Reward Potentials for Planning with Learned Neural Network Transition Models

Buser Say$^{1,2}$*, Scott Sanner$^{1,2}$, Sylvie Thiebaux$^3$

$^1$University of Toronto, Canada
$^2$Vector Institute, Canada
$^3$Australian National University, Australia

*bsay,ssanner}@mie.utoronto.ca
sylvie.thiebaux@anu.edu.au

Abstract

Optimal planning with respect to learned neural network (NN) models in continuous action and state spaces using mixed-integer linear programming (MILP) is a challenging task for branch-and-bound solvers due to the poor linear relaxation of the underlying MILP model. For a given set of features, potential heuristics provide an efficient framework for computing bounds on cost (reward) functions. In this paper, we introduce a finite-time algorithm for computing an optimal potential heuristic for learned NN models. We then strengthen the linear relaxation of the underlying MILP model by introducing constraints to bound the reward function based on the precomputed reward potentials. Experimentally, we show that our algorithm efficiently computes reward potentials for learned NN models, and the overhead of computing reward potentials is justified by the overall strengthening of the underlying MILP model for the task of planning over long-term horizons.

Introduction

In the area of learning and planning, Hybrid Deep MILP Planning (Say et al. 2017) (HD-MILP-Plan) has introduced a two-stage data-driven framework that i) learns transitions models with continuous action and state spaces using NNs, and ii) plans optimally with respect to the learned NNs using a mixed-integer linear programming (MILP) model. It has been experimentally shown that optimal planning with respect to the learned NNs (Say et al. 2017) presents a challenging task for state-of-the-art branch-and-bound (B&B) solvers (IBM 2019) due to the poor linear relaxation of the underlying MILP model that utilize a large number of big-M constraints.

In this paper, we focus on the important problem of improving the effectiveness of the linear relaxation of MILP models for decision making with learned NNs. In order to tackle this challenging problem, we build on potential heuristics (Pomerreening et al. 2015), which provide an efficient STRIPS-based framework for computing a lower bound on the cost of a given state as a function of its features. In this work, we introduce a finite-time constraint generation algorithm for computing an optimal potential heuristic for learned NN models with continuous inputs and outputs (i.e., continuous action and state spaces). Features of our linear potential heuristic are defined over the hidden units of the learned NN model, thus providing a rich and expressive candidate feature space. We use our constraint generation algorithm to compute the potential contribution (i.e., reward potential) of each hidden unit to the reward function of the HD-MILP-Plan problem. The precomputed reward potentials are then used to construct linear constraints that bound the reward function of HD-MILP-Plan, and provide a tighter linear relaxation for B&B optimization.

Experimentally, we show that our constraint generation algorithm efficiently computes reward potentials for learned NNs, and the overhead computation is justified by the overall strengthening of the underlying MILP model for the task of planning over long-term horizons. Overall this work bridges the gap between two seemingly distant literatures – heuristic search and decision making with learned NN models in continuous action and state spaces. Specifically, we show that even data-driven NN models for planning can benefit from advances in heuristics and their impact on the efficiency of search in B&B optimization.

Preliminaries

We briefly review the HD-MILP-Plan framework for optimal planning (Say et al. 2017) with learned NN models as well as potential heuristics (Pomerreening et al. 2015).

Problem Definition

A deterministic factored planning problem is a tuple $\Pi = \langle S, A, C, T, I, G, R \rangle$ where $S$ is a set of state variables with continuous domains, $A$ is a set of action variables with continuous domains, $C : S \times A \rightarrow \{\text{true}, \text{false}\}$ is a function that returns true if action $A$ and state $S$ variables satisfy a set of global constraints, $T : S \times A \rightarrow S$ denotes the stationary transition function, and $R : S \times A \rightarrow \mathbb{R}$ is the reward function. Finally, $I : S \rightarrow \{\text{true}, \text{false}\}$ represents the initial state constraints that assign values to all state variables $S$, and $G : S_G \rightarrow \{\text{true}, \text{false}\}$ represents the goal constraints over the subset of state variables.

