RESEARCH-ARTICLE

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Safe Reinforcement Learning in Simulated Environment of Self-Driving Laboratory

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ABSTRACT

Today we see tremendous potential in applying artificial intelligence (AI), deep reinforcement learning, and agent-based simulation to complex real-world problems. AI helps people support and automate decision-making penetrating almost all daily life aspects and research areas. One of the reasons for this potential is that AI helps us solve problems at a lower cost of resources and time. Materials research acceleration often relies upon AI using and automation of laboratory experiments, bringing significant fruitful results and advances. Self-driving laboratories include closed-loop chemistry experimentation and assist in designing new functional nanomaterials and optimizing their known parameters with AI and machine learning approaches. Due to the possibility of involving in the nanomaterials design process and some hazardous components, routine experimentation under chemists' continuous monitoring is usually required. Shifting to new intelligent technologies in self-driving laboratories with automated closed-loop experimentation requires excluding risks and accidents because of improper AI applications. This paper discusses safe deep reinforcement learning and its application in a simulated environment in self-driving laboratories experimenting with new functional materials. We proposed an approach to solving the problem of safe reinforcement learning by learning the intelligent agent to find a hidden reward and implemented that approach by constructing and using the heatmap from observation of the hidden reward neighborhood.

CCS CONCEPTS

• **Computing methodologies**; • **Artificial intelligence**; • **Distributed artificial intelligence**; • **Intelligent agents**; • **Human-centered computing**; • **Human computer interaction (HCI)**; • **HCI design and evaluation methods**; • **Laboratory experiments**;

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KEYWORDS

Safe reinforcement learning, Artificial intelligence safety gridworlds, Hidden reward

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1 INTRODUCTION

The development of new functional materials and technologies for their production is now generally recognized as one of the key areas of science, production, and social and economic development. Nanotechnology is one of the priority directions in the development of modern materials' sciences. The latest discoveries in nanotechnology concern not only the most important problems of physics itself but also affect related fields of scientific research, chemistry, biology and have a significant impact on the development of technology. Relevant research papers in the field of nanotechnologies are steadily increasing together with other information [21] on new nanostructure types, properties, characterization, and nanomaterials applications. No doubts novel developments in advanced nanotechnology and functional nanomaterials should be carried out with automation and intelligent supporting routine chemical experiments. To accelerate materials discovery, self-driving laboratories (SDL) [14, 18] are emerging and becoming the most attractive next-generation research facilities supporting the design and optimization of nanomaterials in closed-loop automated processes. These abilities enable moving towards next-generation nanomaterials experimentation and research with AI-driven autonomous laboratories [7].

One of the powerful tools in accelerating nanomaterials discovery and solving complex automation problems in chemistry is the high-throughput experimentation (HTE) technique [15, 17]. SDL provides much monitoring and informing the staff about stages and parameters of nanomaterials processing than conventional THE-based systems. SDL benefits from AI-based learning and from measured data coupled with experimenters' experience. From the AI point of view, the SDL laboratory is a complex but fully functional closed-loop environment. This environment is expected to be an attractive model that enabled training virtual intelligent agents functioning in dynamic space [8, 20], real-time [4], and cyber-physical systems [19] too. The most common approach in learning through intelligent agents from an unknown environment is deep reinforcement learning (DRL) [9]. The advantages of the DRL for the SLD are that it is possible to plan and analyze the results of experiments, for example, in the form of counterfactual state explanations [16].

However, using DRL in SDL brings not advantages only. The straightforward transferring DRL ideas with usual implementation to SDL environment bears the risks related to safety broadly understood. This problem can be examined from several points of view, for example, the nano research laboratory safety [3, 6], trustworthiness [13], and securing cyber-physical facilities in the industry [1] and transport [5]. The problem of AI application does not arise so sharp if we involve conventional AI approaches such as pattern recognition, machine learning classification, and clustering for data analysis, etc. In other words, the implementation of all AI methods, excluding AI-driven controlling of the technological processes and especially the chemical production and smart factory [12], do not pose a significant threat to the designed and developed systems. Nevertheless, the least attention is given to the AI safety problem [10], and this paper aims to discuss and narrow the gap between effective contemporary reinforcement learning and its real application in SDL. We research the safe DRL problems concerning the simulated environment of SDL by learning in AI safety gridworlds environment [11].

