LEARNING SOFT CONSTRAINTS FROM CONSTRAINED EXPERT DEMONSTRATIONS

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Paper under double-blind review

ABSTRACT

Inverse reinforcement learning (IRL) methods assume that the expert data is generated by an agent optimizing some reward function. However, in many settings, the agent may optimize a reward function subject to some constraints, where the constraints induce behaviors that may be otherwise difficult to express with just a reward function. We consider the setting where the reward function is given, and the constraints are unknown, and propose a method that is able to recover these constraints satisfactorily from the expert data. While previous work has focused on recovering hard constraints, our method can recover cumulative soft constraints that the agent satisfies on average per episode. In IRL fashion, our method solves this problem by adjusting the constraint function iteratively through a constrained optimization procedure, until the agent behavior matches the expert behavior. We demonstrate our approach on synthetic environments and real world highway driving data.

1 INTRODUCTION

Inverse reinforcement learning (IRL) (Ng et al., 2000; Russell, 1998) refers to the problem of learning a reward function given observed optimal or near optimal behavior. However, in many setups, expert actions may result from a policy that inherently optimizes a reward function subject to certain constraints. While IRL methods are able to learn a reward function that explains the expert demonstrations well, many tasks also require knowing constraints. Constraints can often provide a more interpretable representation of behavior than just the reward function (Chou et al., 2018). In fact, constraints can represent safety requirements more strictly than reward functions, and are therefore are especially useful in safety-critical applications (Chou et al., 2021; Scobee & Sastry, 2019).

Inverse constraint learning (ICL) may therefore be defined as the process of extracting the constraint function(s) associated with the given optimal (or near optimal) expert data, where we assume that the reward function is available. Notably, some prior work (Chou et al., 2018; 2020; 2021; Scobee & Sastry, 2019; Malik et al., 2021) has tackled this problem by learning hard constraints (i.e., functions that indicate which state action-pairs are allowed).

We propose a novel method for ICL (for simplicity, our method is also called ICL) that learns cumulative *soft constraints* from expert demonstrations while assuming that the reward function is known. The difference between hard constraints and soft constraints can be illustrated as follows. Suppose in an environment, we need to obey the constraint "do not use more than 3 units of energy". As a hard constraint, we typically wish to ensure that this constraint is always satisfied for any individual trajectory. The difference between this "hard" constraint and proposed "soft" constraints is that soft constraints are not necessarily satisfied in every trajectory, but rather only satisfied in expectation. This is equivalent to the specification "on average across all trajectories, do not use more than 3 units of energy". In the case of soft constraints, there may be certain trajectories when the constraint is violated, but in expectation, it is satisfied.

To formulate our method, we adopt the framework of constrained Markov decision processes (CMDP) (Altman, 1999), where an agent seeks to maximize expected cumulative rewards subject to constraints on the expected cumulative value of constraint functions. While previous work in constrained RL focuses on finding an optimal policy that respects known constraints, we seek to learn the constraints based on expert demonstrations. We adopt an approach similar to IRL, but the goal is to learn the constraint functions instead of the reward function.

Contributions. Our contributions can be summarized as follows: (a) We propose a novel formulation and method for ICL. Our approach works with any state-action spaces (including continuous state-action spaces) and can learn arbitrary constraint functions represented by flexible neural networks. To the best of our knowledge, our method is the first to learn *cumulative soft constraints* (such constraints can take into account noise in sensor measurements and possible violations in expert demonstrations) bounded in expectation as in constrained MDPs. (b) We demonstrate our approach by learning constraint functions in various synthetic environments, and a driving environment based on real world highway driving data.

The paper is structured as follows. Section 2 provides some background about IRL and ICL. Section 3 summarizes previous work about constraint learning. Section 4 describes our new technique to learn cumulative soft constraints from expert demonstrations. Section 5 demonstrates the approach in synthetic environments as well as real data from human highway driving. Finally, Section 6 concludes by discussing limitations and future work.

2 BACKGROUND

Markov Decision Process (MDP). An MDP is defined as a tuple $(\mathcal{S}, \mathcal{A}, p, \mu, r, \gamma)$, where $\mathcal{S}$ is the state space, $\mathcal{A}$ is the action space, $p(\cdot|s,a)$ are the transition probabilities over the next states given the current state s and current action a, $r : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ is the reward function, $\mu : \mathcal{S} \to [0,1]$ is the initial state distribution and γ is the discount factor. The behavior of an agent in this MDP can be represented by a stochastic policy $\pi : \mathcal{S} \times \mathcal{A} \to [0,1]$, which is a mapping from a state to a probability distribution over actions. A *constrained MDP* augments the MDP structure to contain a constraint function $c : \mathcal{S} \times \mathcal{A} \to \mathbb{R}$ and an episodic constraint threshold β.

Reinforcement learning and Constrained RL. The objective of any standard RL procedure (control) is to obtain a policy that maximizes the (infinite horizon) expected long term discounted reward (Sutton & Barto, 2018):

$$\pi^* = \arg\max_{\pi} \mathbb{E}_{s_0 \sim \mu(\cdot), a_t \sim \pi(\cdot|s_t), s_{t+1} \sim p(\cdot|s_t,a_t)} \left[\sum_{t=0}^{\infty} \gamma^t r(s_t, a_t) \right] =: J_\mu^\pi(r) \tag{1}$$

Similarly, in constrained RL, additionally the expectation of cumulative constraint functions c_i must not exceed associated thresholds β_i:

$$\pi^* = \arg\max_{\pi} J_\mu^\pi(r) \text{ such that } J_\mu^\pi(c_i) \leq \beta_i \forall i \tag{2}$$

For simplicity, in this work we consider constrained RL with only one constraint function.

Inverse reinforcement learning (IRL) and inverse constraint learning (ICL). IRL performs the inverse operation of reinforcement learning, that is, given access to a dataset $\mathcal{D} = \{\tau_j\}_{j=1}^N = \{\{(s_t, a_t)\}_{t=1}^{M_j}\}_{j=1}^N$ sampled using an optimal or near optimal policy π^*, the goal is to obtain a reward function r that best explains the dataset. By "best explanation", we mean that if we perform the RL procedure using r, then the obtained policy captures the behavior demonstrated in $\mathcal{D}$ as closely as possible. In the same way, given access to a dataset $\mathcal{D}$ (just like in IRL), which is sampled using an optimal or near optimal policy π^* (respecting some constraints c_i and maximizing some known reward r), the goal of ICL is to obtain the constraint functions c_i that best explain the dataset, that is, if we perform the constrained RL procedure using $r, c_i \forall i$, then the obtained policy captures the behaviour demonstrated in $\mathcal{D}$.

Setup. Similar to prior work (Chou et al., 2020), we learn only the constraints, but not the reward function. Essentially, it is difficult to say whether a demonstrated behaviour is obeying a constraint, or maximizing a reward, or doing both. So, for simplicity, we assume the (nominal) reward is given, and we just need to learn a (single) constraint function. Without loss of generality, we fix the threshold β to a predetermined value and learn only a constraint function c.[1]

[1]Mathematically equivalent constraints can be obtained by multiplying the constraint function and the threshold by the same value. Therefore there is no loss in fixing β to learn a canonical constraint within the set of equivalent constraints, assuming that the learned constraint function can take arbitrary values.

3 RELATED WORK

Several works in the inverse RL literature consider the framework of constrained MDPs (Kalweit et al., 2020; Fischer et al., 2021; Ding & Xue, 2022). However, those works focus on learning the reward function while assuming that the constraints are known. In contrast, we focus on learning constraints while assuming that the reward function is known.

Initial work in constraint learning focused on learning instantaneous constraints with respect to states and actions. When states and actions are discrete, constraint sets can be learned to distinguish feasible state-action pairs from infeasible ones (Chou et al., 2018; Scobee & Sastry, 2019; McPherson et al., 2021; Park et al., 2020). In continuous domains, various types of constraint functions are learned to infer the boundaries of infeasible state-action pairs. This includes geometric state-space constraints (Armesto et al., 2017; Pérez-D'Arpino & Shah, 2017), task space equality constraints (Lin et al., 2015; 2017), convex constraints (Menner et al., 2021) and parametric non-convex constraint functions (Chou et al., 2020; Malik et al., 2021). Several other works learn local trajectory-based constraints with respect to a single trajectory (Calinon & Billard, 2008; Pais et al., 2013; Li & Berenson, 2016; Mehr et al., 2016; Ye & Alterovitz, 2017).

The vast majority of previous work considers hard constraints, which is fine in deterministic domains. However, in stochastic domains, the probability of violating a constraint can rarely be reduced to zero, making hard constraints inadequate. To that effect, Glazier et al. (2021) learn probabilistic constraints that hold with high probability in expert demonstrations. This approach extends the framework of maximum entropy inverse reinforcement learning to learn a constraint value that is treated as a negative reward added to the given reward function. Since the probability of a trajectory is proportional to the exponential of the rewards, this has the effect of reducing the probability of trajectories with high constraint values. Several other works also extend the inverse entropy RL framework to learn constraints that reduce some transition probabilities to 0 when a constraint is violated, but this amounts to hard constraints again (Scobee & Sastry, 2019; Park et al., 2020; McPherson et al., 2021; Malik et al., 2021). In an other line of work, Bayesian approaches (Chou et al., 2021; Papadimitriou et al., 2021) have also been proposed to learn a distribution over constraints due to the unidentifiability and uncertainty of the true underlying constraints. With the exception of (Papadimitriou et al., 2021), existing techniques that learn probabilistic constraints are restricted to discrete states and actions. Furthermore, the probabilistic constraints that are learned do not correspond to the soft constraints of constrained MDPs. Hence, we fill this gap by proposing a first technique that learns soft cumulative constraint functions bounded in expectations (as in constrained MDPs) for stochastic domains with any state-action spaces.

