: $N = 2.5 \times 10^6$

Since $x \propto 1/M^2$, if we sample uniformly at random M, it means that the zones closer to the cannon are going to be quadratically more frequent than zones further away. With the used parameters, we obtain that the box lands in the zone $A \sim 54\%$ of the times, $\sim 27\%$ in B, $\sim 12\%$ in C and $\sim 7\%$ in zone D. Then our training data for the agent is strongly biased to the closer zones A and B.

In our tests, we found that with not enough training, the agent in an attempt to maximize the reward and minimize the loss learns to exploit this imbalance by choosing always to place the HPNR sensor in zones A and B. This is actually a clever strategy, since it obtains the exact position of the box for 80% of the episodes. However is suboptimal, since by placing first the LPWR sensor and then using its outcome to place the HPNR sensor in the correct place it is possible to obtain the exact position a 100% of the times.

We observed, that if we let the agent train long enough (2.5×10^6 episodes), it finds the optimal strategy even for an unbalanced scenario. This shows that the E-A architecture is potentially valid for getting information about rare events by showing robustness against imbalanced environments. In Fig. 4.4 we have a summary of the training. As we can see in Figs. 4.4a and 4.4b both experimenter learn to cooperate, the experimenter 1 taking always the action 0, and the experimenter 2 using the outcome of the action taken by experimenter 1 to place correctly the HPNR sensor. It results surprising that this can be achieved only with the rewards generated from the at first untrained analyzer. The working principle is supposed to be the same than for the multi-armed bandit: to let the analyzer exploit the correlations during the exploration phase to start a feedback loop in which all agents improvement improves each other performance.

Changing the DQN algorithm of the experimenter 2 to a more sophisticated dual DQN algorithm with experience replay reduced the number of episodes needed to find the optimal strategy by a factor of 10, needing only 2.5×10^5 episodes to show almost identical results. However, both algorithms took a similar amount of computation time ($\sim$ 5 h in an average laptop). This is because the dual DQN algorithm fits several points from the memory in each episode, taking longer to compute each episode.

This shows us that there is a lot of room for improvement by choosing different reinforcement learning agents or hyper-parameters. It also manifest one of the strength of this architecture: its modularity. With very few changes on the learning architecture we can set up completely different agents.

Chapter 5

Conclusion and future work

In this section we are going to discuss the conclusions extracted from this project and outline future work to expand the E-A architecture.

5.1 Conclusion

In this work we have proposed a new machine learning architecture that successfully finds the correct strategies for some given type of experiments, i.e. it finds the experimental strategies that lead to the relevant data allowing to correctly predict the physical properties of the system. We found that it works by exploiting the existing correlations between data obtained with specific actions and the empirical value of the asked property to start a feedback loop. Such correlations are found in a random exploration phase of the action space with an at first untrained predictor function that is trained with a gradient descent like algorithm. These architecture achieved the following milestones:

- It successfully finds the correct strategies for multi-armed bandit like experiments in every tested case. However, the computation time scales poorly to large action spaces (5h on an average laptop [1] for an action space of $\sim 10^3$ possible actions). Although these type of problems are from limited interest, they are useful to show the ability of the E-A architecture to find unknown correlations solely by empirical validation.
- It showed its ability to solve sequential experiments, i.e. experiments where the actions of future steps may depend on the chosen actions and observations from previous steps. This is done by concatenating reinforcement

[1] Surface Pro 2017, i5-7300U, 8GB of RAM.

learning agents. Based on the feedback obtained through empirical validation, they learn to find the optimal strategy for the experiment. Parallel to that, the feedforward neural network that produces the predictions learns to efficiently interpret the data to make accurate predictions.

We show that performance can vary widely depending on the machine learning tools used for the experimenters and the analyzers. We explored the use of agents with memory and they tend to perform better (learn the correct strategy in less episodes). Although the memory should be carefully implemented to not break the feedback loop, e.g. allowing only a small size memory. This is mainly for two reasons: first because analyzers that use memories with random access might be using some wrong actions to train the model when a good action was taken, hindering the formation of the feedback loop. Secondly, because if the agents are getting better at collecting data and emitting predictions, we do not want them to be trained with old data of less quality from when they were worse.

We also find some weaknesses on the architecture that are not solved yet. The structure of the specific E-A model used for a given experiment strongly influences the development of the experiment. For example, in sequential experiments we need to fix the number D of actions or, in general, what actions are allowed. This prior assumptions are yet unavoidable in this kind of set-ups. We suggest that many of this prior assumptions can be loosened by introducing the use of recurrent neural networks, variational methods and common machine learning techniques, like automatic feature selection or hyper-parameter optimization. Another weakness relates to its scalability. For experiments with large D, training at least D separate agents becomes computationally intractable. Finally, we do not have any approach yet yet that allows to understand how or why the machine learning system chooses its experimental strategy. This is relevant for complex experiments with complicated sequences of actions. It could be difficult to understand why the agent chose a specific strategy even if the strategy performs well on the predictions. In the next section we are going to discuss our suggestions and upcoming work to solve some of these weaknesses.