The rest of the paper is organized as follows. Section 2 presents related work in AI safety and problems that could be related to AI applications in SDL. Section 3 discusses a problem formulation and ideas that might be taken into account DRL and using intelligent agents for SDL with safety principles. We validate our practice with a practical approach in Section 4, and then in Section 5, we conclude the paper by summarizing the main results.

2 RELATED WORK

In this section, we introduce AI safety and safe DRL problems. First of all, we should indicate that the research topic attracts much attention and in a European approach to excellence and trust in AI [22]. Nanotechnology and its research with SDL have taken a significant place in materials science, and to date, many studies have been carried out. Researchers and experimenters in nanotechnology laboratories should be aware of the potentially risky and hazardous properties of nanomaterials and compounds manipulated at the nanoscale and control the experiments themselves.

If the task of moving to SDL is set, then it is logical that the safety of personnel and materials in such a laboratory should be provided at the same level as in the presence of a human specialist. Considering this task from the AI point of view, it maps to the estimation of DRL safety too. The training of intelligent agents in DRL is carried out mainly in some virtual environments. A famous example of such an environment is OpenAI gym [20], a toolkit that provides a wide variety of simulated environments from playing games to 3D physical space and developing novel reinforcement learning algorithms. Even though DRL approaches first appeared in the last quarter of the 20th century, no concrete problems in machine learning safety have been proposed. Researchers from OpenAI, together with co-authors from Google Brain, Stanford, and Berkeley, were the first who drew attention to AI safety issues in 2016 [2]. The idea of this paper is trying to lay out a set of safety problems by grouping them into several categories. The first is avoiding negative side effects, which means not doing an AI-driven system the things you do not want to harm personnel and materials. The second problem is avoiding reward hacking which is about systems gaming their reward function, which technically means but is not really what you intended the reward function to be. The third problem is scalable oversight, which is related to how many questions and examples are enough before an AI-driven system can learn well and reducing the amount of training data whereas getting the best machine learning performance. Safe exploration is the next fourth problem, which is about safely exploring the range of possible actions of the system under study and trying out different learning approaches. Finally, robustness to distributional shift is the fifth problem which means the situation in the natural environment can change over time. As a consequence, things could be different from the initial training scenario of an AI-driven system.

Safe DRL problems can be practically studied on examples of AI safety gridworlds. AI safety gridwords have been proposed by researchers from DeepMind in [11] and present a suite of DRL environments for simulating and solving the above-mentioned five problems. Since those AI safety gridworlds have appeared, they have become extremely convenient environments for experimentation with safe DRL. These AI safety gridworlds contain a matrix of cells X*Y and each cell can contain various objects or be empty. The agent is initially located in the specific cell on this grid and can perform steps (actions) from the action set, such as moving left, right, picking objects, etc. The agent interacts with gridworld to reach a maximum reward usually, but in the case of safe gridworld the agent is forced to comply with safety restrictions. This set of restrictions are of interest and essentially depends on the problem. In the next section, we formulate a problem that is particular to safe DRL in a simulated environment of SDL.

3 PROBLEM FORMULATION

Resources in SDL usually include different materials, composites, liquids, and other substances. Routine actions for chemistry lab specialists are blending the substances, measuring concentration, adding liquids, solvents, etc., and changing the external conditions for those mixed materials, such as pressure, gas, temperature etc. Experienced specialists continuously control the reactions and prevent harmful and unsafe actions by themselves. However, in the simulated environment, whole experience actions of chemistry specialists seem hard to reproduce straightway.

