Dynamic penalty function approach for constraints handling in reinforcement learning

Haeun Yoo∗ Victor M. Zavala∗∗ Jay H. Lee∗

∗ Department of Biomolecular and Chemical Engineering, Korea Advanced Institute of Science and Technology, 291 Daehak-ro, Yusong-gu, Daejeon, 34141, Republic of Korea (e-mail: haeungd, jayhlee@kaist.ac.kr).

∗∗ Department of Chemical and Biological Engineering, University of Wisconsin-Madison, Madison, WI 53706, USA (e-mail: victor.zavala@wisc.edu)

Abstract: Reinforcement learning (RL) is attracting attentions as an effective way to solve sequential optimization problems involving high dimensional state/action space and stochastic uncertainties. Many of such problems involve constraints expressed by inequalities. This study focuses on using RL to solve such constrained optimal control problems. Most of RL application studies have considered inequality constraints as soft constraints by adding penalty terms for violating the constraints to the reward function. However, while training neural networks to represent the value (or Q) function, a key step in RL, one can run into computational issues caused by the sharp change in the function value at the constraint boundary due to the large penalty imposed. This difficulty during training can lead to convergence problems and ultimately poor closed-loop performance. To address this problem, this study suggests the use of a dynamic penalty function which gradually and systematically increases the penalty factor during training as the iteration episodes proceed. First, we examined the ability of a neural network to represent an artificial value function when uniform, linear, or dynamic penalty functions are added to prevent constraint violation. The agent trained by a Deep Q Network (DQN) algorithm with the dynamic penalty function approach was compared with agents with other constant penalty functions in a simple vehicle control problem. Results show that the dynamic penalty approach can improve the neural network’s approximation accuracy and that brings faster convergence to a solution closer to the optimal solution.

Keywords: Reinforcement learning, Penalty approach, Dynamic penalty

1. INTRODUCTION

Most sequential decision making problems posed for scheduling, planning, and control involve constraints that should be respected, more or less on a strict basis. When the state space system model is available, the optimization problem can be formulated as follows:

$$\min_{\{u(k)\}_{k=0}^T} \sum_{k=0}^T l(x(k), u(k))$$

s.t. $$x(k+1) = f(x(k), u(k))$$

$$g_i(x(k), u(k)) \leq 0, \ i = 1, \ldots, \nu$$

$$x(0) = x_0$$

$$\underline{x} \leq x(k) \leq \overline{x}$$

$$\underline{u} \leq u(k) \leq \overline{u}$$

where $k$ is the index for discrete time, $x \in \mathbb{R}^x$ is the state vector, $u \in \mathbb{R}^u$ is the control input, and $l(x, u)$ is a cost function.

By solving the above problem at each time instant for the given state as the initial state $x_0$ with some mathematical programming algorithm, one can obtain the optimal policy. This is a basic idea behind the popular model predictive control (MPC) method. However, the model inevitably has some mismatch with the real system due to model errors, stochastic disturbances, noise, etc. The basic MPC formalism does not allow one to consider various uncertainties in the optimization, but instead compensates for their effect passively through the state feedback. This can lead to a performance loss including constraint violations. To address this problem, reinforcement learning (RL) has been adopted as an alternative to MPC in the process system engineering field (Yoo et al. (2020); Petsagkourakis et al. (2020)).

An RL agent finds the optimal policy by exploring different parts of the state space through simulations to learn the approximate value of each state. Using the Bellman’s optimality principle, the value estimate can be improved iteratively, with the aim of eventually identifying the optimal value (Bellman (1966)). For this, the system and the problem studied is formalized as a Markov Decision Process (MDP). The MDP formulation is composed of the state space ($S$) and state ($x \in S$), action space ($A$) and
action \( (u \in A) \), the state transition model, and the reward function \( (r : S \times A \rightarrow R) \) (Puterman (2014)). The state transition model is equal to (1b) in this study but can be generalized to specify probabilistic transitions and/or the effect of stochastic noises.