---

*This work is done during author’s visit to the Australian National University.
ward function (i.e., reward potential) of each hidden unit circles in Figure 1), and compute the potential contribution $U$ of the learned NN over its set of hidden units in our HD-MILP-Plan compilation. We define the features as the sum of potentials for all the features that are true in the context of cost-optimal Potential Heuristics we turn to potential heuristics that will be used to strengthen the free action $A$ and state variables $S$.

For horizon $H$, a solution $\pi = \langle \bar{A}^1, \ldots, \bar{A}^H \rangle$ to problem II (i.e. a plan for II) is a value assignment to action $A^t$ and state $S^t$ variables such that $T(S^t, \bar{A}^t) = S^{t+1}$ and $C(S^t, \bar{A}^t) = \text{true}$ for time steps $t \in \{1, \ldots, H\}$, and the initial and goal state constraints are satisfied, i.e. $I(S^0) = \text{true}$ and $G(\{s^t | s \in S_T\}) = \text{true}$, respectively. Similarly, an optimal solution to II is a plan that maximizes the total reward function $\sum_{t=1}^{H} R(S^{t+1}, A^t)$. Given the description of the planning problem, we next describe a data-driven framework for planning using learned NNs.

Planning with Neural Network Learned Transition Models

Hybrid Deep MILP Planning (Say et al. 2017) (HD-MILP-Plan) is a two-stage data-driven framework for learning and solving planning problems. Given samples of state transition data, the first stage of the HD-MILP-Plan process learns the transition function $T$ using a NN with Rectified Linear Units (ReLUs) (Nair and Hinton 2010) and linear activation units. In the second stage, the learned transition function $T$ is used to construct the learned planning problem $\Pi = (S, A, C, T, I, G, R)$. As shown in Figure 1, the learned transition function $T$ is sequentially chained over the horizon $t \in \{1, \ldots, H\}$, and compiled into a MILP. Next, we turn to potential heuristics that will be used to strengthen the MILP compilation of HD-MILP-Plan.

Potential Heuristics

Potential heuristics (Pomerening et al. 2015; Seipp et al. 2015) are a family of heuristics that map a set of features to their numerical potentials. In the context of cost-optimal classical planning, the heuristic value of a state is defined as the sum of potentials for all the features that are true in that state. Potential heuristics provide an efficient method for computing a lower bound on the cost of a given state.

In this paper, we introduce an alternative use of potential functions to tighten the linear relaxation of ReLU units in our HD-MILP-Plan compilation. We define the features of the learned NN over its set of hidden units $U$ (i.e., gray circles in Figure 1), and compute the potential contribution (i.e., reward potential) of each hidden unit $w \in U$ to the reward function $R$ for any time step $t$. These reward potentials are then used to introduce additional constraints on ReLU activations that help guide B&B search in HD-MILP-Plan.

Reward Potentials for Learned NNs

In this section, we present the optimal reward potentials problem and an efficient constraint generation framework for computing reward potentials for learned NNs.

Optimal Reward Potentials Problem

The problem of finding the optimal reward potentials over a set of ReLUs $U$ for any time step $t$ can be defined as the following bilevel optimization problem:

$$\begin{align*}
\min_{v_u^{on}, v_u^{off}} \sum_{u \in U} v_u^{on} + v_u^{off} \\
\text{subject to} \sum_{u \in U} v_u^{on} x_u + v_u^{off} (1 - x_u) & \geq R(S^1, A^0) \\
\max_{S^0, S^1, A^0, x_u} R(S^1, A^0) - \sum_{u \in U} v_u^{on} x_u + v_u^{off} (1 - x_u) & \leq v_u^{on} + v_u^{off} (1 - x_u) \\
\text{subject to} \hat{T}(S^0, A^0, \{x_u | u \in U\}) = S^1 \\
C(S^0, A^0) = \text{true}
\end{align*}$$

where auxiliary variable $x_u(S^0, A^0)$ ($x_u$ for short) represents the activation (i.e., $x_u = 1$) or deactivation (i.e., $x_u = 0$) of ReLU $u \in U$ in the learned NN transition model $\tilde{T}$, and continuous variables $v_u^{on}$ and $v_u^{off}$ represent the potentials for ReLU activation and deactivation, respectively. Next, we describe a finite-time constraint generation algorithm for computing reward potentials.