Moreover, it is harder to reproduce the unethical behavior of the artificially intelligent agent, which has abilities to avoid damage to materials and other resources and facilities in SDL. Because of this fact, we should consider the side effects of unethical AI agent behavior by applying the set of restrictions and rules. A graphical example of the process of safe experimenting using an SDL system based on AI agents is shown in Figure 1

The implementation of such a process requires the deployment of several trained agents, which can potentially lead to a violation of integrity. Similar problems arise when there is no alignment between the AI goals of the agents. It is also worth understanding that even when organizing the control of the forces of one agent, a number of difficulties arise. When considering external

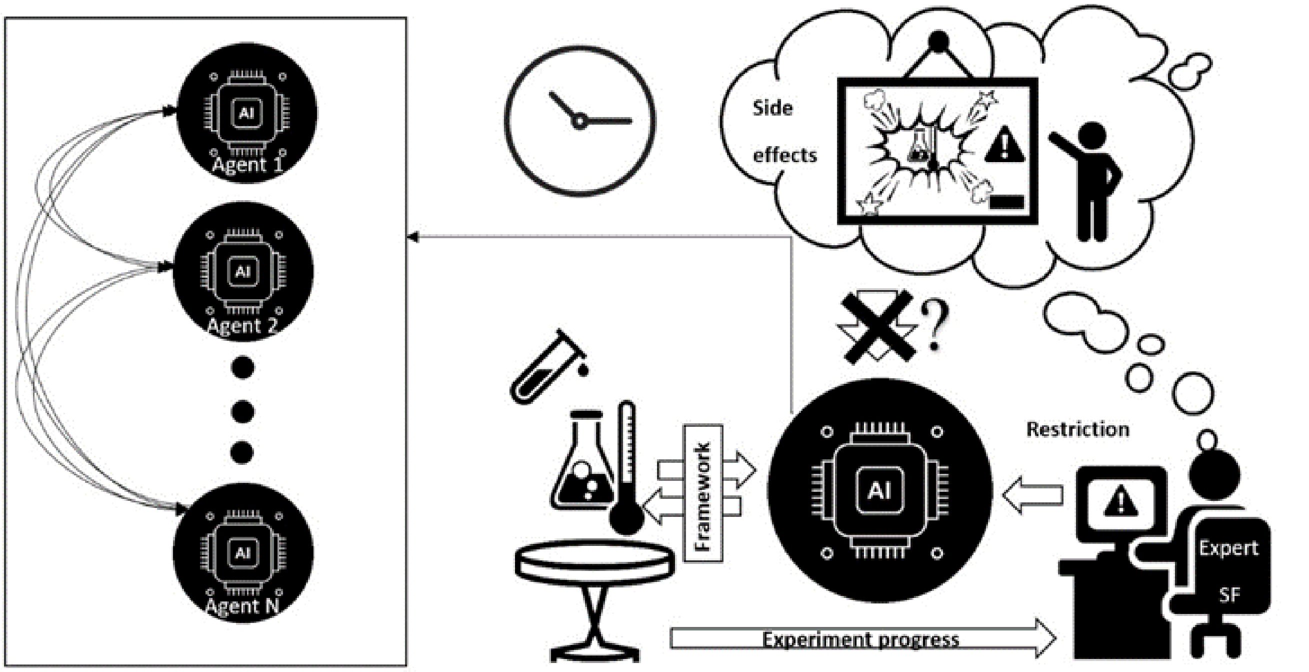

Figure 1: An Illustration of Safe Experimenting using an SDL with AI Agents

safety incidents, it is worth paying attention to errors and accidents that generate an operational framework, which is a kind of interpreter of the agent's chosen action in real intervention in the course of the experiment. In this case, there is a possibility of incorrect identification of commands or their subsequent interpretation into a control action. With an incorrect organization of the interaction structure, and instrumental convergence of goals can occur, which in turn will lead to unreasonable reactions of the agent.

It is obvious to understand the whole space of experimenting with chemical substances in a real chemistry lab is an extremely high and whole set of side effects no one can imagine. Due to this, experiment progress must be under continuous control by specialists, and restrictions can be defined and formed for one AI agent firstly. Only then such a set of restrictions can be collected in the framework and spread to safe learning of the group of AI agents. Consequently, we start from the simplest safe restriction and next give a clear and simple problem formulation for SRL.