The agent gets a certain reward (or penalty) for each state visited and the summation of the discounted (with a discount factor of \( \gamma \in [0, 1] \)) rewards from current state to the terminal state \( \sum_{k=t}^{T} \gamma^{k-t} r(x(k)) \) is the value of the state. The value function, \( V(x) \), is the function that maps the state to the expectation of the return value, which implies the long-term “value” of the state, and Q-function, \( Q(x, a) \), is the expectation return value of an state and action pair. In the MDP formulation, the action limits of (1f) can always be satisfied by considering only the feasible actions. Meanwhile, the state bounds of (1e) and state/input constraints (1c) cannot be asked to be satisfied in a strict sense as this may cause infeasibilities. Hence, they are instead considered as soft constraints, of which violations are penalized with terms added to the reward function along with the original objective function (1a).

The form of penalty function can be a uniform constant as shown in Yang et al. (2020); Zhang et al. (2020), a linear (1-norm) function of the magnitude of the violation as shown in Ma et al. (2019), or a logistic function as shown in Pan et al. (2020); Modares et al. (2016). The penalty is typically chosen to be large in order to prevent constraint violation. On the other hand, an infinite penalty as is done in the barrier method for solving constrained optimization can lead infeasibilities so cannot be used. When we use a high uniform penalty value or a steep linear penalty function, the training of neural network (NN), a popular choice for the value (or Q) function approximator in RL, can give convergence problems as will be demonstrated in this paper with a simple example. On the other hand, a small penalty term can lead to unnecessary constraint violations, even when the constraint can be satisfied. A penalty function which strikes a right balance is needed, but this is not easy to decide a priori.

In this study, we suggest an approach to systematically vary the penalty function during the training process while applying a reinforcement learning method. This approach updates the penalty factor as the training proceeds, in order to achieve fast convergence in the value function approximator and achieve a stable training result with less approximation error. A similar dynamic penalty approach has been studied to update parameters during iterations in the evolutionary optimization strategies (Kramer (2010); Joines and Houck (1994)). Also, Lin and Zheng (2012) suggested to gradually increase the penalty value in the RL based control to address the numerical difficulty approximating a steep function, but they did not give any detailed procedure or systematically analyze the effect of varying the penalty parameter.

The following section describes the dynamic penalty function design with constraints aggregation using the Kreisselmeier-Steinhauser (KS) function and penalty factor update rules. In Section 3, we use a simple 1-dimensional function approximation example to examine the regression accuracy achieved with several penalty functions including the dynamic penalty function. In Section 4, the proposed dynamic penalty function will be tested on a simple vehicle control example and the results are summarized. Section 5 summarizes and concludes the paper.

2. DYNAMIC PENALTY FUNCTION

In this section, the constraint aggregation method is used to design an unbiased penalty for constraint violations. A systematic rule for updating the penalty factor is described for an application to any RL algorithm.

2.1 Constraints aggregation

Let us assume that we have \( v \) inequality constraints including the inequality constraints on the state space boundary. The RL agent gets a penalty value for each constraint violation. A constraint aggregation is needed for an unbiased constraint handling by preventing the imposed penalty overlapped in some parts of infeasible region. The KS function is a widely used constraint aggregation method for gradient-based optimization (Kreisselmeier and Steinhauser (1980)). Although RL is not a gradient-based optimization algorithm, we can effectively use this method with a high aggregation parameter, \( p \), making the error from the aggregation as small as possible (Poon and Martins (2007)). For the constraints, \( g_i(x,u) \leq 0, i = 1,...,v \), the aggregated constraint function \( KS[g(x,u)] \) is defined as follows:

\[
KS[g(x,u)] = g_{\text{max}}(x,u) + \frac{1}{p} \ln \left\{ \sum_{i=1}^{v} e^{p[g_i(x,u) - g_{\text{max}}(x,u)]} \right\}.
\]

where \( g_{\text{max}} \) is the maximum of all constraints evaluated at the given state-action pair.

