Optimizing Percentile Criterion Using Robust MDPs

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Abstract

We address the problem of computing reliable policies in reinforcement learning problems with limited data. In particular, we compute policies that achieve good returns with high confidence when deployed. This objective, known as the *percentile criterion*, can be optimized using Robust MDPs (RMDPs). RMDPs generalize MDPs to allow for uncertain transition probabilities chosen adversarially from given ambiguity sets. We show that the RMDP solution's sub-optimality depends on the spans of the ambiguity sets along the value function. We then propose new algorithms that minimize the span of ambiguity sets defined by weighted L_1 and L_∞ norms. Our primary focus is on Bayesian guarantees, but we also describe how our methods apply to frequentist guarantees and derive new concentration inequalities for weighted L_1 and L_∞ norms. Experimental results indicate that our optimized ambiguity sets improve significantly on prior construction methods.

1 Introduction

Applying reinforcement learning to problem domains that involve high-stakes decisions, such as medicine or robotics, demands that we have high confidence in the quality of a policy before deploying it. Markov Decision Processes (MDPs) represent a well-established model in reinforcement learning (Puterman, 2005; Sutton and Barto, 2018), but their sequential nature makes them particularly sensitive to parameter errors, which can quickly accumulate (Mannor et al., 2007; Tirinzoni et al., 2018; Xu and Mannor, 2009). Parameter errors are unavoidable when estimating MDPs from

data (Laroche et al., 2019). We focus on computing policies that maximize high-confidence return guarantees in the batch settings. Such guarantees reduce the chance of disappointing the stakeholders after deploying the policy and give them a choice to gather more data or switch to an alternative strategy (Petrik et al., 2016).

We propose a new method for computing reliable policies that achieve, with high confidence, good returns once deployed. This objective is also known as the *percentile criterion* (Delage and Mannor, 2010) and can be modeled as risk-aversion to epistemic uncertainty (Petrik and Russel, 2019). Because optimizing the percentile criterion is NP-hard (Delage and Mannor, 2010), we use Robust MDPs (RMDPs) (Iyengar, 2005) to optimize it approximately. We establish new error bounds on the performance loss of the RMDPs' policy compared to the optimal percentile solution. Using these new bounds when constructing the RMDPs leads to policies with significantly better return guarantees than reported in prior work (Delage and Mannor, 2010; Petrik and Russel, 2019).

RMDPs generalize MDPs to allow for uncertain, or unknown, transition probabilities (Iyengar, 2005; Nilim and Ghaoui, 2005; Wiesemann et al., 2013). Transition probabilities are hard to estimate from data, and even small errors significantly impact the returns and policies. RMDPs consider transition probabilities to be chosen adversarially from a so-called *ambiguity set* (or an uncertainty set). The optimal policy is computed by solving a specific zero-sum game in which the agent chooses the best policy, and an adversarial nature chooses the worst transition probabilities from the ambiguity sets. RMDPs are tractable when their ambiguity sets satisfy so-called rectangularity assumptions (Goyal and Grand-Clement, 2018; Mannor et al., 2016; Wiesemann et al., 2013).

Given the goal is to optimize the percentile criterion, the critical question is how to construct the ambiguity sets from state transition samples to optimize the percentile criterion. Prior work constructs ambiguity sets as confidence regions bounded by a distance from a nominal (expected) transition probability (Auer et al.,

2009; Gupta, 2019; Iyengar, 2005; Petrik et al., 2016; Petrik and Russel, 2019; Strehl and Littman, 2004). In most cases, the ambiguity sets are represented as L_1-norm (also referred to as total variation) balls around the nominal probability. In comparison with other probability distance measures, like KL-divergence, the polyhedral nature of the L_1-norm allows more efficient computation (Ho et al., 2018).

The main contribution of this paper is a new technique for optimizing the *shape* of ambiguity sets in RMDPs. Prior work simply constructs ambiguity sets with the smallest size, or volume, that is sufficient to provide the desired high-confidence guarantees. Our new bounds show that the *span* of the ambiguity set along a specific direction is much more important than its volume. To minimize their span, we consider asymmetric ambiguity sets defined in terms of weighted L_1 and L_∞ balls. Recent results shows that RMDPs with such ambiguity sets can be solved very efficiently (Ho et al., 2018, 2020). Although our primary focus is on the Bayesian setup, we also discuss the frequentist setup and derive new high-confidence concentration inequalities for the weighted L_1 and L_∞ norms.

The remainder of the paper is organized as follows. We first describe the necessary background in Section 2 and bound the performance loss of RMDPs as a function of the ambiguity sets' span in Section 3. Section 4 describes algorithms that minimize the span of ambiguity sets by optimizing the weights of the norms used in their definition. Then, Section 5 describes methods for choosing the size of the weighted-norm ambiguity sets. In Section 6, we outline the approach in the frequentist setup and present new concentration inequalities for weighted L_1 and L_∞ ambiguity sets. Finally, the experimental results in Section 7 show that minimizing ambiguity sets' span greatly improves the RMDPs' solution quality.