4 APPROACH

4.1 INVERSE CONSTRAINT LEARNING: TWO PHASES

We propose an approach to do ICL, that is, given a reward r and demonstrations $\mathcal{D}$, this strategy obtains a constraint function c such that when r, c are used in the constrained RL procedure (any algorithm that optimizes Equation (2)), the obtained policy π^* explains the behavior in $\mathcal{D}$. Our approach is based on the template of IRL, where we typically alternate between a policy optimization phase and a reward adjustment phase (Arora & Doshi, 2021). We first describe a theoretical procedure that captures the essence of our approach and then later adapt it into a practical algorithm. The theoretical approach starts with an empty set of policies (i.e., $\Pi = \emptyset$) and then grows this set of policies by alternating between two optimization procedures until convergence:

$$\text{POLICY OPTIMIZATION: } \pi^* := \arg\max_{\pi} J_\mu^\pi(r) \text{ such that } J_\mu^\pi(c) \leq \beta \text{ and } \Pi \leftarrow \Pi \cup \{\pi^*\} \tag{3}$$

$$\text{CONSTRAINT ADJUSTMENT: } c^* := \arg\max_{c} \min_{\pi \in \Pi} J_\mu^\pi(c) \text{ such that } J_\mu^{\pi_E}(c) \leq \beta \tag{4}$$

The optimization procedure in Equation (3) performs forward constrained RL (see Section 2 - Background and Equation (2) for the definition of constrained RL and the notation J_μ^π) to find an optimal policy π^* given a reward function r and a constraint function c. This optimal policy is then added to the set of policies Π. This is followed by the optimization procedure in Equation (4), which adjusts the constraint function c to increase the constraint values of the policies in Π while keeping the constraint value of the expert policy π_E bounded by β. This is achieved by maximizing the

accumulated constraint value for the most feasible (lowest total constraint value) policy in Π. This selectively increases the constraint function until the most feasible optimal policies become infeasible. At each iteration of those two optimization procedures a new policy is found but its constraint value will be increased past β unless it corresponds to the expert policy (which is enforced by the constraint in Equation (4)). By doing so, this approach will converge to the expert policy (or an equivalent policy when multiple policies can generate the same trajectories) as shown in Theorem 1. Intuitively, this happens because all policies and trajectories except the expert's are made infeasible in the long run.

Theorem 1. *Assuming there is a unique policy π^E that achieves $J_\mu^{\pi^E}(r)$, the alternation of optimization procedures in Equation* (3) *and Equation* (4) *converges to a set of policies Π such that the last policy π^* added to Π is equivalent to the expert policy π^E in the sense that π^* and π^E generate the same trajectories.*

Proof See Appendix A. ■

In practice, there are several challenges in implementing the optimization procedures proposed in Equation (3) and Equation (4). First, we do not have the expert policy π_E, but rather trajectories generated based on the expert policy. Also, the set Π of policies can grow to become very large before convergence is achieved. Furthermore, convergence may not occur or may occur prematurely due to numerical issues and whether the policy space contains the expert policy. The optimization procedures include constraints and one of them requires min-max optimization. Therefore, we approximate the theoretical approach in Equation (3) and Equation (4) into the practical approach described in Algorithm 1.

As a first step, we replace the optimization procedure in Equation (4) by a simpler optimization described in Equation (5). More precisely, we replace the max-min optimization (which is a continuous-discrete optimization problem) of the constraint values of the policies in Π by a maximization of the constraint value of the mixture π_{mix} of policies in Π. In this case, the mixture π_{mix} is a collection of optimal policies where each policy has a weight, which is used in the computation of $J_\mu^{\pi_{mix}}(c)$ in Equation (5). The details of this computation are stated in Algorithm 3. Overall, changing the objective avoids a challenging max-min optimization, but we lose the theoretical guarantee of convergence to a policy equivalent to the expert policy. However, we find in our experiments that the algorithm still converges empirically.

$$c^* := \arg\max J_\mu^{\pi_{mix}}(c) \text{ such that } J_\mu^{\pi_E}(c) \leq \beta \tag{5}$$

Maximizing the constraint values of a mixture of policies Π usually tends to increase the constraint values for all policies in Π most of the time, and when a policy's constraint value is not increased beyond β it will usually be a policy close to the expert policy.

4.2 Solving the constrained optimizations through the penalty method

The constrained optimization problems Equation (3), Equation (4), Equation (5), described in the preceding subsection belong to the following general class of optimization problems (here, f, g are potentially non-linear and non-convex):

$$\min_y f(y) \text{ such that } g(y) \leq 0 \tag{6}$$

While many existing constrained RL algorithms formulate the constrained optimization from a Lagrangian perspective (Borkar, 2005; Bhatnagar & Lakshmanan, 2012; Tessler et al., 2018; Bohez et al., 2019) as a min-max problem that can be handled by gradient ascent-descent type algorithms, these are still challenging in terms of empirical convergence, notably suffering from oscillatory behaviour (demonstrated in Appendix B.4).

Therefore, we use a less commonly used optimization framework, namely, the **penalty method** (Bertsekas, 2014; Donti et al., 2020) which converts a constrained problem into an unconstrained problem with a non differentiable ReLU term. Roughly, the approach starts by instantiating $y = y_0$, and then two (sub) procedures are repeated for a few steps each until convergence: (a) first a *feasible* solution is found by repeatedly modifying y in the direction of $-\nabla g(y)$ until $g(y) \leq 0$ (note that this is equivalent to $-\nabla ReLU(g(y))$, also called *feasibility projection*, then (b) a soft loss is optimized that simultaneously minimizes $f(y)$ while trying to keep y within the feasible region. This soft loss

is as follows: (here, λ is a hyperparameter):

$$\min_y L_{\text{soft}}(y) := f(y) + \lambda \text{ReLU}(g(y)) \tag{7}$$

As an alternative to Lagrangian based approaches, the penalty method has the advantage of simpler algorithmic implementation. Further, as we will demonstrate later in our experiments, it also performs well empirically.

Note that the choice of λ is crucial here. In fact, we plan to use the penalty method to optimize both Equation (3) and Equation (5), using different λ for each case. A small λ means that in the soft loss optimization subprocedure (Equation (7)), the gradient update of $\text{ReLU}(g(y))$ is miniscule in comparison to the gradient update of $f(y)$, because of which y may not stay within the feasible region during the soft loss optimization. In this case, the feasibility projection subprocedure is important to ensure the overall requirement of feasibility is met (even if exact feasibility cannot be guaranteed). Conversely, a large λ means that minimizing the soft loss is likely to ensure feasibility, and the feasibility projection subprocedure may therefore be omitted. This forms the basis for our proposed optimization procedures (see Algorithms 2 and 3 for the exact steps of these procedures). Namely, we perform forward constrained RL (Equation (3)) using $\lambda = 0$ with the feasibility projection subprocedure, and constraint adjustment (Equation (4) / Equation (5)) using a moderate/high λ and without the feasibility projection subprocedure.

4.3 Improving Constraint Adjustment

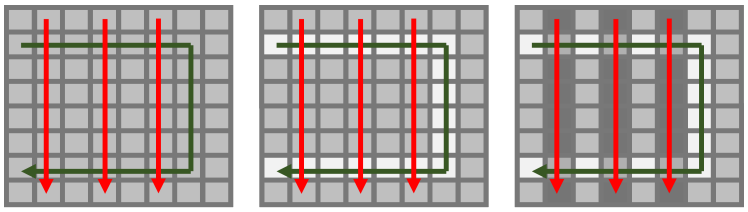


Figure 1: Given expert (green) and agent (red) behaviour for an arbitrary Gridworld environment (first figure), the proposed algorithm decreases the constraint value for the expert behaviour (second figure) and increases the constraint value for the agent behaviour (third figure). Constraint learning is slower if there is overlap between the two behaviours since there exist some states for which the algorithm tries to simultaneously increase and decrease the constraint value. Note that dark gray represents a higher constraint value, light gray a medium constraint value and white represents a lower constraint value.

We can further improve the constraint adjustment subprocedure by noticing that an overlap in expert and agent data used in computing the terms $J_\mu^{\pi_E}(c)$ and $J_\mu^{\pi_{mix}}(c)$ respectively in Equation (5) hampers convergence in learning constraints. We can see this in the following way. We know that constraint adjustment (Equation (4), Equation (5)) is finding the decision boundary between expert and agent trajectories (see Figure 1 for an illustration). Consider the soft loss objective for Equation (5):

$$\min_c L_{\text{soft}}(c) := -J_\mu^{\pi_{mix}}(c) + \lambda \text{ReLU}(J_\mu^{\pi_E}(c) - \beta)$$

Here, the expert data is used to compute $J_\mu^{\pi_E}(c)$, and the agent data is used to compute $J_\mu^{\pi_{mix}}(c)$. Depending on whether $J_\mu^{\pi_E}(c) - \beta \leq 0$ or not, the ReLU term vanishes in $L_{\text{soft}}(c)$. There are two cases. **(I)** If $J_\mu^{\pi_E}(c) - \beta \leq 0$, then c is already feasible, that is, for this value of c, the average constraint value across expert trajectories is less than or equal to β. If there are expert (or expert-like) trajectories in agent data (used to compute $-J_\mu^{\pi_{mix}}(c)$), then we will then end up increasing the constraint value across these expert trajectories (on average), which is not desirable since it will lead to c becoming more infeasible. This will lead to requiring more iterations to converge in learning the constraint function c. **(II)** If $J_\mu^{\pi_E}(c) - \beta > 0$, then there is a nonzero ReLU term in $L_{\text{soft}}(c)$. If there are some expert or expert-like trajectories in agent data (and subsequently in $-J_\mu^{\pi_{mix}}(c)$), and we take the gradient of $L_{\text{soft}}(c)$, we will get two contrasting gradient terms trying to increase and decrease the constraint value across the same expert (or expert-like) trajectories. The gradient update associated with the ReLU term is required since we want c to become feasible, but having

expert (or expert-like) trajectories in $-J_\mu^{\pi_{mix}}(c)$ diminishes the effect of the ReLU term and then more iterations are needed for convergence of constraint function c.