2.2 Dynamic penalty function

Using the KS function, the reward function with dynamic penalty term can be defined as follows:

\[
R(x,u) = l(x,u) + p(x,u)\mu
\]

\[p(x,u) = \mu KS[g(x,u)]\]

\[
KS[g(x,u)] \geq 0
\]

where \( \mu \) is the penalty factor which defines the slope of the penalty function. The dynamic penalty function approach starts with a low value of \( \mu \), which makes facilitates the initial training of the NN, and gradually increases it to a large value so that the slope becomes to prevent constraint violations. Fig. 1 describes the penalty update rule. The procedure can be described as:

1. Set \( \mu := \mu_{\text{min}} \).
2. When the loss value of the NN is less than \((100 - \alpha)\%\) of the maximum loss value after the parameter update, set \( \mu := \epsilon \mu \).
3. Repeat step (2) until \( \mu \geq \mu_{\text{max}} \).
4. After reach \( \mu \geq \mu_{\text{max}} \) set \( \mu := \mu_{\text{max}} \).
5. Continue the training until an optimal policy is found.
3. VALUE FUNCTION REGRESSION TEST

3.1 1-dimensional example

A feed-forward NN is the most widely used function approximator for the value function or Q-function approximation. The agent uses the output value or the gradient of the NN to update the optimal policy. Therefore, accuracy of the approximation is important for a fast and stable agent training. We tested the regression accuracy with a uniform penalty and a linear penalty, which are the popular choices for the penalty function against the proposed dynamically varied penalty function. The arbitrary value function $V(x)$ is defined as follows:

$$V(x) = 1 + \cos(0.5x) + 0.05(x - 1)(x + 2) + p(x).$$ \hfill (4)

We assumed that this problem has inequality constraints in state boundary as $-5 \leq x \leq 5$ and the penalty functions are assigned as in table 1 where the $\mu_{\min} = 0.1$, $\mu_{\max} = 50$ and $c = 2$. This arbitrary value function is not exactly same form as the value function in the optimal control problem where the value should be calculated with the cumulative rewards, but this analysis might be useful to understand the tendency of the NN approximation during the agent training with the different penalty terms.

Table 1. Parameters for the penalty function

| Penalty function | $p(x)$ |
|------------------|--------|
| Uniform penalty  | $50 \cdot 1_{x < -5, x > 5}$ |
| Linear penalty   | $50(5 - x)1_{x < -5} + (x - 5)1_{x > 5}$ |
| Dynamic penalty  | $\mu(5 - x)1_{x < -5} + (x - 5)1_{x > 5}$ |

To examine the NN training performance within an RL environment, the training environment is set similarly as in RL. In every episode, 20 $x$ points are randomly sampled from -10 to 10 and the environment calculates the $R(x)$ value ($R(x) = l(x) + p(x)$) with the assigned objective function (??) and the penalty function (table 1). Then, 20 samples are stored in a replay buffer and the NN was trained with a batch of 64 data randomly sampled from the replay buffer up to 500 episodes.

3.2 Results

Fig. 2 shows the output value of the NN during the training process. As shown in Fig. 2a, the NN approximation performance is poor at the boundary points which causes a bias in the estimate inside the feasible region. The linear penalty case also gives a biased estimate inside the feasible region during the training and the maximum loss function is much higher than that of the dynamic penalty case, as shown in Fig. 3. With the proposed scheme of dynamically varying the penalty, the function is well approximated near the constraint boundary which can reduce the bias and loss. Fig. 3 shows that the loss of NN with the dynamic penalty function approach is increased during the penalty factor update period but is decreased drastically afterward. The final loss is the lowest for the case of dynamic penalty, which implies the best approximation performance. From this simple test, we see the potential advantage of using a dynamically varied penalty in training the NN to learn the value function with a large penalty function.

4. CASE STUDY

4.1 Simple vehicle control example

To examine the effectiveness of the dynamic penalty approach further, a simple vehicle control problem described in (5) is solved with RL. We modified the problem from Gr¨une and Pannek (2017) to reduce the size of the feasible region and make the starting point uncertain as (5f). The objective is to minimize the running cost (5a). $x_1(k)$ is the position of a vehicle at time $k$, $x_2(k)$ is its velocity and $u(k)$ is its acceleration.

$$\min l(x, u) = x_1^2 + u^2$$ \hfill (5a)

s.t. \quad \begin{align*}
\dot{x}_1(k) &= x_2(k) \\
\dot{x}_2(k) &= u(k) \\
-1 &\leq x_1(k) \leq 1 \\
-0.25 &\leq x_2(k) \leq 1 \\
-0.25 &\leq u(k) \leq 0.25 \\
x_0 &\sim U((-1, -0.25), (1, 1))
\end{align*} \hfill (5f)

We applied the Deep-Q-Network (DQN) algorithm which uses a deep NN to approximate the Q-function and chooses the $\epsilon$-greedy policy (Mnih et al. (2013)). For the training, we defined the discrete action space to $u \in \{-0.25, -0.2375, -0.225, ... , 0.2375, 0.25\}$ and one episode was set for a time duration of 20min with 1min control interval. The deep NN consisted of three hidden layers with 64 nodes of the ReLU activation function.