Constraint Generation for Computing Reward Potentials

The optimal reward potentials problem can be solved efficiently through the following constraint generation framework that decomposes the problem into a master problem and a subproblem. The master problem finds the values of ReLU potentials $\bar{v}_u^{on}$ and $\bar{v}_u^{off}$. The subproblem finds the values of ReLU variables $x_u^{\bar{R}_u}$ that violate constraint (2) the most for given $\bar{v}_u^{on}$ and $\bar{v}_u^{off}$, and computes the maximum value of $\bar{R}_u$ for given $x_u^{\bar{R}_u}$.

Subproblem $S$: For a complete value assignment to ReLU potential variables $\bar{v}_u^{on}$ and $\bar{v}_u^{off}$, the subproblem optimizes the violation defined by the rearrangement of expressions in constraint (2) with respect to constraints (4-5) as follows.

$$\begin{align*}
\max_{S^0, S^1, A^0, x_u} & R(S^1, A^0) - \sum_{u \in U} \bar{v}_u^{on} x_u + \bar{v}_u^{off} (1 - x_u) \\
\text{subject to} \hat{T}(S^0, A^0, \{x_u | u \in U\}) = S^1 \\
C(S^0, A^0) = \text{true}
\end{align*}$$
We denote the optimal values of ReLU variables $x_u$, found by solving the subproblem as $\bar{x}_u$, and denote the value of the reward function $R$ found by solving the subproblem as $R^* \left( \{ \bar{x}_u | u \in U \} \right)$. Further, we refer to subproblem as $S$.

**Master problem $M$:** Given the set of complete value assignments $K$ to ReLU variables $\bar{x}_u^k$ and optimal objective values $R^* \left( \{ \bar{x}_u^k | u \in U \} \right)$ for all $k \in K$, the master problem optimizes the regularized $1$ sum of reward potentials (1) with respect to constraint (2) as follows.

$$
\min_{v_{uo}^+, v_{o}^f} \sum_{u \in U} v_{uo}^+ + v_{o}^f + \lambda \sum_{u \in U} (v_{uo}^+)^2 + (v_{o}^f)^2 \tag{9}
$$

subject to

$$
\sum_{u \in U} v_{uo}^+ x_u^k + v_{o}^f (1 - x_u^k) \geq R^* \left( \{ \bar{x}_u^k | u \in U \} \right) \\
\forall k \in K \tag{10}
$$

We denote the optimal values of ReLU potentials $v_{uo}^+$ and $v_{o}^f$, found by solving the master problem as $\bar{v}_{uo}^+$ and $\bar{v}_{o}^f$, respectively. Further, we refer to master problem as $M$.

**Reward Potentials Algorithm:** Given the definitions of the master problem $M$ and the subproblem $S$, the constraint generation algorithm for computing an optimal reward potential is outlined as follows.

**Algorithm 1 Reward Potentials Algorithm**

1: $k \leftarrow 1$, violation $\leftarrow \infty$, $M \leftarrow$ objective function (9)
2: while violation $> 0$ do
3: $\bar{v}_{uo}^+, \bar{v}_{o}^f \leftarrow M$
4: $\bar{x}_u, \bar{A}, \bar{S}, R^* \left( \{ \bar{x}_u^k | u \in U \} \right) \leftarrow S (\bar{v}_{uo}^+, \bar{v}_{o}^f)$
5: violation $\leftarrow R (\bar{S}, \bar{A}) - \sum_{u \in U} \bar{v}_{uo}^+ \bar{x}_u^k + \bar{v}_{o}^f (1 - \bar{x}_u^k)$
6: $M \leftarrow M$
7: $\sum_{u \in U} v_{uo}^+ x_u^k + v_{o}^f (1 - x_u^k) \geq R^* \left( \{ \bar{x}_u^k | u \in U \} \right)$
8: $k \leftarrow k + 1$