To improve empirical convergence, we propose two reweightings: (a) we reweight the policies in π_{mix} (line 6 in Algorithm 3) so that policies dissimilar to the expert policy are favoured more in the calculation of $-J_\mu^{\pi_{mix}}(c)$, and (b) we reweight the individual trajectories in the expectation $-J_\mu^{\pi_{mix}}(c)$ (line 8 in Algorithm 3) to ensure that there is less or negligible weight associated with the expert or expert-like trajectories. We can perform both these reweightings using a density estimator (specifically, RealNVP flow (Dinh et al., 2016)). The idea is to learn the density of expert or expert-like state-action pairs and compute the negative log-probability (NLP) of any given trajectory's state-action pairs at test time to determine if it is expert or expert-like, or not. Practically, this is estimated by computing the mean and std. deviation of the NLP of expert state-action pairs, and then at test time, checking if the NLP of the given state-action pairs is within one std. deviation of the mean or not. Please refer to lines 1-3 in Algorithm 3 for the exact pseudocode.

Our complete algorithm is provided in Algorithm 1. As mentioned in Section 4.1, the algorithm repeatedly optimizes the objectives defined in Equation (3) and Equation (5) on lines 6 and 7. The procedures for these optimizations are provided in Algorithms 2 and 3, which use the penalty method as described in Section 4.2. Further, Algorithm 3 describes constraint adjustment using a normalizing flow as described in this subsection. *Inputs and outputs to each algorithm have also been specified.*

Algorithm 1 INVERSE-CONSTRAINT-LEARNING

hyper-parameters: number of ICL iterations n, tolerance ϵ
input: expert dataset $\mathcal{D} = \{\tau\}_{\tau\in\mathcal{D}} := \{\{(s_t, a_t)\}_{1\le t\le|\tau|}\}_{\tau\in\mathcal{D}}$
1: **initialize** normalizing flow f
2: **optimize** likelihood of f on expert state action data: $\max_f \textsc{Sum}_{(s,a)\in\tau,\tau\in\mathcal{D}}(\log p_f(s,a))$
3: **initialize** constraint function c (parameterized by $\boldsymbol{\phi}$)
4: **for** $1 \le i \le n$ **do**
5: **initialize** policy π_i (parameterized by $\boldsymbol{\theta}_i$)
6: **perform** $\pi_i := \textsc{Constrained-RL}(\pi_i, c)$
7: **perform** $c := \textsc{Constraint-Adjustment}(\pi_{1:i}, c, \mathcal{D}, f)$
8: **break** if $\textsc{Normalized-Accrual-Dissimilarity}(\mathcal{D}, \mathcal{D}_{\pi_i}) \le \epsilon$
▷ *See Section 5 for normalized accrual dissimilarity metric*
9: **end for**
output: learned constraint function c (neural network with sigmoid output),
learned most recent policy π_i

Algorithm 2 CONSTRAINED-RL

hyper-parameters: learning rates η_1, η_2, constraint threshold β, constrained RL epochs m
input: policy π_i parameterized by $\boldsymbol{\theta}_i$, constraint function c
1: **for** $1 \le j \le m$ **do**
2: **correct** π_i to be feasible: (iterate) $\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \eta_1 \nabla_{\boldsymbol{\theta}_i} \textsc{ReLU}(J_\mu^{\pi_i}(c) - \beta)$
3: **optimize** expected discounted reward: $\boldsymbol{\theta}_i \leftarrow \boldsymbol{\theta}_i - \eta_2 \nabla_{\boldsymbol{\theta}_i} \textsc{PPO-Loss}(\pi_i)$
▷ *Proximal Policy Optimization* (Schulman et al., 2017)
4: **end for**
output: learned policy π_i

5 EXPERIMENTS

Environments. We conduct several experiments on the following environments: (a) *Gridworld (A, B)*, which are 7x7 gridworld environments, (b) *CartPole (MR or Move Right, Mid)* are variants of the CartPole environment from OpenAI Gym (Brockman et al., 2016), and (c) *Highway driving environment* based on HighD dataset (Krajewski et al., 2018). Due to space requirements, we have provided further details on these environments (with figures) in Appendix C.1.

Baselines and metrics. We use two baselines to compare against our method: (a) *GAIL-Constraint*, which is based on Generative adversarial imitation learning method (Ho & Ermon, 2016), and (b)

Algorithm 3 CONSTRAINT-ADJUSTMENT

hyper-parameters: learning rate η_3, penalty wt. λ, constraint threshold β, constraint adjustment epochs e
input: policies $\pi_{1:i}$, constraint function c, trained normalizing flow f, expert dataset $\mathcal{D} = \{\tau\}_{\tau \in \mathcal{D}} := \{\{(s_t, a_t)\}_{1 \leq t \leq |\tau|}\}_{\tau \in \mathcal{D}}$
given: $c^\gamma(\tau) := \text{SUM}_{1 \leq t \leq |\tau|}(\gamma^{t-1} c(s_t, a_t))$, $\text{SAMPLE}_\tau(\Pi, p)$ which generates $|\mathcal{D}|$ trajectories $\tau = \{(s_t, a_t)\}_{1 \leq t \leq |\tau|}$, where for each τ, we choose $\pi \in \Pi$ with prob. $p(\pi)$, then, $s_1 \sim \mu(\cdot), a_t \sim \pi(\cdot|s_t), s_{t+1} \sim p(\cdot|s_t, a_t)$

$\mu_E := \text{MEAN}_{(s,a) \in \tau, \tau \in \mathcal{D}}(-\log p_f(s, a))$
$\sigma_E := \text{STD-DEV}_{(s,a) \in \tau, \tau \in \mathcal{D}}(-\log p_f(s, a))$
$w(\tau) := \text{MEAN}_{(s,a) \in \tau}(\mathbf{1}(-\log p_f(s, a) > \mu_E + \sigma_E))$ ▷ *trajectory dissimilarity w.r.t. expert*
construct policy dataset $\mathcal{D}_{\pi_i} = \text{SAMPLE}_\tau(\Pi = \{\pi_i\}, p = \{1\})$
$\tilde{w}_i := \text{MEAN}_{\tau \in \mathcal{D}_{\pi_i}} w(\tau)$ ▷ *unnormalized policy weights*
construct agent dataset $\mathcal{D}_A = \text{SAMPLE}_\tau(\Pi = \pi_{1:i}, p(\pi_i) \propto \tilde{w}_i)$ ▷ *policy reweighting*
for $1 \leq j \leq e$ **do** ▷ *constraint function adjustment*
  compute $J_\mu^{\pi_{mix}}(c) := \text{SUM}_{\tau \in \mathcal{D}_A} \frac{w(\tau) c^\gamma(\tau)}{\text{SUM}_{\tau \in \mathcal{D}_A} w(\tau)}$ ▷ *trajectory reweighting*
  compute $J_\mu^{\pi_E}(c) := \text{MEAN}_{\tau \in \mathcal{D}}(c^\gamma(\tau))$
  compute soft loss $L_{\text{soft}}(c) := -J_\mu^{\pi_{mix}}(c) + \lambda \text{RELU}(J_\mu^{\pi_E}(c) - \beta)$
  optimize constraint function c: $\boldsymbol{\phi} \leftarrow \boldsymbol{\phi} - \eta_3 \nabla_{\boldsymbol{\phi}} L_{\text{soft}}(c)$
end for
output: constraint function c

Inverse constrained reinforcement learning (ICRL) (Malik et al., 2021), which is a recent method that can learn arbitrary neural network constraints. In the absence of any other neural network constraint learning technique, only those two relevant baselines are compared to empirically. We provide further details in Appendix C.2. Next, we define two metrics for our experiments: (a) *Constraint Mean Squared Error (CMSE)*, which is the mean squared error between the true constraint and the recovered constraint, and (b) *Normalized Accrual Dissimilarity (NAD)*, which is a dissimilarity measure computed between the expert and agent accruals (state-action visitations of policy/dataset). Further details can be found in Appendix C.3.

Finally, we use a constraint neural network with a sigmoid output, so that we can also interpret the outputs as safeness values. Our results are reported in Tables 1 and 2. The average recovered constraint functions and accruals are provided in Appendix D. For the highway dataset, our results are reported in Figure 2. The hyperparameter configuration (e.g., choice of λ) and training strategy are elaborated in Appendix C.

Table 1: Constraint Mean Squared Error (Mean $\pm$ Std. Deviation across 5 seeds)

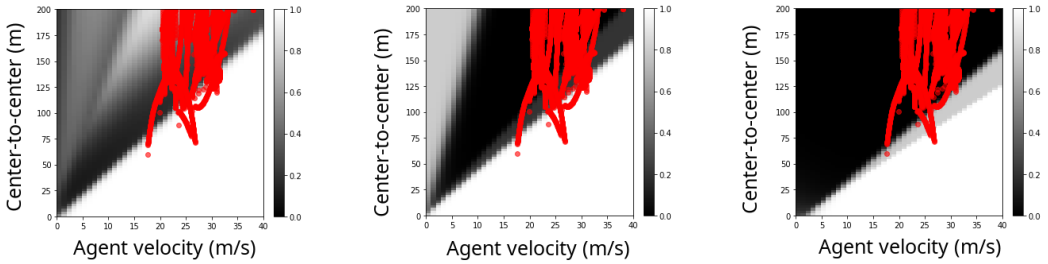
Algorithm↓, Environment→	Gridworld (A)	Gridworld (B)	CartPole (MR)	CartPole (Mid)
GAIL-Constraint	0.31 ± 0.01	0.25 ± 0.01	0.12 ± 0.03	0.25 ± 0.02
ICRL	0.11 ± 0.02	0.21 ± 0.04	0.21 ± 0.16	0.27 ± 0.03
ICL (ours)	**0.08 ± 0.01**	**0.04 ± 0.01**	**0.02 ± 0.00**	**0.08 ± 0.05**

Table 2: Normalized Accrual Dissimilarity (Mean $\pm$ Std. Deviation across 5 seeds)

Algorithm↓, Environment→	Gridworld (A)	Gridworld (B)	CartPole (MR)	CartPole (Mid)
GAIL-Constraint	1.76 ± 0.25	1.29 ± 0.07	1.80 ± 0.24	7.23 ± 3.88
ICRL	1.73 ± 0.47	2.15 ± 0.92	12.32 ± 0.48	13.21 ± 1.81
ICL (ours)	**0.36 ± 0.10**	**1.26 ± 0.62**	**1.63 ± 0.89**	**3.04 ± 1.93**

5.1 RESULTS FOR SYNTHETIC EXPERIMENTS

Accuracy of learned constraints. While our (practical) method is not guaranteed to produce the true constraint function (constraint unidentifiability is a known problem (Chou et al., 2020)), empirically,



GAIL-Constraint ICRL ICL ($\beta = 0.1$) (ours)

Figure 2: Constraint functions (averaged across 5 seeds) recovered for the HighD highway driving environment. X-axis is the agent (ego car) velocity v (ms^{-1}), Y-axis is the gap from the ego car to the vehicle (center-to-center distance) in front g (m). Red points are (discretized) binary expert accruals, i.e. the states that the agent has been in. Both the baselines, GAIL-Constraint and ICRL assign a high (white) constraint value to more expert states compared to our method, ICL, which overlaps less with the expert states. Ideally, it is expected that the constraint value should be less for expert states, since they are acceptable states.

we find that our method is still able to learn constraint functions that strongly resemble the true constraint function, as can be seen by our low CMSE scores (Table 1).