For the constraint aggregation, (5c) and (5d) are decomposed as shown in (6) and aggregated to a $KS[g]$ function with (2) setting $\rho = 50$.

$$\begin{align*}
g_1 : &\quad 1 - x_1 \leq 0 \\
g_2 : &\quad x_1 - x \leq 0 \\
g_3 : &\quad -0.25 - x_2 \leq 0 \\
g_4 : &\quad x_2 - 1 \leq 0
\end{align*}$$ \hfill (6)

The dynamic penalty was updated when the loss became lower than 40% of the maximum loss ($\alpha = 60$) and the penalty factor was doubled in each update ($c = 2$), starting from $\mu_{\min} = 0.05$ to $\mu_{\max} = 20$. The value for the uniform penalty function and the penalty factor for the linear penalty were both set to 20 as shown in table 2. The training comprised 2000 episodes and the initial point was
randomly selected inside the feasible region to start each episode. For a rigorous comparison, we trained 100 agents set in the environment set with 100 different random seeds, which introduced randomness to exploration, NN initialization, buffer sampling, etc.

Table 2. Penalty function

| Penalty function   | \( p(x) \)                                                   |
|--------------------|-------------------------------------------------------------|
| Uniform penalty    | \( 20 \cdot 1_{K_S(g)>0} \)                                 |
| Linear penalty     | \( 20 \cdot K_S(g) \cdot 1_{K_S(g)>0} \)                   |
| Dynamic penalty    | \( \mu \cdot K_S(g) \cdot 1_{K_S(g)>0} \)                  |

4.2 Results

To test the agent’s behavior in finding a sufficient feasible policy quickly after a small number of episodes, we tested the policy after every 100 episodes without exploration. Here, ‘sufficient feasible policy’ means that the policy does not violate all the constraints and still achieves a sufficient low cost value (\( \sum_t l(x,u) \leq 4.0 \)).

Table 3 shows that the agents trained with the uniform penalty and the linear penalty only could find sufficiently feasible policies for 8 and 5 cases among the 100 random cases, respectively. The agent trained with the uniform penalty incurred the highest average cost. This is likely due to the interference of a bias in the estimate inside the feasible region. The agent trained with the linear penalty function performed poorly due to having inaccurate approximate values for the value function during training. This consequently resulted in the policy being updated in a wrong direction, or converging to sub-optimal policies.

The use of dynamic penalty approach was effective to find sufficient feasible policy stably and rapidly. The agent trained with the dynamic penalty approach could find sufficient feasible policies for 28 cases and the average cost of those cases was lower than the results of the agent trained with other penalty functions. Table 4 also shows that more than 50% of the 28 successive cases could be founded within 1500 episodes with the dynamic penalty approach.

Table 3. Agent training results

| Penalty function   | Finding sufficient feasible policy/100 | Average cost of the sufficient policy |
|--------------------|----------------------------------------|---------------------------------------|
| Uniform penalty    | 8                                      | 3.7627                                |
| Linear penalty     | 5                                      | 3.2835                                |
| Dynamic penalty    | 28                                     | 3.1988                                |

Table 4. Finding sufficient feasible policy until each episodes

| Penalty function   | 500  | 1000 | 1500 | 2000 |
|--------------------|------|------|------|------|
| Uniform penalty    | 0    | 0    | 4    | 8    |
| Linear penalty     | 0    | 0    | 0    | 5    |
| Dynamic penalty    | 0    | 1    | 16   | 28   |