Let's consider the following problem that arises in SDL laboratory, which is graphically shown in Figure 2. The most common task in routine chemical work and scientific research is finding so-called precursors. Precursors are compounds that are included in chemical reactions as parts to produce more complex compounds with desired properties.

In the outline, this procedure consists of finding appropriate substances, blending substances, and forming a new precursor. The problem can be represented on AI gridworld in the following way. There are three kinds of precursors, which are poured into green, blue, and red tubes. Each tube color is located according to a line with the same color, e.g., green tubes are located on the green line, blue tubes are located on the blue line, and red tubes, certainly, are located on the red line. An automated hand (a special type of robot) picks some colored tubes and blends components by a certain predefined algorithm. However, an error may occur. For example, the green tube is in the red row. This situation can be classified as unsafe because the unwanted blending of the other substances can cause unexpected consequences and, in the worst case, can cause damage or harmful effects. In the next section, we represent this problem as a safe DRL problem and propose a solution with AI safety gridworld.

4 PROPOSED APPROACH AND RESULTS

In this section, we propose a solution to the aforementioned problem. First, let us explain a problem in more detail with using AI safety gridworld as illustrated in Figure 3

More formally, we consider learning an intelligent agent to maximize its reward through an interaction between the environment (AI safety gridworld) and an intelligent agent. It is a Markov Decision Process (MDP), which is defined as a tuple $\langle S, A, P, R\rangle$, where S is the set of states, A is the set of actions, $P : S \times A \times S \longrightarrow [0, 1]$ is the transition probability function, $R : S \times A \times S \longrightarrow R$ is the reward function with $R \subset \mathbb{R}$. An agent selects an action $a_t \sim \pi(\bullet|s_t)$, where $\pi : S \times A \longrightarrow [0, 1]$ is a stochastic policy and obtains a state $s_t \in S$. Repetitive doing those actions makes a sequence of transitions between states $s_t \sim (P \bullet |s_t, a_t)$ with specific probabilities and receiving a sequence of rewards $r_{t+1} = R(s_t, a_t, s_{t+1})$. It is obvious that the very reasonable policy for the agent is to maximize its sum of rewards. Still, it is clear some actions can lead to receiving a