Sharpness of learned constraints. GAIL-Constraint method is able to find the correct constraint function for all environments except CartPole (Mid), however, the recovered constraint is more diffused throughout the state action space (see Appendix D for training plots). In contrast, our recovered constraint is pretty sharp, even without a regularizer.

Ability to learn complex constraints. From the training plots, we find that the ICRL method is able to find the correct constraint function only for CartPole (MR) and to a less acceptable degree for Gridworld (A). This is surprising as ICRL should be able to theoretically learn any arbitrary constraint function (note that we used the settings in (Malik et al., 2021) except for common hyperparameters), and expect it to perform better than GAIL-Constraint. Our justification for this is two-fold. One, the authors of ICRL have only demonstrated their approach with simple single-proposition constraints, and for more complex settings, ICRL may not be able to perform as well. Second, ICRL may require more careful hyperparameter tuning for each constraint function setting, even with the same environment, depending on the constraint. On the other hand, our method is able to learn these relatively complex constraints satisfactorily with relatively fewer hyperparameters.

Similarity of learned policy to expert policy. We find a strong resemblance between the accruals recovered by our method and the expert, as can be seen by our low NAD scores (Table 2). In these scores, there is some variability (e.g., in Cartpole (MR) and Gridworld (B) environments) which is expected, since the policies are stochastic. For baselines, GAIL-Constraint accruals are similar to the expert accruals except for CartPole (Mid) environment, where it is also unable to learn the correct constraint function. Overall, this indicates that GAIL is able to correctly imitate the constrained expert across most environments, as one would expect. On the other hand, ICRL accruals are even worse than GAIL, indicating that it is unable to satisfactorily imitate the constrained expert, even on the environments for which it is able to generate a somewhat satisfactory constraint function. Training plots are provided in Appendix D.

5.2 Results for real world experiments

We report the results for the HighD driving environment in Figure 2. Overall, all the methods are able to find a constraint function that shows that as the agent's velocity increases, the center-to-center distance that must be maintained between the cars also must increase. The time gap that must be maintained can be calculated by dividing the requisite center-to-center distance by the agent's velocity. For all the methods, this time gap is approximately between 3-4.5 seconds. More precisely, at $v = 20\text{ms}^{-1} = 72\text{kmh}^{-1}$, the gap is roughly between 60-80 m (equivalently, 3-4 seconds) for all methods, while close to $v = 40\text{ms}^{-1} = 144\text{kmh}^{-1}$, the gap is between 125-150 m (equivalently

≈3-4 seconds) for our method, and 160-180 m (equivalently 4-4.5 seconds) for GAIL-Constraint and ICRL. Note that our method is the only one which doesn't assign high constraint value to large center-to-center gaps (no white areas in the black regions in Figure 2). The possible justification for this is that the other methods are unable to explicitly ensure that expert trajectories are assigned low constraint value, while our method is able to do so through the constraint adjustment step. Moreover, our method has fewer accrual points (red) in the white (high constraint value) region compared to the baselines.

5.3 Ablations and Questions

Use of penalty method vs. Lagrangian. As mentioned in Section 4.2, Lagrangian formulations are quite popular in the literature, however, they are inherently min-max problems that admit gradient ascent-descent solutions which are prone to oscillatory behavior, as we observe in Appendix B.4. Thus, we prefer the simpler framework of penalty method optimization which works well empirically.

Stochastic dynamics. Our algorithm can also be applied to stochastic environments, which we demonstrate in Appendix B.3 with slippery Gridworld environments. Stochasticity would lead to noisier demonstrations, and we find that a little noise in the demonstrations helps in the quality of the recovered constraint, but too much noise can hamper the constraint learning.

Quality of learned policy w.r.t. imitation learning. We reiterate that our objective is to learn constraints, while the goal of imitation learning techniques (e.g., behavior cloning) is to directly learn a policy that mimics the expert without inferring any reward or constraint function. Even then, once the constraints have been learned, they can be used with the given reward to learn a constrained policy. Depending on factors like quality of expert data etc., ICL can learn a better or worse policy compared to an imitation learning method. We do not have definitive evidence to conclude that either is true.

Entropy regularized approaches and overfitting. Maximum entropy techniques (e.g., (Scobee & Sastry, 2019; Malik et al., 2021)) have been previously proposed in the literature. Entropy maximization can indeed help in reducing overfitting, but they require a completely different mathematical setup. Our method doesn't belong to this family of approaches, but we hope to incorporate these strategies in the future to reap the mentioned benefits. We still note that empirically, our approach doesn't seem to suffer from any overfitting issues.

Use of normalizing flow and reweighting. We justify our choice of using a normalizing flow to reweigh policies and trajectories (Algorithm 3) in Appendix B.2. We find that ICL with reweighting performs better than ICL without reweighting, although the improvement is minor.

6 Conclusion, Limitations and Future Work

This paper introduces a new technique to learn (soft) constraints from expert demonstrations. While several techniques have been proposed to learn constraints in stochastic domains, they adapt the maximum entropy inverse RL framework to constraint learning (Scobee & Sastry, 2019; Park et al., 2020; McPherson et al., 2021; Glazier et al., 2021; Malik et al., 2021). We propose the first approach that can recover soft cumulative constraints common in constrained MDPs.

Limitations. First, the proposed technique assumes that the reward function is known and can only learn a single constraint function. The challenge with simultaneously learning the reward function as well as multiple constraints is that there can be many equivalent configurations of reward and constraint functions that can generate the same trajectories (unidentifiability (Ng et al., 2000)). Second, it is possible that expert demonstrations are sub-optimal. In that case, we hypothesize that our method would learn alternative constraints such that the provided demonstrations become optimal for these constraints. Finally, our approach requires several outer iterations of forward CRL and constraint adjustment, and as a result, it needs more training time than the existing baselines.

Future work. First, for learning rewards and/or multiple constraints, we need a way to specify preference for specific combinations of reward and constraint functions. Second, it may be more desirable to express constraints not through expectations, but through probabilistic notions, e.g., a cumulative soft constraint which holds (i.e., is $\leq \beta$) with probability $\geq p$. Finally, we hope to extend our work to handle demonstrations from multiple experts and incorporate entropy regularization into our framework for its benefits.

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APPENDIX

A PROOF OF THEOREM 1

We give a proof by contradiction under 3 assumptions. The 3 assumptions are:

(i) The reward function is non-negative.

(ii) The space of policies is finite.

(iii) There is a unique policy π^E that achieves $J_\mu^{\pi^E}(r)$. In other words no other policy achieves the same expected cumulative reward as π^E.

Note that the first assumption is not restrictive since we can always shift a reward function by adding a sufficiently positive constant to the reward of all state-action pairs such that the new reward function is always non-negative. This new reward function is equivalent to the original one since it does not change the value ordering of policies.

We argue that the second assumption is reasonable in practice. Even if we consider what appears to be a continuous policy space because the parameterization of the policy space is continuous, in practice, parameters have a finite precision and therefore the space of policies is necessarily finite (albeit possibly very large).

Based on assumption (ii), it should be clear that the alternation of the optimization procedures in Equation (3) and Equation (4) will converge to a fixed point. Since there are finitely many policies, and we add a new policy to Π at each iteration (until we reach the fixed point), in the worst case, the alternation will terminate once all policies have been added to Π.

When the algorithm converges to a fixed point, let π^* be the optimal policy found by policy optimization in Equation (3) and c^* be the optimal constraint function found by constraint adjustment in Equation (4). According to Equation (3), we know that $J_\mu^{\pi^*}(c^*) \leq \beta$. Similarly, we show that the objective in Equation (4) is less than or equal to β:

$$\max_c \min_{\pi \in \Pi} J_\mu^\pi(c) \text{ subject to } J_\mu^{\pi^E}(c) \leq \beta \tag{8}$$

$$= \min_{\pi \in \Pi} J_\mu^\pi(c^*) \qquad \text{since } c^* \text{ is the optimal solution of equation 4} \tag{9}$$

$$\leq \beta \qquad \text{since } \pi^* \in \Pi \text{ and } J_\mu^{\pi^*}(c^*) \leq \beta \tag{10}$$

Next, if we assume that π^* is not equivalent to π^E, then we can show that the objective in Equation (4) is greater than β.

$$\max_c \min_{\pi \in \Pi} J_\mu^\pi(c) \text{ such that } J_\mu^{\pi^E}(c) \leq \beta \tag{11}$$

$$\geq \min_{\pi \in \Pi} J_\mu^\pi(\hat{c}) \qquad \text{where we choose } \hat{c}(s,a) = \frac{r(s,a)\beta}{J_\mu^{\pi^E}(r)} \tag{12}$$

$$= \min_{\pi \in \Pi} J_\mu^\pi(r)\beta / J_\mu^{\pi^E}(r) \qquad \text{by substituting } \hat{c} \text{ by its definition} \tag{13}$$

$$> J_\mu^{\pi^E}(r)\beta / J_\mu^{\pi^E}(r) = \beta \qquad \text{since } J_\mu^\pi(r) \geq J_\mu^{\pi^E}(r)\ \forall \pi \in \Pi \text{ according to equation 3 and } J_\mu^\pi(r) \neq J_\mu^{\pi^E}(r) \text{ by assumption (iii)} \tag{14}$$

The key step in the above derivation is Equation (12), where we choose a specific constraint function $\hat{c}$. Intuitively, this constraint function is selected to be parallel to the reward function while making sure that $J_\mu^{\pi^E}(c) \leq \beta$. We know that all policies in Π achieve higher expected cumulative rewards than π^E. This follows from the fact that the optimization procedure in Equation (3) finds an optimal policy π^* at each iteration and this optimal policy is not equivalent to π^E based on our earlier assumption. So the policies in Π must earn higher expected cumulative rewards than π^E. So if we select a constraint

function parallel to the reward function then the policies in Π will have constraint values greater than the constraint value of π^E and therefore they should be ruled out in the constrained policy optimization Equation (3).