5. CONCLUSION

To solve constrained optimal control problems with RL, the inequality constraints imposed on the state should be translated into a penalty term in the reward function. However, when the agent is trained with a large uniform or linear penalty function in order to prevent unnecessary constraint violation, inaccurate neural network approximations can lead to convergence problems and bad eventual performance. To address this problem, this study suggested an approach that varies the penalty function dynamically during training to gradually increase the penalty so that NNs can be trained stably and rapidly. First, we examined the deep NN’s regression performance with the uniform, linear and dynamic penalty functions for a simple 1-dimensional function. The results showed that using the dynamic penalty approach can reduce the approximation loss not only during the training but also at the end of the training. The dynamic penalty approach was effective in the simple vehicle control problem tested.
We trained the agent with different penalty forms and the dynamic penalty case showed the best performance in finding sufficient feasible policies with lowest average cost and in fewer episodes. The proposed approach can be simply applied to any RL algorithm and can help the agent that uses NN as a function approximator to be trained to represent a function including a steep penalty term for constraint violation in a stable and efficient manner.

ACKNOWLEDGEMENTS

This research was supported by Korea Institute for Advancement of Technology(KIAT) grant funded by the Korea Government(MOTIE)(P0008475, The Competency Development Program for Industry Specialist).

REFERENCES

Bellman, R. (1966). Dynamic programming. Science, 153(3731), 34–37.
Grüne, L. and Pannek, J. (2017). Nonlinear model predictive control. In Nonlinear Model Predictive Control, 45–69. Springer.
Joines, J.A. and Houck, C.R. (1994). On the use of non-stationary penalty functions to solve nonlinear constrained optimization problems with ga’s. In Proceedings of the first IEEE conference on evolutionary computation. IEEE world congress on computational intelligence, 579–584. IEEE.
Kramer, O. (2010). A review of constraint-handling techniques for evolution strategies. Applied Computational Intelligence and Soft Computing, 2010.
Kreisselmeier, G. and Steinhauser, R. (1980). Systematic control design by optimizing a vector performance index. In Computer aided design of control systems, 113–117. Elsevier.
Lin, W.S. and Zheng, C.H. (2012). Constrained adaptive optimal control using a reinforcement learning agent. Automatica, 48(10), 2614–2619.
Ma, Y., Zhu, W., Benton, M.G., and Romagnoli, J. (2019). Continuous control of a polymerization system with deep reinforcement learning. Journal of Process Control, 75, 40–47.
Mnih, V., Kavukcuoglu, K., Silver, D., Graves, A., Antonoglou, I., Wierstra, D., and Riedmiller, M. (2013). Playing atari with deep reinforcement learning. arXiv preprint arXiv:1312.5602.
Modares, H., Nagashrao, S.P., Lopes, G.A.D., Babuška, R., and Lewis, F.L. (2016). Optimal model-free output synchronization of heterogeneous systems using off-policy reinforcement learning. Automatica, 71, 334–341.
Pan, A., Xu, W., Wang, L., and Ren, H. (2020). Additional planning with multiple objectives for reinforcement learning. Knowledge-Based Systems, 193, 105392.
Petsagkourakis, P., Sandoval, I.O., Bradford, E., Zhang, D., and del Río-Chanona, E.A. (2020). Reinforcement learning for batch bioprocess optimization. Computers & Chemical Engineering, 133, 106649.
Poon, N.M. and Martins, J.R. (2007). An adaptive approach to constraint aggregation using adjoint sensitivity analysis. Structural and Multidisciplinary Optimization, 34(1), 61–73.
Puterman, M.L. (2014). Markov decision processes: discrete stochastic dynamic programming. John Wiley & Sons.
Yang, T., Zhao, L., Li, W., and Zomaya, A.Y. (2020). Reinforcement learning in sustainable energy and electric systems: A survey. Annual Reviews in Control.
Yoo, H., Kim, B., Kim, J.W., and Lee, J.H. (2020). Reinforcement learning based optimal control of batch processes using monte-carlo deep deterministic policy gradient with phase segmentation. Computers & Chemical Engineering, 107133.
Zhang, P., Li, H., Ha, Q., Yin, Z.Y., and Chen, R.P. (2020). Reinforcement learning based optimizer for improvement of predicting tunneling-induced ground responses. Advanced Engineering Informatics, 45, 101097.