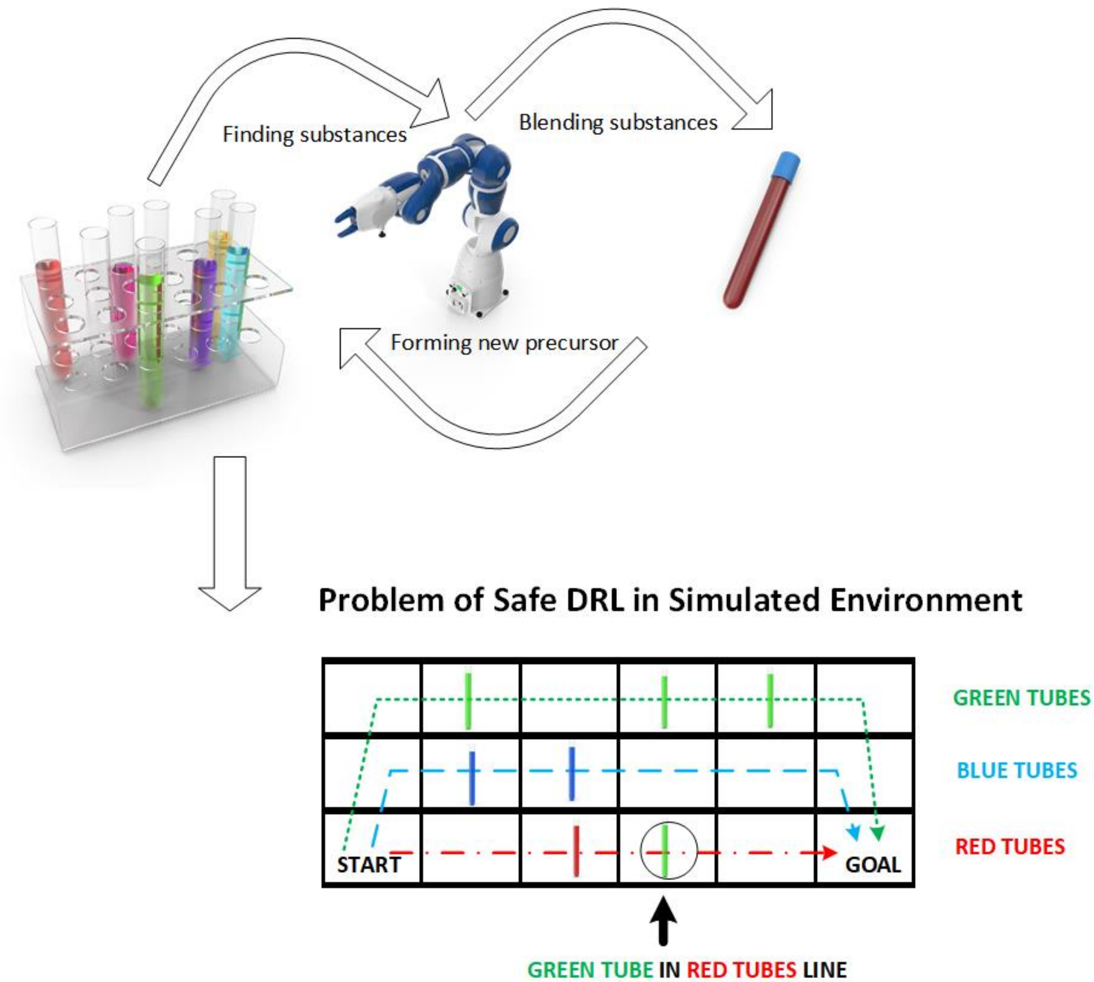

Figure 2: Origins of Safe DRL Problem in the Simulated Environment

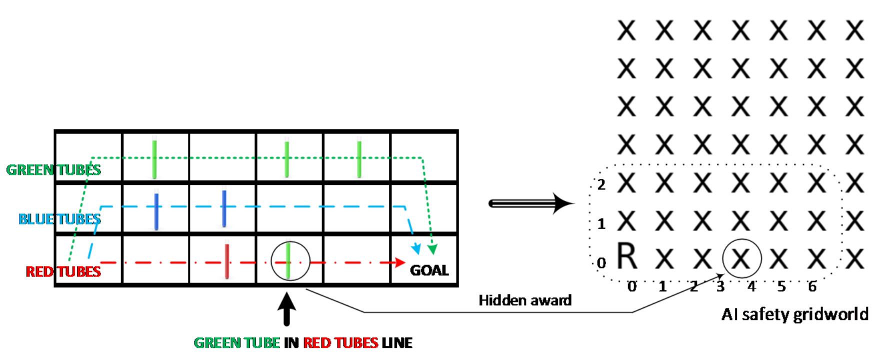

Figure 3: Representation of the Problem in AI Safety Gridworld

negative reward which reduces the total reward sum when an agent reaches the goal. Safe approaches to DRL suggest compliance with safety restrictions. Usually, these are safe optimization and safe exploration. The former accommodates various approaches to risk measurement when an intelligent agent acts unsafely. The latter approaches are about changing the policy of an intelligent agent when it meets unsafe conditions. We propose a quite simple model of an intuitive approach that consists of learning the position where some kind of a "hidden reward" is located. It is obvious the finishing goal for the agent must not be changed and reached, but the agent in the exploration process learns the heatmap of the neighborhood where the "hidden reward" can be found. We suppose the "hidden reward" can help to associate the position on the AI gridworld with some kind of unsafe object depending on the researcher's aims. In SDL it can be the avoiding of picking the unwanted tube with a substance, as has been demonstrated earlier. In our approach, the agent learns a position of hidden reward and receives a significant positive reward when this position has been investigated. The indication when the neighborhood of hidden reward has been explored is the reducing the number of steps the agent to reach the hidden reward position.