Since the inequalities 8-10 contradict the inequalities 11-14, we conclude that π^* must be equivalent to π^E. ■

B Additional Discussion

B.1 Constrained PPO

For our forward constrained RL step, we use a modification of the PPO algorithm (Schulman et al., 2017) that approximately ensures constraint feasibility. This modification is based on the penalty method mentioned in Section 4.2. This modified PPO works in two steps. First, we update the policy parameters to ensure constraint feasibility. Then, we update the policy parameters to optimize the PPO objective. If the policy π is parameterized by $\boldsymbol{\theta}$, then these two steps are:

$$\text{Feasibility Projection: } \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta_1 \nabla_{\boldsymbol{\theta}} \text{ReLU}(J_\mu^\pi(c) - \beta)$$
$$\text{PPO Update: } \boldsymbol{\theta} \leftarrow \boldsymbol{\theta} - \eta_2 \nabla_{\boldsymbol{\theta}} \text{PPO-Loss}(\pi)$$

The gradient for the feasibility projection step can be computed just like policy gradient:

$$G_{t_0}(c) := \sum_{t=t_0}^{\infty} \gamma^{t-t_0} c(s_t, a_t) \tag{15}$$

$$\nabla_{\boldsymbol{\theta}} J_\mu^\pi(c) = E_{s_0 \sim \mu, a_t \sim \pi(\cdot|s_t), s_{t+1} \sim p(\cdot|s_t, a_t)} \left[\sum_{t=0}^{\infty} G_t(c) \nabla_{\boldsymbol{\theta}} \log \pi(a_t|s_t) \right] \tag{16}$$

$$\nabla_{\boldsymbol{\theta}} \text{ReLU}(J_\mu^\pi(c) - \beta) = \mathbf{I}(J_\mu^\pi(c) > \beta) \nabla_{\boldsymbol{\theta}} J_\mu^\pi(c) \tag{17}$$

The PPO-Loss(π) term is computed over a minibatch as follows (note that $A(s_t, a_t)$ is an advantage estimate). This is the same as the original paper (Schulman et al., 2017), except for an entropy term.

$$r_t := \frac{\pi(a_t|s_t; \boldsymbol{\theta})}{\pi(a_t|s_t; \boldsymbol{\theta}_{old})} \tag{18}$$

$$\text{PPO-Loss}(\pi) := -\mathbb{E}_t \left[\min(r_t, \text{clip}(r_t, 1 - \epsilon_{PPO}, 1 + \epsilon_{PPO})) A(s_t, a_t) \right] - \lambda_{ent} H(\pi) \tag{19}$$

This gradient can be computed through automatic differentiation.

Overall, we do not have a ReLU term in the PPO update, since its gradient would interfere with the PPO update and cause difficulty in learning. Instead, the feasibility projection step tries to ensure feasibility of the solution before every PPO update. While this doesn't guarantee that feasibility will hold during and after the PPO update, we see empirically that feasibility approximately holds.

The feasibility projection step is comparable to a projection step, since it projects the solution into the feasibility region, although not necessarily the closest feasible point.

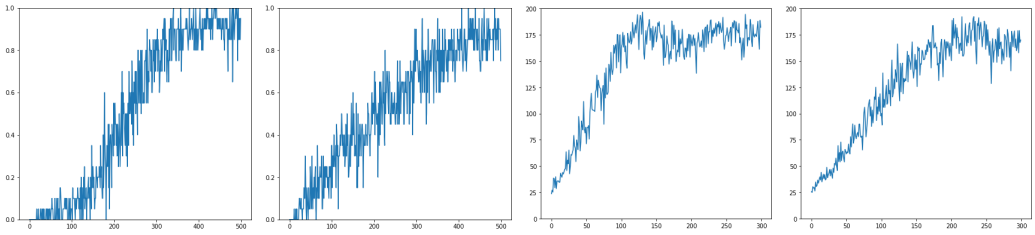
Our results are reported in Figures 3, 4.

B.2 Ablation: Effect of Policy Mixture and Reweighting

To assess the effect of having a policy mixture and reweighting, we conduct experiments with two more variants of ICL on all the synthetic environments:

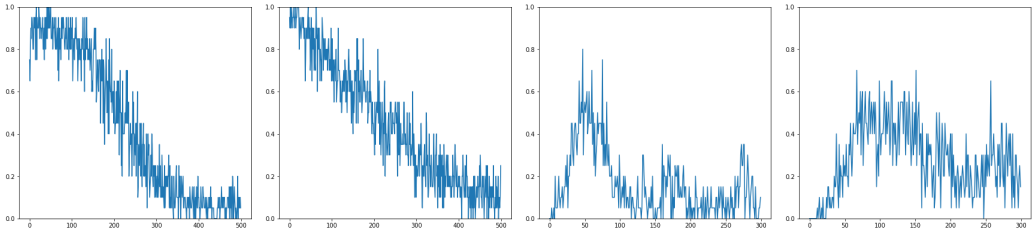
- ICL wihout a mixture policy or reweighting (use the policy learned in constrained RL step instead of π_{mix} to do constraint adjustment step)
- ICL with a mixture policy but with no reweighting (use uniform weights)

Our results are reported in Figure 5. We find that ICL without a mixture policy or reweighting is unable to perform as well as other methods with Gridworld (A) environment. Empirically, it is



Gridworld (A) ($\beta = 0.99$) | Gridworld (B) ($\beta = 0.99$) | CartPole (MR) ($\beta = 50$) | CartPole (Mid) ($\beta = 30$)

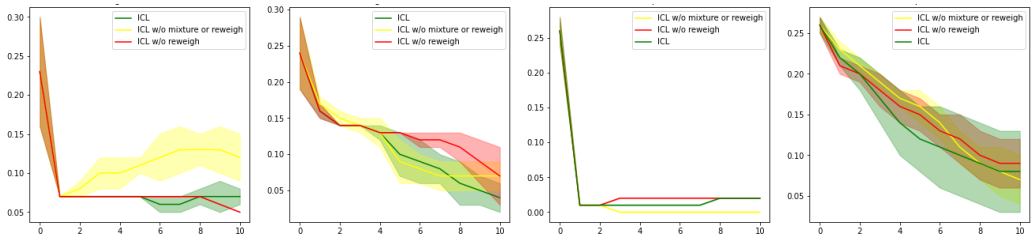
Figure 3: Avg reward per PPO epoch for the expert (1 seed). As seen, the modified PPO is able to learn a good policy that achieves a high reward.



Gridworld (A) ($\beta = 0.99$) | Gridworld (B) ($\beta = 0.99$) | CartPole (MR) ($\beta = 50$) | CartPole (Mid) ($\beta = 30$)

Figure 4: Avg constraint violations per PPO epoch for the expert (1 seed). As seen, the modified PPO is able to learn a good policy that reduces the constraint violations as the training progresses.

prone to divergence and cyclic behavior. This divergent behavior can be observed in the Gridworld (A) case. ICL with a mixture policy but with no reweighting is unable to converge as fast as ICL with mixture policy and reweighting in the Gridworld (B) and CartPole (Mid) environments. For the CartPole (MR) environment, all the methods converge fairly quickly and have almost the same performance. We also note that there is significant variance in the result for ICL on the CartPole (Mid) environment. Despite this, overall, ICL with a mixture policy and reweighting performs better than the other variants (or close to the best). Thus, we report this variant (with mixture policy and reweighting) in Table 1 and Table 2.



Gridworld (A) ($\beta = 0.99$) | Gridworld (B) ($\beta = 0.99$) | CartPole (MR) ($\beta = 50$) | CartPole (Mid) ($\beta = 30$)

Figure 5: CMSE (Y-axis) vs ICL Iteration i (X-axis). In each iteration, we do one complete procedure of constrained RL and one complete procedure of constraint function adjustment.

B.3 Environment Stochasticity

To assess the effect of environment stochasticity on the performance of our algorithm, we conduct experiments with a stochastic variant of Gridworld (A) environment. More specifically, we apply the

Table 3: Constraint Mean Squared Error

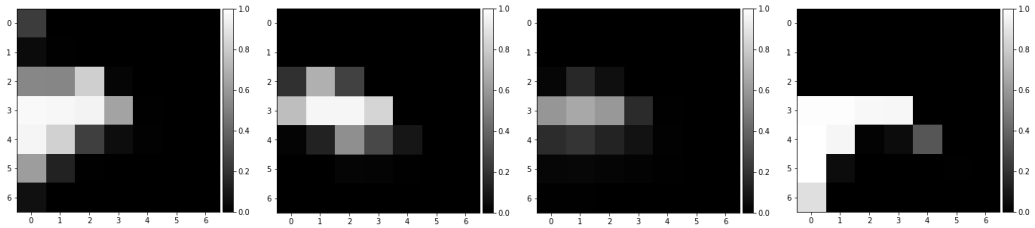
Algorithm↓, Environment→	$p_{slip} = 0.1$	$p_{slip} = 0.3$	$p_{slip} = 0.5$
ICL	0.02 ± 0.00	0.03 ± 0.01	0.08 ± 0.00

Table 4: Normalized Accrual Dissimilarity

Algorithm↓, Environment→	$p_{slip} = 0.1$	$p_{slip} = 0.3$	$p_{slip} = 0.5$
ICL	0.45 ± 0.10	1.13 ± 0.37	1.29 ± 0.20

Reported metrics (Mean $\pm$ Std. Deviation across 5 seeds) for the experiments on stochastic Gridworld (A) environments.