Algorithm 1 iteratively computes reward potentials $\bar{v}_{uo}^+$ and $\bar{v}_{o}^f$ (i.e., line 3), and first checks if there exists an activation pattern, that is a complete value assignment to ReLU variables $\bar{x}_u$, that violates constraint (2) (i.e., lines 4 and 5), and then returns the optimal reward value $R^* \left( \{ \bar{x}_u^k | u \in U \} \right)$ for the violating activation pattern. Given the optimal reward value $R^* \left( \{ \bar{x}_u^k | u \in U \} \right)$ for the violating activation pattern, constraint (10) is updated (i.e., lines 6-7). Since there are finite number of activation patterns and solving $\bar{S}$ gives the maximum value of $R^* \left( \{ \bar{x}_u^k | u \in U \} \right)$ for each pattern $k \in \{1, \ldots, K\}$, the Reward Potentials Algorithm 1 terminates in at most $k \leq 2^{U/2}$ iterations with an optimal reward potential for the learned NN.

**Increasing the Granularity of the Reward Potentials Algorithm:** The feature space of Algorithm 1 can be enhanced to include information on each ReLUs input and/or output. Instead of computing reward potentials for only the activation $\bar{v}_{uo}^+$ and deactivation $\bar{v}_{o}^f$ of ReLU $u \in U$, we (i) introduce an interval parameter $N$ to split the output range of each ReLU $u$ into $N$ equal size intervals, (ii) introduce auxiliary Boolean decision variables $y_{u,n}$ to represent the activation interval of ReLU $u$ such that $y_{u,n} = 1$ if and only if the output of ReLU $u$ is within interval $i \in \{1, \ldots, N\}$, and $y_{u,n} = 0$ otherwise, and (iii) compute reward potentials for each activation interval $\bar{v}_{uo}^+, \ldots, \bar{v}_{uo}^N$ and deactivation $\bar{v}_{o}^f$ of ReLU $u \in U$.

**Strengthening HD-MILP-Plan**

Given optimal reward potentials $\bar{v}_{uo}^+, \ldots, \bar{v}_{uo}^N$ and $\bar{v}_{o}^f$, the MILP compilation of HD-MILP-Plan is strengthened through the addition of following constraint:

$$
\sum_{u \in U} \sum_{i=1}^{N} v_{uo}^+ y_{u,i} + v_{o}^f (1 - y_{u,i}) \geq R(S^{t+1}, A^t) \tag{11}
$$

for all time steps $t \in \{1, \ldots, H\}$. Next, we present our experimental results to demonstrate the efficiency and the utility of computing reward potential and strengthening HD-MILP-Plan.

**Preliminary Experimental Results**

In this section, we present preliminary computational results of two sets of experiments. First, we present results on the convergence of Algorithm 1 for computing an optimal reward potential for the learned NN. Second, we present results on the overall strengthening of HD-MILP-Plan with respect to its underlying linear relaxation and search efficiency, for the task of long-term planning.

**Experimental Setup**

The experiments were run on a MacBookPro with 2.8 GHz Intel Core i7 16GB memory. Two instances from the Navigation (Say et al. 2017) domain, namely Navigation with maze sizes (i) 8-by-8 and (ii) 10-by-10, were selected. The learned transition function $\bar{T}$ for both domains are ReLU based NNs with 2 hidden layers of 32 ReLUs. The planning horizon was set to $H = 100$, and the action bounds were constrained to $[-0.1, 0.1]$. CPLEX 12.9.0 (IBM 2019) solver was used to optimize both Algorithm 1, and HD-MILP-Plan, with 6000 seconds of total time limit per domain instance. We show results for the values of interval parameter $N = 2, 3$. Finally in the master problem, we have chosen the regularizer constant $\lambda$ in the objective function (9) to be $\frac{1}{\sqrt{M}}$ where $M$ is the large constant used in the big-M constraints of HD-MILP-Plan.