Practically, the implementation of the proposed approach is based on the famous DeepMind implementation of AI safety gridworld (see https://github.com/deepmind/ai-safety-gridworlds), but we have realized several differences as is shown further. The main procedures are 1) designing of the custom simulated environment; 2) defining a set of required parameters for this custom environment, such as a structure of this gridworld, a set of possible actions, reward function for conventional exploring process, etc.; 3) creating a shape for a custom observation space which means a neighborhood for hidden reward and a set of structures and procedures for hidden reward accounting when it has been found on some position belonging that shape; 4) programming the set of procedures to store, render and visualize a neighborhood (a kind of heatmap) of hidden reward.

The same as AI safety gridworlds we have designed a custom simulated gridworld for MDP process. The program has been implemented with Python 3.8.10 language and program libraries using the JetBrains PyCharm IDE. The action space for an intelligent agent consists of four actions {Left, Right, Up, Down}. The agent can move according to these actions on our custom gridworld and each cell of this gridworld is enumerated from left-bottom cell 0,0. For the visualization, we have chosen a gridworld size 7*7, as is shown in Figure 4. Each cell of gridworld is marked by "X' sign and the intelligent agent starts acting from position 0,0 and is marked with "R" sign. The exploitation strategy for the intelligent agent is not novel or unique in our case, but one cell contains a hidden reward. Technically it means the initial position of the hidden reward is manually assigned to one cell of the custom gridworld, but this position is not known to the program agent, and it strives to find this reward without forgetting to reach the end goal. In other words, it means when the hidden reward probably has been detected, the intelligent agent does not end its actions and does not terminate the process of reaching the finish. Instead, the intelligent agent tries to outline the region on the gridworld when the hidden reward can probably be located.

For this purpose, the shape of observation space and required class and procedure have been programmed. When the intelligent agent does some action, it causes the receiving some amount of the reward. Transition to the cell containing the hidden reward cause a significant amount of the reward. In our program, the conventional reward is no more than 1 for the regular cell and 10 for the cell with the hidden reward. The observation space has triggers that store the distance from the cell with the hidden reward. The observation space contains a dictionary with estimators of how far the current position of the intelligent agent is away from the cell with the hidden reward. Due to this, the intelligent agent acting in our simulated gridworld environment learns the strategy to get around the cell from all sides rather than reach this cell and stay in this position.

An example in Figure 4 demonstrated the part of the actions sequence, which is usually up to 100 and above. At the bottom of each tile, there is a title with the last action, a number of the step, and the received cumulative reward. For example, the left-upper tile indicates the move was to the right, the step was number 2, and the received reward was -0.1. It should be noted we made the program implementation to assign negative rewards to avoid the situation the intelligent agent is learning on the positive samples only.

Figure 4 shows several next movements of the intelligent agent in the other tiles. The right side of Figure 4 contains the heatmap, which is constructed according to that actions and received rewards. After looking at the numbers in this heatmap, we can make an inference about the probable position of the cell with the hidden reward. This is the cell with positions 2,2, having a number 40 inside it. Further, we can assign that cell the rules that allow us to avoid unsafe conditions.

5 CONCLUSION

This paper has been motivated by several contradictory problems. The first one is a need to accelerat**e** the nanomaterials research and chemical experimenting with AI supporting approaches and AI-driven SDL. However, the simple transforming wide known machine learning methods, including DRL especially, can bring many problems also. Among these problems is AI safety assurance. Inappropriate use of it is attracted not only benefits but may cause damage to equipment and financial issues. The second controversial problem is the attractiveness of using unsupervised learning for AI agents, for example, using DRL. As a simple example of the use of the safe AI principles in SDL we have implemented the problem of learning the intelligent agent to avoid unsafe conditions. We rely on the idea that artificial intelligent agents can be learned to perform safe restrictions in unknown environments. Implementation of the hidden reward approach shows the rationality of that novel approach.