ICL algorithm (Algorithm 1) to the Gridworld (A) environment, with varying values of the transition probability. A transition probability of 1 implies deterministic transition to the next state. A transition probability of $1 - p_{slip}$ implies a stochastic transition, such that the agent can enter the intended next state with this probability, and go to any other random direction with overall probability p_{slip}. Our results are reported in Tables 3 and 4, and in Figure 6.



ICL ($p_{slip} = 0$) ICL ($p_{slip} = 0.1$) ICL ($p_{slip} = 0.3$) ICL ($p_{slip} = 0.5$)

Figure 6: Average constraint function value (averaged across 5 training seeds) for stochastic Gridworld (A) environment, demonstrating the effect of changing p_{slip}.

Empirically, we observe that the increase in environment stochasticity leads to a decrease in the performance of the constrained RL algorithm. Additionally, with a higher stochasticity, there is more noise in the demonstrations. When we increase the stochasticity slightly (going from a deterministic environment to $p_{slip} = 0.1$), we find that the recovered constraint function has lower error (see Figure 6). This happens because with a little stochasticity, there is more exploration in terms of states visited, which leads to a more accurate constraint function since the algorithm tries to avoid more states. However, with more stochasticity ($p_{slip} = 0.5$), the demonstrations themselves become more noisy, and hence the algorithm recovers a worse constraint function than in the case with little stochasticity (see Table 3). Finally, we also find that accruals of the learned policy also have more error w.r.t. provided demonstrations as the stochasticity increases (see Table 4).

B.4 Comparison w.r.t. a Lagrangian implementation

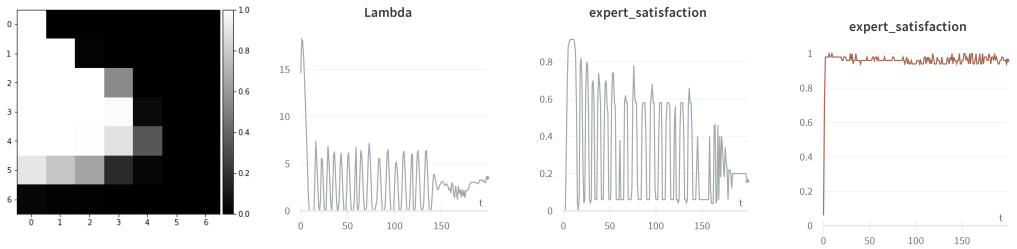
Equation (5) can also be represented using a min-max optimization:

$$\min_{\lambda \geq 0} \max_{c} J_{\mu}^{\pi_{mix}}(c) - \lambda(J_{\mu}^{\pi_E}(c) - \beta) \tag{20}$$

It is possible to perform this optimization instead of the penalty based strategy proposed in this paper. In terms of implementation, this would amount to an alternating gradient ascent descent procedure, where we first ascent on c, followed by descent on λ, and we repeat these steps until convergence. However, as is the case with min-max optimizations, this is prone to training instability and oscillatory behavior. We demonstrate this with the Gridworld (A) environment. In particular, we can see this oscillatory behavior in the plot for the Lagrange multiplier λ (Figure 7, second subfigure). We also

plot the expert satisfaction % for the Lagrangian and non Lagrangian implementation (ICL) (see third and fourth subfigure in Figure 7). The expert satisfaction % is computed as the percentage of expert demonstrations satisfying the constraint using the current constraint function, during training. As the plots show, the Lagrangian implementation is prone to oscillatory behavior. Initially it does achieve a high satisfaction, but over time, the satisfaction degrades. This does not happen in the ICL implementation. This is our primary rationale for using a penalty based method.

In terms of the recovered constraint function, we find that the Lagrangian implementation is still able to achieve a noisy yet reasonable constraint function (see the first subfigure in Figure 7). Therefore, the Lagrangian approach is indeed correct in principle and can be used to recover a constraint function. However, in terms of other training metrics, the Lagrangian approach does not perform well. Our proposed method is able to mitigate this.

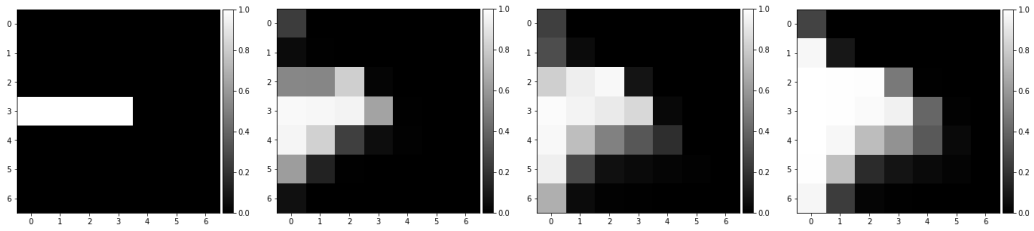


Avg. constraint value (5 seeds) on Gridworld (A) | Lagrange multiplier λ for Lagrangian implementation | Expert satisfaction over time for Lagrangian implementation | Expert satisfaction over time for ICL

Figure 7: The first figure shows the avg. constraint function (averaged across 5 seeds) for the Lagrangian implementation. The second figure shows the value of the Lagrange multiplier during training for 1 seed (X-axis denotes the adjustment iteration). The last two figures show the value of the expert satisfaction (%) for the Lagrangian implementation and the regular implementation (ICL).

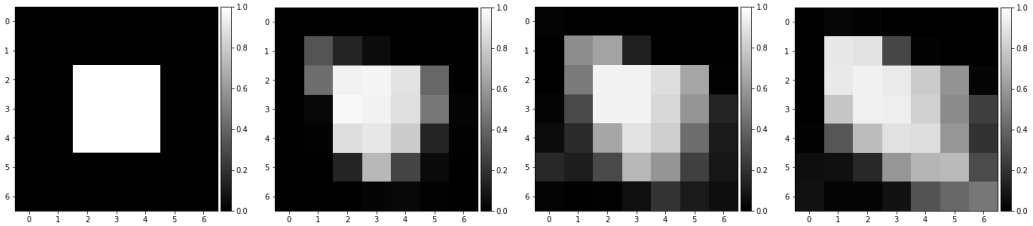
B.5 Effect of Constraint Threshold β

We also assess the effect of β with the Gridworld (A, B) environments. We do not assess the effect of β on the CartPole (MR, Mid) environments since our claim can be easily verified by just observing the learned costs for the Gridworld (A, B) environments. Our claim is as follows. With a higher β, the learned constraint function should have a higher CMSE and more state-action pairs with higher constraint values. This is because since β is higher, the agent is allowed to visit more high constraint value state-action pairs, as the constraint threshold is more relaxed. To verify this claim, we run experiments on the Gridworld (A, B) environments. Specifically, in addition to $\beta = 0.99$ (which corresponds to the results in Tables 1 and 2), we also run experiments with $\beta = 2.99, 5.99$. Our results are reported in Figures 8, 9. From the figures, it is apparent that our claim is correct.



True constraint function | ICL ($\beta = 0.99$) | ICL ($\beta = 2.99$) | ICL ($\beta = 5.99$)

Figure 8: Average constraint function value (averaged across 5 training seeds) for Gridworld (A) environment, demonstrating the effect of changing β.



True constraint function | ICL ($\beta = 0.99$) | ICL ($\beta = 2.99$) | ICL ($\beta = 5.99$)

Figure 9: Average constraint function value (averaged across 5 training seeds) for Gridworld (B) environment, demonstrating the effect of changing β.

C Training Setup and Experimental Details

All PPO variants mentioned in this paper are single-process for simplicity. For the tables, we abbreviate the Gridworld (A, B), CartPole (MR, Mid) environments as GA, GB, CMR, CMid.

C.1 Environments

We use the following environments in this work:

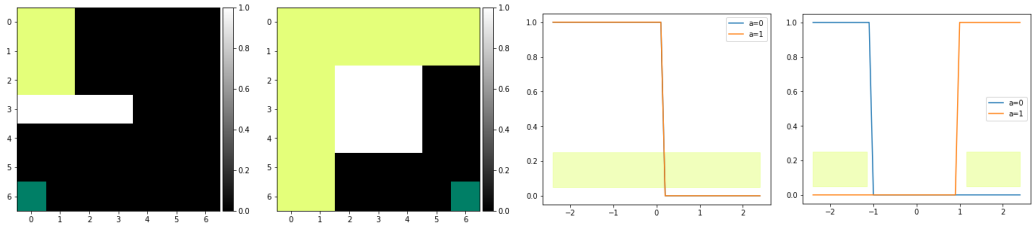
- **Gridworld (A, B)** are 7x7 gridworld environments (adapted from `yrlu`'s repository (Lu, 2019)). The start states, true constraint function and the goal state are indicated in Figure 10. The action space consists of 8 discrete actions including 4 nominal directions and 4 diagonal directions.
- **CartPole (MR, Mid)** (MR means Move Right) are variants of CartPole environment from OpenAI Gym (Brockman et al., 2016) where the objective is to balance a pole for as long as possible (maximum episode length is 200). The start regions and the true constraint function are indicated in Figure 10. Both variants may start in a region of high constraint value, and the objective is to move to a region of low constraint value and balance the pole there, while the constraint function is being learned.
- **HighD environment**: We construct an environment using ≈ 100 trajectories of length ≤ 1000 from the HighD highway driving dataset (Krajewski et al., 2018) (see Figure 11). The environment is adapted from the Wise-Move framework (Lee et al., 2019). For each trajectory, the agent starts on a straight road on the left side of the highway, and the objective is to reach the right side of the highway without colliding into any longitudinally moving cars. The action space consists of a single continuous action, i.e. the acceleration. Note that for this environment, we do not have the true constraint function. Instead, we aim to learn a constraint function that is able to capture the relationship between agent's velocity and the distance to car in the front.

