Synthesizing Chemical Plant Operation Procedures using Knowledge, Dynamic Simulation and Deep Reinforcement Learning

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Abstract: Chemical plants are complex and dynamical systems consisting of many components for manipulation and sensing, whose state transitions depend on various factors such as time, disturbance, and operation procedures. For the purpose of supporting human operators of chemical plants, we are developing an AI system that can semi-automatically synthesize operation procedures for efficient and stable operation. Our system can provide not only appropriate operation procedures but also reasons why the procedures are considered to be valid. This is achieved by integrating automated reasoning and deep reinforcement learning technologies with a chemical plant simulator and external knowledge. Our preliminary experimental results demonstrate that it can synthesize a procedure that achieves a much faster recovery from a malfunction compared to standard PID control.

Keywords: Process Optimization, Dynamic Simulation, Automated Reasoning, Deep Reinforcement Learning

1. INTRODUCTION

Chemical plants are complex and dynamical systems consisting of many components for manipulation and sensing. Operation of chemical plants is thus not straightforward and requires skilled and experienced operators. Such operators are, however, rapidly retiring in the aging population of Japan, and the industry is likely to face a serious shortage of experienced and skilled operators in the near future.

To tackle this problem, we develop an artificial intelligence (AI) system that can assist human operators of chemical plants. More specifically, our AI system is designed to suggest appropriate operation procedures to human operators and present reasons why those procedures are considered to be appropriate. The ability of explaining the reasoning process of AI is especially important since human operators would not adopt a suggested operation procedure unless they are convinced with its validity.

Our system is based on simulation models for chemical plants and the combination of deep learning and reinforcement learning, which is often called deep reinforcement learning and has recently been applied to control problems in various domains such as robotics \cite{1}. Although deep reinforcement learning has proven successful in many control problems, finding appropriate operation procedures for chemical plants is a highly challenging problem due to the vast search space of possible operation procedures that result from many continuous control variables in plant simulation models. To narrow down the search space, our system uses qualitative knowledge derived from manuals and focus only on promising operation procedures.

Our approach differs from previous work on automatic synthesis of operation procedures in some significant ways. While the models used in previous studies \cite{2,3} are functional or qualitative, our system employs a quantitative and dynamic model for simulation and thus can produce precise procedures with numerical control values. Quantitative and dynamic simulation models have been used for the purpose of training human operators \cite{4}, but not for the purpose of finding appropriate operation procedures. Numerical approaches based on model predictive control (MPC) could be used to find quantitative operation procedures \cite{4}, but MPC requires the model to be differentiable and is not as flexible as deep reinforcement learning in terms of problem formulation.

In this paper, we use a simple model and a malfunction scenario shown in Fig. 1 to evaluate the effectiveness of our approach. Our system computes possible operation procedures for a raw material feed section of a vinyl acetate monomer (VAM) plant to recover from a malfunction of feed pressure. Our preliminary experiments demonstrate that it can synthesize a procedure that

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achieves a much faster recovery from a malfunction compared to standard PID control.

2. BACKGROUNDS

2.1. Classical planning

Classical planning is a field of AI that studies how to explore action sequences from one state to another based on a discrete state representation and a discrete action (state transition rule) set. Classical planning techniques can derive a sequence of elements to be manipulated using qualitative behavioral models of a plant and has been applied to operation procedure synthesis for chemical plants [5].

2.2. Reinforcement learning

Reinforcement learning is a branch of machine learning that studies how an agent can acquire action sequences which maximize the total reward given by an environment. Unlike classical planning, reinforcement learning covers continuous control problems, and has been applied to the problem of optimizing parameters of PID controllers [6].