**Convergence Results**

In the first set of experiments, we demonstrate the convergence capabilities of Algorithm 1 for computing an optimal reward potential for the learned NN.

Figure 2 visualizes the violation of constraint (2) as a function of time over the computation of optimal reward potentials using the Reward Potentials Algorithm 1 for the learned NNs of both Navigation 8-by-8 (i.e., top) and Navigation 10-by-10 (i.e., bottom) planning instances. In both
instances, we observe that the violation of constraint (2) decreases exponentially and terminates with optimal reward potentials.

**Strengthening Results**

In the second set of experiments, we demonstrate the overall strengthening of HD-MILP-Plan with respect to its underlying linear relaxation and search efficiency as a result of constraint (11), for the task of long-term planning.

Figure 3 visualizes the overall effect of incorporating constraint (11) into HD-MILP-Plan as a function of time for the Navigation domain with (a) 8-by-8 and (b) 10-by-10 maze sizes. In both Figures 3 (a-b), linear relaxation (i.e. top), number of closed nodes (i.e., middle), and number open nodes (i.e., bottom), are displayed as a function of time.

The inspection of both Figures 3 (a-b) show that once the reward potentials are computed, the addition of constraint (11) allows HD-MILP-Plan to obtain a tighter bound by exploring significantly less number of nodes. In the 8-by-8 maze instance, we observe that HD-MILP-Plan with constraint (11) outperforms the base HD-MILP-Plan by 1,700 and 3,300 seconds with interval parameter $N = 2, 3$, respectively. In the 10-by-10 maze instance, we observe that HD-MILP-Plan with constraint (11) obtains a tighter bound compared to the base HD-MILP-Plan by 3,750 seconds and reaches almost the same bound by the time limit (i.e., 6000 seconds) with interval parameter $N = 2, 3$, respectively. For both instances, we observe that increasing the value of the interval parameter $N$ increases its computation time, but can also increase the search efficiency of the B&B solver by better exploration and pruning capabilities (i.e., middle and bottom figures).

**Conclusion**

In this paper, we have focused on the problem of improving the linear relaxation and the search efficiency of MILP models for decision making with learned NNs. In order to tackle this problem, we have introduced a finite-time constraint generation algorithm for computing the potential contribution of each hidden unit to the reward function of the planning problem. We have introduced constraints to tighten the bound on the reward function of the planning problem. Experimentally, we have shown that our constraint generation algorithm efficiently computes reward potentials for learned NNs, and the overhead computation is justified by the overall strengthening of the underlying MILP model as demonstrated on the task of planning over long-term horizons. With this paper, we have shown the potential of bridging the gap between two seemingly distant literatures; heuristics search and decision making with learned NN models in continuous action and state spaces.
References

IBM. 2019. *IBM ILOG CPLEX Optimization Studio CPLEX User’s Manual*.

Nair, V., and Hinton, G. E. 2010. Rectified linear units improve restricted boltzmann machines. In *Twenty-Seventh International Conference on Machine Learning*, 807–814.

Pommerening, F.; Helmert, M.; Roger, G.; and Seipp, J. 2015. From non-negative to general operator cost partitioning. In *Twenty-Ninth AAAI Conference on Artificial Intelligence*, 3335–3341.

Say, B.; Wu, G.; Zhou, Y. Q.; and Sanner, S. 2017. Nonlinear hybrid planning with deep net learned transition models and mixed-integer linear programming. In *Twenty-Sixth International Joint Conference on Artificial Intelligence*, 750–756.

Seipp, J.; Pommerening, F.; Helmert, M.; and Roger. 2015. New optimization functions for potential heuristics. In *Twenty-Fifth International Conference on Automated Planning and Scheduling*, 193–201.