The environments are more clearly illustrated in Figures 10 and 11.

C.2 Description of baseline methods

We use the following two baselines to compare against our method:

- **GAIL-Constraint**: Generative adversarial imitation learning (Ho & Ermon, 2016) is an imitation learning method that can be used to learn a policy that mimics the expert policy. The discriminator can be considered as a local reward function that incentivizes the agent to mimic the expert. We assume that the agent is maximizing the reward $r(s, a) := r_0(s, a) + \log(1 - c(s, a))$ where r_0 is the given true reward, and then the log term corresponds to the GAIL's discriminator. Note that when $c(s, a) = 0$, the discriminator reward is 0, and when $c(s, a) = 1$, the discriminator reward tends to $-\infty$.



Gridworld (A) Gridworld (B) CartPole (MR) CartPole (Mid)

Figure 10: Environments used in the experiments. White regions indicate constraint value of 1. Light green (or yellow) regions correspond to start states. Dark green regions correspond to the goal state. Gridworld environments have discrete states and discrete actions. Cartpole environments have continuous states and discrete actions.

Figure 11: HighD driving dataset environment. Leftmost white region indicates start region and rightmost white region indicates end region. Ego car is in blue, other cars are in red. This environment has both discrete and continuous states, and a continuous action.

- **Inverse constrained reinforcement learning (ICRL)** (Malik et al., 2021) is a recent method that is able to learn arbitrary Markovian neural network constraint functions, however, it can only handle hard constraints.

For both these methods, we use a similar training regime as adopted by (Malik et al., 2021), however, we try to keep the constraint function architecture fixed across all experiments (baselines and our method). *Note* that we did not include the method in Scobee and Sastry (Scobee & Sastry, 2019) as it is unable to handle continuous state spaces. Similarly, we did not include the binary constraint (BC) method described in (Malik et al., 2021) as GC and ICRL empirically perform better than BC, according to their experiments.

C.3 METRICS

We define two metrics for our experiments.

- **Constraint Mean Squared Error (CMSE)** is computed as the mean squared error between the true constraint function and the recovered constraint function on a uniformly discretized state-action space for the respective environment.
- **Normalized Accrual Dissimilarity (NAD)** is computed as follows. Given a policy learned by the method, we compute an agent dataset of trajectories. Then, the accrual (state-action visitation frequency) is computed for both the agent dataset and the expert dataset over a uniformly discretized state-action space, which is the same as the one used for CMSE. Finally, the accruals are normalized to sum to 1, and the Wasserstein distance is computed between the accruals.

More concretely, the NAD metric is computed as follows. Given the policy π learned by any method (ICL or a baseline), we sample a dataset $\mathcal{D}_\pi$ of agent trajectories (note that $|\mathcal{D}_\pi| = |\mathcal{D}|$, where $\mathcal{D}$ is the expert dataset):

$$\mathcal{D}_\pi := \textsc{Sample}_\tau(\Pi = \{\pi\}, p = \{1\}), \ \textsc{Sample} \text{ is defined in Algorithm 1}$$

Then, the accrual (state-action visitation frequency) is computed for both the agent dataset and the expert dataset over a uniformly discretized state-action space (this depends on the constraint function inputs). For the various environments, these are:

- **Gridworld (A, B)**: $\{(x, y) | x, y \in \{0, 1, ..., 6\}\}$

- **CartPole (MR, Mid)**: $\{(x, a)|x \in \{-2.4, -2.3, \cdots, 2.4\}, a \in \{0, 1\}\}$
- **HighD**: $\{(v, g)|v \in \{0, 1, \cdots, 40\}, g \in \{0, 1, \cdots, 80\}\}$ (here, v is in ms^{-1} and g is in pixels, where 1 pixel = 2.5m)

Finally, the accruals are normalized to sum to 1, and the Wasserstein distance is computed between the accruals. If the environment is CartPole, the 1D distance is computed and summed across actions. Otherwise, the 2D distance is computed. We use the Python Optimal Transport library (Flamary et al., 2021), specifically the `emd2` function to achieve this.

C.4 Common Hyperparameters

Hyperparameters common to all the experiments are listed in Table 5.

Table 5: Common Hyperparameters

Hyperparameter	Value(s)
PPO learning rate (η_2)	5×10^{-4}
Constraint function learning rate (η_3)	5×10^{-4}
Constraint function hidden layers	64+ReLU, 64+ReLU
Constraint function final activation	Sigmoid
PPO policy layers	64+ReLU, 64+ReLU
PPO value fn. layers	64+ReLU, 64+ReLU
Minibatch size	64
PPO clip parameter (ϵ_{PPO})	0.1
PPO entropy coefficient (λ_{ent})	0.01
PPO updates per epoch	25
No. of trajectories for any dataset	50
Training seeds	1, 2, 3, 4, 5

Since HighD is a continuous action space environment, we use Tanh activation for the policy, which outputs the mean and std. deviation of a learned Gaussian action distribution.

The inputs to the constraint functions are as follows:

- **Gridworld (A, B)**: x, y coordinates of the agent's position in the 7x7 grid
- **CartPole (MR, Mid)**: x position of the cart, and the discrete action (0/1 corresponding to left or right)
- **HighD**: velocity (ms^{-1}) of the ego, and the distance of the ego to the front vehicle in pixels (1 pixel $\approx$ 2.5 m)

The environment maximum horizons (episodes are terminated after these many steps) are as follows:

- **Gridworld (A, B)**: 50 steps
- **CartPole (MR, Mid)**: 200 steps
- **HighD**: 1000 steps

C.5 Hyperparameters for GAIL-Constraint

Hyperparameters specific to the GAIL-Constraint method are listed in Table 6. This method was adapted from Malik et al. (Malik et al., 2021) and they performed 1M timesteps of training on all environments. To be sure that this method performs as expected, we did 2M timesteps of training (except for the HighD environment where we do 0.4M timesteps of training, since it was computationally expensive to simulate).

C.6 Hyperparameters for ICRL

Similar to GAIL-Constraint, we performed 2M timesteps of training on all environments except HighD, where we performed 0.4M timesteps of training. Hyperparameters are listed in Table 7.

Table 6: GAIL-Constraint Hyperparameters

Hyperparameter	Value(s)				
	GA	GB	CMR	CMid	HighD
Discount factor (γ)	1.0	1.0	0.99	0.99	0.99
PPO steps per epoch	2000	2000	2000	2000	2000
PPO value fn. loss coefficient	0.5	0.5	0.5	0.5	0.5
PPO gradient clip value	0.5	0.5	0.5	0.5	0.5
PPO total steps	2M	2M	2M	2M	0.4M

ICRL did not perform as expected on two out of the four environments, that is, Gridworld (B) and the CartPole (Mid) environments, and may require further environment specific hyperparameter tuning. Nevertheless, we use these parameters since they (somewhat) worked on Gridworld (A) and CartPole (MR) environments. Note that for a fair comparison, we tried to ensure that for some of the parameters, we use the same value as our method, ICL (these parameters are number of rollouts, batch size, learning rate, γ, constraint function architecture etc.).

Table 7: ICRL Hyperparameters

Hyperparameter	Value(s)				
	GA	GB	CMR	CMid	HighD
Discount factor (γ)	1.0	1.0	0.99	0.99	0.99
PPO steps per epoch	2000	2000	2000	2000	2000
PPO value fn. loss coefficient	0.5	0.5	0.5	0.5	0.5
Constraint value fn. loss coefficient	0.5	0.5	0.5	0.5	0.5
PPO gradient clip value	0.5	0.5	0.5	0.5	0.5
Eval episodes	100	100	100	100	100
ICRL Iterations	200	200	200	200	40
Forward PPO timesteps	10000	10000	10000	10000	10000
PPO Budget	0	0	0	0	0
Penalty initial value (ν)	0.1	0.1	0.1	0.1	0.1
Penalty learning rate	0.01	0.01	0.01	0.01	0.01
Per step importance sampling	Yes	Yes	Yes	Yes	Yes
Forward KL (Old/New)	10	10	10	10	10
Backward KL (New/Old)	2.5	2.5	2.5	2.5	2.5
Backward iterations	5	5	5	5	5
Constraint network reg. coefficient	0.6	0.6	0.6	0.6	0.6

C.7 Hyperparameters for ICL (Our method)

The hyperparameters for our method are listed in Table 8. Our PPO implementation differs from the baselines (the baseline code was adapted from Malik et al. (Malik et al., 2021) official repository) as it does a fixed number of episodes per epoch rather than doing a fixed number of environment steps per epoch. We adjusted the number of PPO epochs in ICL so that each PPO procedure is roughly the same length (or less) as the ICRL/GAIL PPO procedure. Even then, the entire ICL training process requires a lot more steps than the GAIL-Constraint/ICRL baselines, since every iteration requires a complete PPO procedure. We have mentioned this in our conclusions section.

For the Gridworld (A, B) environments, we chose $\beta = 0.99$ to disallow any state of constraint value 1. For the CartPole (MR, Mid) environments, the cartpole may start in a high constraint value region. To allow it to navigate to a low constraint value region, we chose a high β. We chose β by doing a hyperparameter search on $\beta \in \{30, 50\}$ for the CartPole environments.

To choose λ, we tried values 1.5, 15, 150 and found that 1.5 was insufficient for the optimization. We know that λ is the ReLU multiplier term in the soft loss objective, and it cannot be a low value for constraint adjustment procedure. Hence, we chose a value of 15 which was appropriate for our experiments.