In order to deal with complex problems where no hand-engineered input features are available, Deep Q-Networks (DQNs) [7] combine deep learning and reinforcement learning and achieved higher performance than humans in the domain of video games. In reinforcement learning, deep neural networks are often used as function approximators for policy and value functions of the agent. However, the high representation power of deep neural networks often results in unstable performance due to its drastic changes in behavior while updating parameters. Proximal Policy Optimization (PPO) [8] is a relatively recent deep reinforcement learning algorithm and has outperformed other state-of-the-art algorithms on a virtual robot control problem on physical simulators by introducing constraints for the amount of parameter changes on each update to avoid the instability problem.

2.3. Dynamic simulation

Dynamic simulation is used for reproducing behavior and responses of a dynamical system based on physical models. It has been applied for the purpose of training operators [4] and optimizing operation procedures of industrial process plants [9]. The VAM plant model [10, 11] is one of those simulation environments.

2.4. Procedure synthesis

Automatic synthesis of operation procedures is a challenging theme of plant control and has long been studied [2]. A recent study [3] uses a qualitative functional model based on Multilevel Flow Modeling (MFM) for a plant and derives procedures for leading a plant to a desired state by tracing back the influence propagation rules between plant elements such as valves and pipes. Since this type of method focuses on discrete qualitative models, it cannot deal with continuous manipulation values of each operation element and optimize them.

3. PROPOSED SYSTEM

We develop an AI system that can automatically synthesize operation procedures for chemical plants. It is designed to assist human operators who are working to get the plant to recover from an undesirable (malfunction) situation. Our system uses both qualitative and quantitative (dynamic simulation) models of a plant and outputs operation procedures including actual manipulation values that results from automatic exploration of maximizing specified objective functions (rewards). The system also outputs explanations about the validity of the procedures that are human-understandable.

Figure 2 shows the block diagram of our system. It consists of three modules, namely, the dynamic simulator of a plant, the automated planner and the reinforcement learning agent. The planner explores operation sequences and the agent explores the amount of manipulation on each step of the sequence by interacting with the simulator. The detailed process flow is as follows:

1. The users of the system first prepare a knowledge base (qualitative models) of the target plant and provide it to the automated planner. Table 1 describes an example of the knowledge. Users also set the malfunction scenario to configure the undesirable state on the dynamic simulator, and design the objective function to be satisfied by the output procedure as the rewards of reinforcement learning.

2. The dynamic simulator reproduces the undesired state according to the scenario.

3. Given the observed undesirable state on the simulator, the automated planner synthesizes operation sequences, i.e. which component to manipulate in what order. The planner also outputs an explanation as to why the sequence is valid. The explanation consists of a reasoning process, utilized knowledge and the corresponding parts...
of the reference documents.

4. The reinforcement learning agent hypothesizes an operation procedure, tries it on the simulator and receives sensor values as its response. The agent considers a plan to be better if it yields greater rewards calculated from observed sensor values. The agent repeats this exploration many times until a certain termination condition, e.g. a threshold of cumulative reward, is met.

5. The human plant operator decides whether to adopt the procedure output by the system or not according to the explanation of its validity.

This method utilizes knowledge not only for composing the explanation but also for narrowing the space of possible procedures in order to explore them in a practical computational time.

At the time of this writing, the reinforcement learning agent connected to the dynamic simulator automatically explores operation procedures. However, the module for automated planning is manually emulated.

4. PRELIMINARY EXPERIMENTS

We conducted preliminary experiments to evaluate the efficiency of the synthesized procedures for a recovery from a malfunction.

We used the VAM plant model [10, 11] as the dynamic simulator. The materials used by a VAM plant are acetic acid, ethylene and oxygen. They are processed through eight sections: (1) a raw material feed, (2) a reactor, (3) a separator and a compressor, (4) an absorber, (5) a CO2 remover and a purge line, (6) a buffer tank, (7) a distillation column, and (8) a decanter. There are recycling systems of ethylene and acetic acid, and the behavior of the plant is dynamic and complex. The model has 36 malfunction scenarios, and they can reproduce unsteady states caused by disturbances or process failures such as feed composition change, heavy rain and failure of pumps.