5.2 Future work

In the following section, we outline some future work and some ideas that could be implemented to solve some of the current drawbacks of the architecture.

5.2.1 Experimenters for continuous action spaces

So far we only explored experiments with discrete action spaces, but many experiments require to set continuous values in each taken action. For instance, in the example of the sliding box of Chapter 5, instead of placing the HPNR sensor in a discrete zone we could let the agent to place it anywhere within a given interval.

The reason why we have not explored yet this kind of experiments comes from the fact that all reinforcement learning agents used to portray the experimenter role were based in methods that compute the value function $Q(x, a)$ for every action $a \in \mathcal{A}$ and state $x \in \mathcal{X}$. The state space $\mathcal{X}$ can be continuous for this kind of algorithms since we can use neural networks to produce an estimate of Q for each action even for continuous inputs. However, for the action space $\mathcal{A}$ this is not the case, since we decide which action to take by computing the $\arg\max_{a \in \mathcal{A}} Q(x, a)$. Therefore, we need to compute the value of Q for every action, which is impossible for a continuous action space.

To solve this issue we can use reinforcement learning agents with policies independent from the value function. One example of these kind of agents are the actor-critic algorithms [21]. This kind of algorithm divide the process of policy generation in two: an actor that consists of a parametric function independent from the value function and a critic that evaluates the actions taken by the actor by using an estimation of the expected reward. We suspect that this kind of agents can be seamlessly implemented in the E-A architecture.

5.2.2 Combination of the Experimenter-Analyzer architecture with SciNet

In [17], the authors explore the use of variational auto-encoders to extract autonomously physically relevant parameters from physical data without prior assumptions about the physical system. They proposed a neural network architecture called *SciNet* where they use a variational auto-encoder to find the minimal latent representation that contains relevant physical parameters. This architecture can be combined with the Experimenter-Analyzer architecture to create an agent that autonomously collect the data and finds the relevant physical parameters, using only only feedback about the quality of its predictions (and the relevant parameters are learned in an unsupervised way). This can be achieve by substituting the regular regression neural networks used in this work as the analyzer with the architecture used for SciNet.

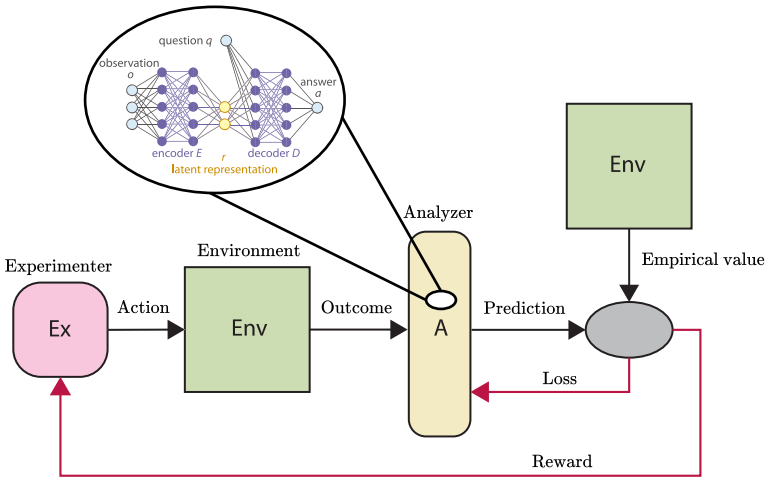


Figure 5.1: Diagram of a Experimenter-Analyzer structure combined with SciNet to extract the relevant physical parameters from the data collected by the experimenter. The image of the auto-encoder was taken from the original paper [17] with the permission of the authors.

5.2.3 Recurrent Neural Networks for sequential experiments with constant action spaces

There are some sequential experiments, like the beam scale experiment of Ex. 4.1.1, where every event of the sequence shares the same action space. In this cases we may be able to substitute sequential reinforcement agents with a single recurrent neural network. LSTM networks [22] are a promising technology for this kind of approach. This method could be a partial solution to the scalability issue and might proportionate tools to infer the optimal D automatically.

5.2.4 Application of the architecture to real physical systems

It might be interesting to explore real life experiments where we can try the E-A architecture. Potential candidates should be experiments on systems that allow for fast measurements. In the run simulations, each full iteration of the learning loop takes on average $\sim$ 10 ms. Many experimental set-ups allow to manipulate and read measurements of physical systems in much smaller timescales, e.g. electrical circuits or condensed matter systems.

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