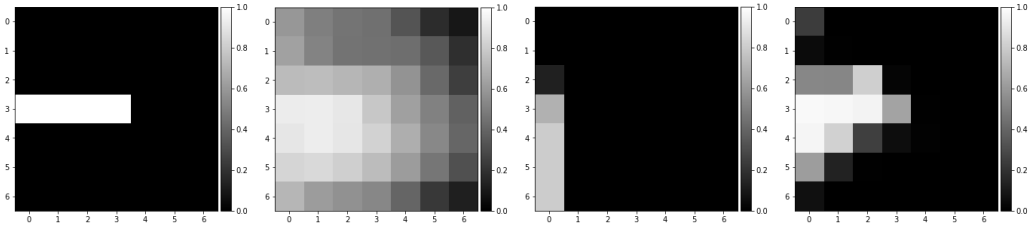
Table 8: ICL Hyperparameters

Hyperparameter	Value(s)				
	GA	GB	CMR	CMid	HighD
Discount factor (γ)	1.0	1.0	0.99	0.99	0.99
ICL Iterations (n)	10	10	10	10	3
Correction learning rate (η_1)	2.5×10^{-5}	2.5×10^{-5}	2.5×10^{-5}	2.5×10^{-5}	2.5×10^{-5}
PPO episodes per epoch	20	20	20	20	20
β	0.99	0.99	50	30	0.1
Constraint update epochs (e)	20	20	20	20	25
PPO epochs (m)	500	500	300	300	50
Soft loss coefficient λ	15	15	15	15	15

D TRAINING PLOTS

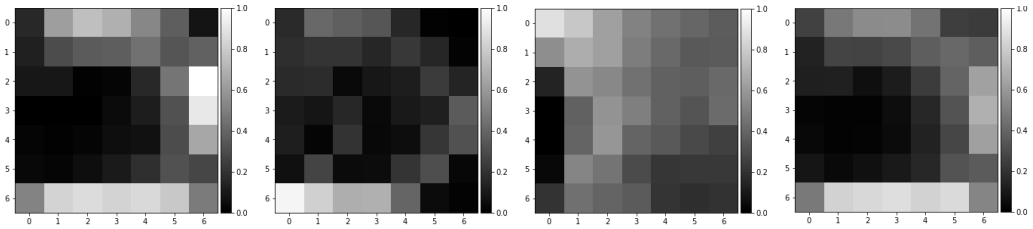
For completeness, we provide the training plots for the recovered constraint functions (Figures 12, 14, 16, 18) and their respective accruals (Figures 13, 15, 17, 19, 20). Note that we have reported the costs for the HighD environment in the main paper (Figure 2).

Please note that we have omitted the individual reward and constraint value plots, since there aren't any interesting insights. In all the environments, the reward goes up over time and the constraint value goes down over time, similar to Figures 3 and 4.



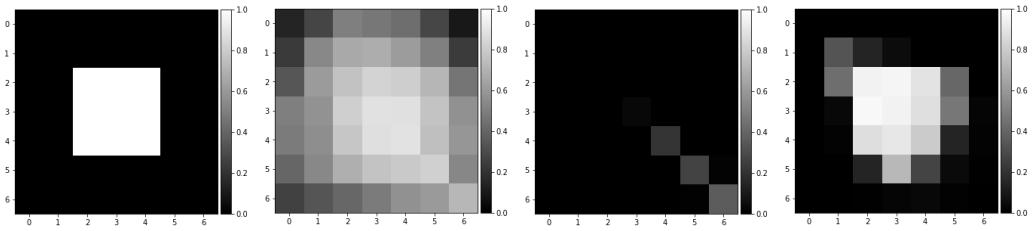
True constraint fn. GAIL-Constraint ICRL ICL ($\beta = 0.99$)

Figure 12: Average constraint function value (averaged across 5 training seeds) for Gridworld (A) environment.



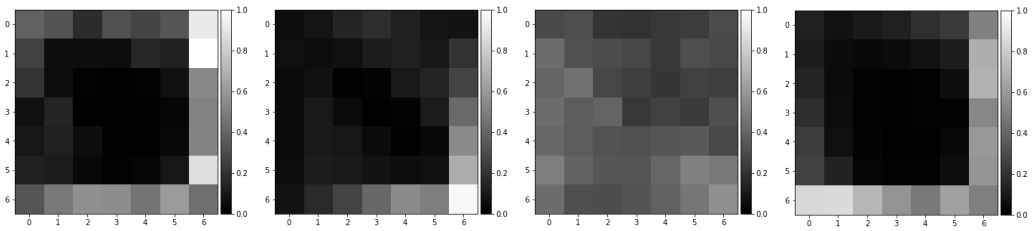
Expert accruals GAIL-Constraint ICRL ICL ($\beta = 0.99$)

Figure 13: Average normalized accruals (averaged across 5 training seeds) for Gridworld (A) environment.



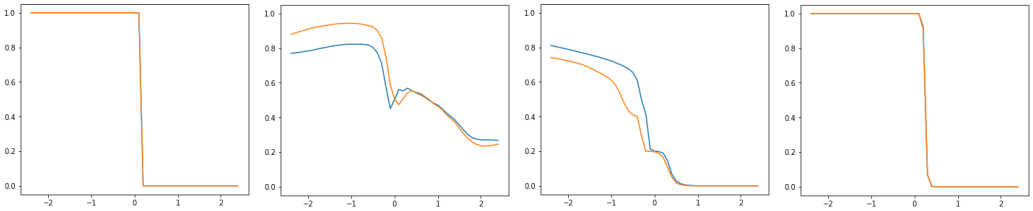
True constraint fn. GAIL-Constraint ICRL ICL ($\beta = 0.99$)

Figure 14: Average constraint function value (averaged across 5 training seeds) for Gridworld (B) environment.



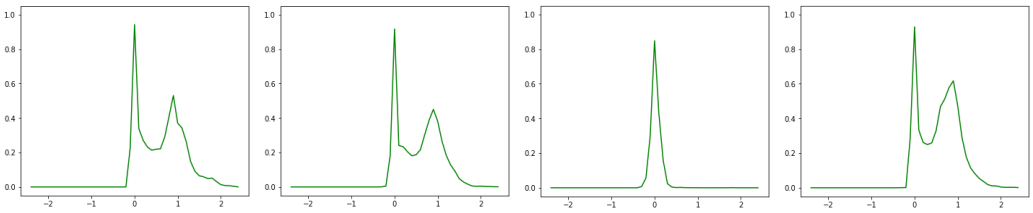
Expert accruals GAIL-Constraint ICRL ICL ($\beta = 0.99$)

Figure 15: Average normalized accruals (averaged across 5 training seeds) for Gridworld (B) environment.



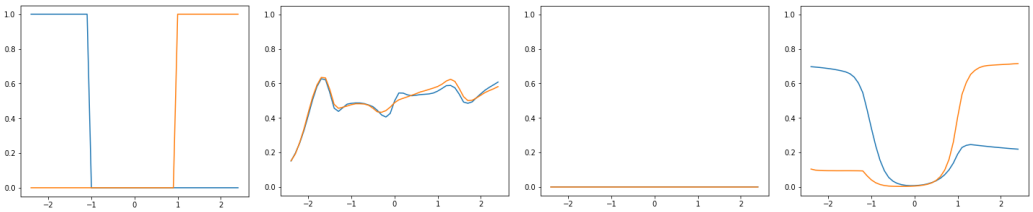
True constraint fn. GAIL-Constraint ICRL ICL ($\beta = 50$)

Figure 16: Average constraint function value (averaged across 5 training seeds) for CartPole (MR) environment. Blue line represents the constraint value for $a = 0$ (going left) and the orange line represents the constraint value for $a = 1$ (going right).



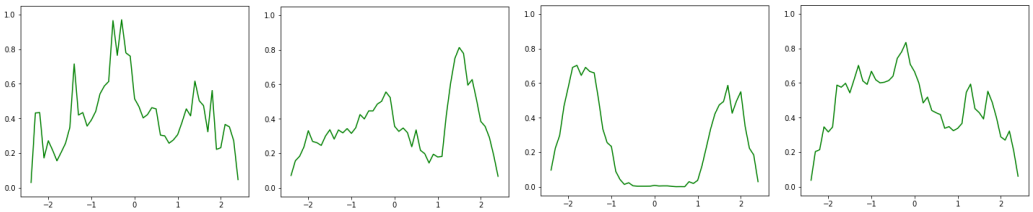
Expert accruals GAIL-Constraint ICRL ICL ($\beta = 50$)

Figure 17: Average normalized accruals (averaged across 5 training seeds) for CartPole (MR) environment.



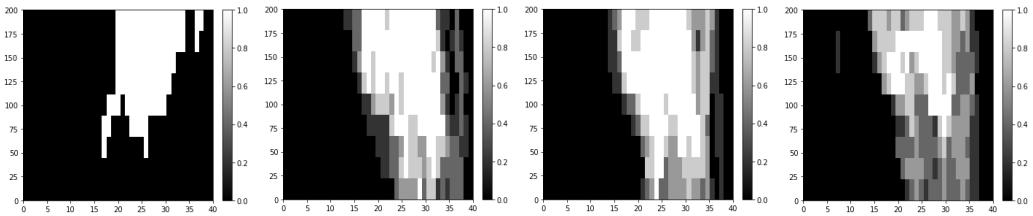
True constraint fn. GAIL-Constraint ICRL ICL ($\beta = 30$)

Figure 18: Average constraint function value (averaged across 5 training seeds) for CartPole (Mid) environment. Blue line represents the constraint value for $a = 0$ (going left) and the orange line represents the constraint value for $a = 1$ (going right).



Expert accruals GAIL-Constraint ICRL ICL ($\beta = 30$)

Figure 19: Average normalized accruals (averaged across 5 training seeds) for CartPole (Mid) environment.



Expert accruals GAIL-Constraint ICRL ICL ($\beta = 0.1$)

Figure 20: Average normalized accruals (averaged across 5 training seeds) for HighD environment. The X-axis and Y-axis are ego velocity in ms^{-1} and gap to the front vehicle g in m respectively.