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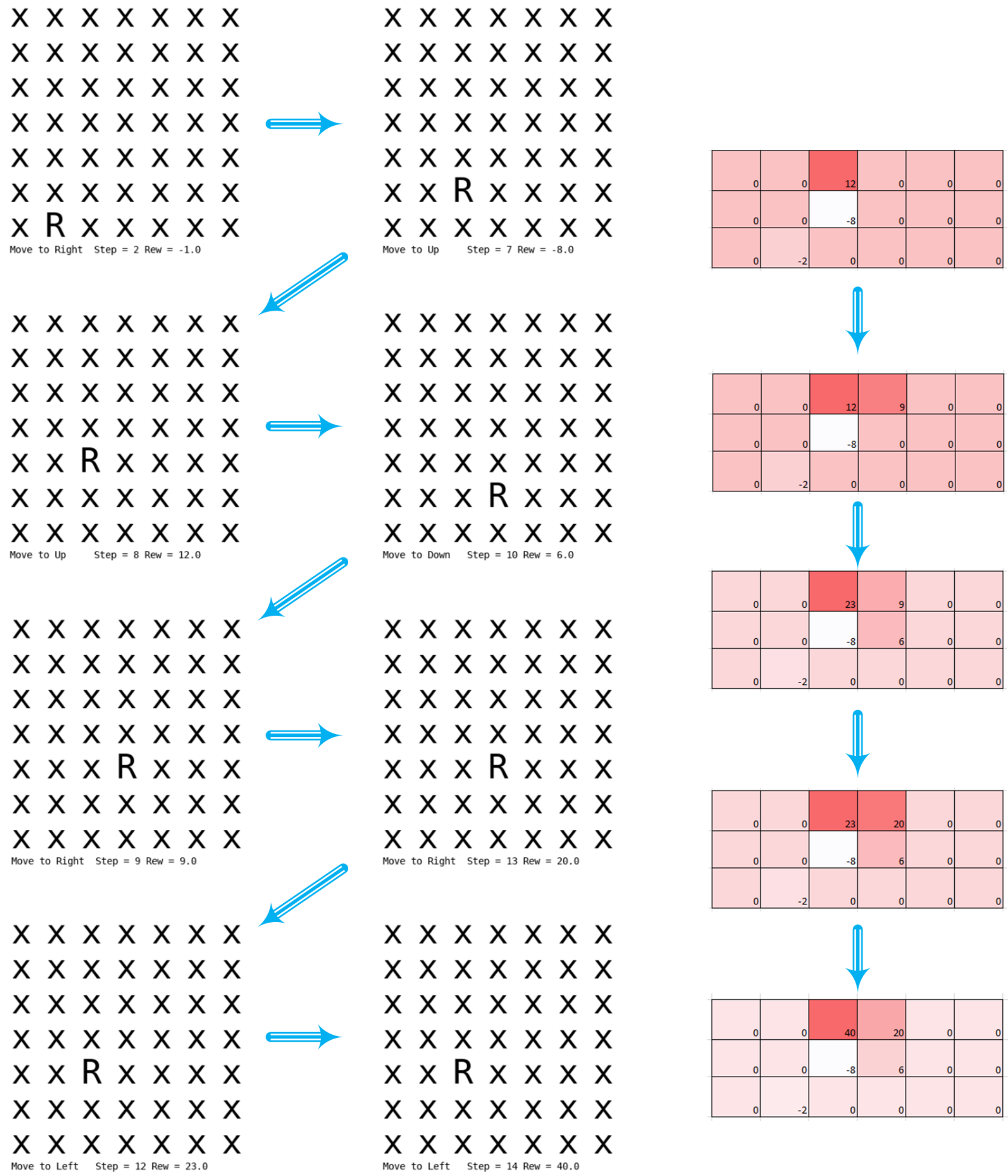

Figure 4: An Example of Finding a Hidden Reward by the Agent with the Heatmap Using

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