We used the malfunction scenario, “MAL03 Change C2H4 Feed Pressure” (raw material ethylene (C2H4) feed pressure change, hereinafter called MAL03) available on the plant model. MAL03 mainly affects the raw material feed section on the plant. Figure 1 shows the related components of the section. The PID controller, which monitors the pressure of the vaporizer, controls the flow volume of the fresh ethylene by adjusting the control valve. In this malfunction scenario, the goal is to maintain the pressure of the vaporizer while the feed pressure of the fresh ethylene changes. The occurrence of the malfunction can be detected by observing the flowmeter attached on the fresh ethylene feed pipe. By manual reasoning based on the plant knowledge base and the qualitative observations, we specified one target element for manipulation, which is the set point value (SV) of the PID controller.

In the following experiments, the reinforcement learning agent observes real-valued seven dimensional vector of the sensor values around the section and acts to decide the continuous scalar value of the SV at each time step.

4.1. Simple malfunction

We compared the output procedure to standard PID control with respect to the time required for recovery from malfunction.

The parameters of MAL03 are fixed through this experiment and the change in the ethylene feed pressure (increase to 120%) caused by the malfunction occurs as a step function. The objective for the agent to minimize is the difference between the value of the sensor on each time and that of a normal state. We translated this into the reward function as \( \max(0, 1 - \alpha |s_t - \sigma|) \) where \( \alpha \) is a constant scale factor (we set it to 50 in this experiment), \( s_t \) is the value of the sensor at time \( t \) and \( \sigma \) is the value of the normal state. An episode (each procedure trial) consists of a 30-minutes simulation and actions executed on every one minute. The agent receives a reward after each action. Thus, the cumulative reward would be 30 if the plant kept steady during the whole episode, i.e. if \( s_t = \sigma \) for all \( t \). We employed PPO as the reinforcement learning agent.

Figure 3 shows the cumulative rewards that the agent received while the learning progresses. The thick black line located at the bottom indicates the cumulative reward value of standard PID control. This graph shows that the cumulative reward the agent achieved after learning is much higher than in the case of standard PID control.

Figure 4 shows the graphs of the target sensor value (pressure of the vaporator) on the simulator. The straight horizontal line (the value of 0.784) indicates the value of the normal state. While the dashed line which indicates the response of the standard PID controller does not achieve the steady state in the 30-minute simulation, the proposed procedure quickly recovers from the unsteady state in a few minutes. In other words, the agent successfully acquired a procedure that enables a faster recovery.
4.2. Variable malfunction

We also evaluated the response ability of PPO in more complicated settings. Figure 5 shows the set of parameters on MAL03 which occurs as a ramp function. In this case, there are three parameters, namely, the amount of difference from steady-state value, the period to complete the malfunction and the period to start procedure (depicted as thick arrows on the figure). To make MAL03 more complicated, we randomized the malfunction parameters for each episode. The ranges of each parameter uniformly sampled from are as follows:
- the amount of difference: from 90% to 120%,
- the period to complete: 0 min. to 30 min.,
- the period to start procedure: 0 min. to 60 min.

Other settings are almost the same as the simple case (simulate for 30 minutes). We also used PPO as the agent.

Figure 6 shows the cumulative reward during the training of the agent. The bold line indicates the moving average of 20 episodes. The reward value tends to increase along with the number of episodes. This suggests that PPO allows the agent to learn procedures for dynamic and complex ramp-wise disturbance which is not well suited for MPC since it assumes step-wise changes.

5. CONCLUSION

We have introduced an AI system for synthesizing plant operation procedures, which we are developing for assisting human plant operators. The inputs of the system are plant knowledge, a scenario for leading the plant to an undesirable state, and an objective function. It outputs operation procedures including detailed manipulation values and explanations of the validity of the procedure that are understandable to human operators. We have verified the efficiency of the output procedure by preliminary experiments. We plan to evaluate the optimality of the output procedure and the utility of explanation in collaboration with plant operators as the next step of this work.

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