Notation: Bold letters, like $\boldsymbol{x}_s$, indicate an s-th vector, while y_s would indicate the s-th element of a vector $\boldsymbol{y}$. The symbol Δ^N denotes the N-dimensional probability simplex (non-negative vectors that sum to 1). We also use $\mathcal{A}^\mathcal{B}$ to denote the set of all functions $\mathcal{A} \to \mathcal{B}$.

2   Framework and Related Work

We consider the standard infinite-horizon MDP setting with finite states $\mathcal{S} = \{1, \dots, S\}$ and actions $\mathcal{A} = \{1, \dots, A\}$. The agent can take any action $a \in \mathcal{A}$ in every state $s \in \mathcal{S}$ and transitions to the next state s' according to the *true* transition function $P^\star : \mathcal{S} \times \mathcal{A} \to \Delta^S$, where Δ^S is a probability simplex. For any transition function $P : \mathcal{S} \times \mathcal{A} \to \Delta^S$, we use the shorthand $\boldsymbol{p}_{s,a} = P(s,a)$ to denote the vector of transition probabilities from a state $s \in \mathcal{S}$ and

an action $a \in \mathcal{A}$. The agent also receives a reward $r_{s,a,s'} \in \mathbb{R}$; we use $\boldsymbol{r}_{s,a} = (r_{s,a,s'})_{s' \in \mathcal{S}} \in \mathbb{R}^S$ to denote the vector of rewards. The goal is to compute a deterministic policy $\pi : \mathcal{S} \to \mathcal{A}$ that maximizes the γ-discounted return (Puterman, 2005):

$$\max_{\pi \in \Pi} \ \rho(\pi, P) = \max_{\pi \in \Pi} \ \mathbb{E}\left[\sum_{t=0}^{\infty} \gamma^t \cdot r_{S_t, \pi(S_t), S_{t+1}}\right] \ ,$$

where $S_0 \sim \boldsymbol{p}_0$, $S_{t+1} \sim P^\star(S_t, \pi(S_t))$, $\boldsymbol{p}_0 \in \Delta^S$ is the initial probability distribution, and Π is the set of all deterministic policies. The return function ρ is parameterized by P, because we assume them to be uncertain or unknown.

We consider the batch RL setting in which the transition function must be estimated from a fixed dataset $D = (s_t, a_t, s'_t)_{t=1,\dots,T}$ generated by a behavior policy. We describe the Bayesian setup first and outline the frequentist extension in Section 6. Bayesian techniques start with a prior distribution over the transition function $P^\star$ and then derive a posterior distribution f over $P^\star$ (Delage and Mannor, 2010; Gelman et al., 2014; Xu and Mannor, 2009). We use the concise notation $\tilde{P} = P^\star \,|\, D$ to represent the posterior over the transition function conditioned on the data D. In other words, $\mathbb{E}[\tilde{P}] = \mathbb{E}[P^\star \,|\, D]$.

Percentile citerion   The Bayesian *percentile criterion* optimization simultaneously optimizes for the policy π and a *high-confidence lower bound* on its performance y:

$$\max_{\pi \in \Pi} \max_{y \in \mathbb{R}} \ \left\{ y \mid \mathbb{P}_{\tilde{P} \sim f}\left[\rho(\pi, \tilde{P}) \geq y \right] \geq 1 - \delta \right\} \ . \quad (1)$$

The confidence parameter $\delta \in [0, 1/2)$ bounds the probability that the optimized policy π fails to achieve a return of at least y when deployed. For example, $\delta = 0$ maximizes the worst-case return, and $\delta = 0.5$ maximizes the median return. It is common in practice to choose a small positive value, such as $\delta = 0.05$, in order to achieve meaningful guarantees without being overly conservative. Also, the constraint $\delta < 1/2$ is important as our results (Theorem 3.2) do not hold for the risk-seeking setting with $\delta \geq 1/2$.

There are several important practical advantages to optimizing the percentile criterion instead of the average return (Delage and Mannor, 2010). First, the output policy is more robust and less likely to fail catastrophically due to model errors. Second, the objective value y in (1) provides a high-confidence lower bound on the true return. Having such a guarantee on its return helps to avoid an unpleasant surprise when the policy π is deployed. If the guarantee y is insufficiently low, the stakeholder may decide to collect more data

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or choose a different methodology for guiding their decisions.

We emphasize that we develop algorithms that are independent of how the posterior distribution f is computed. Bayesian priors can be as simple as independent Dirichlet distributions over $\boldsymbol{p}_{s,a}^{\star}$ for each state s and action a. However, hierarchical Bayesian models are more practical since they can generalize among states even when $|D| \ll S$ (Delage and Mannor, 2010; Petrik and Russel, 2019). Many tools, such as Stan (Stan Development Team, 2017) or JAGS, now exist that allow for convenient and efficient computation of the posterior distribution f using MCMC.

Robust MDPs Because the optimization in (1) is NP-hard (Delage and Mannor, 2010), we seek new algorithms that can approximate it efficiently. Robust MDPs (RMDPs), which extend regular MDPs, are a convenient and powerful framework that can be used to optimize the percentile criterion. In particular, RMDPs allow for a generic ambiguity set $\hat{\mathcal{P}} \subseteq \left\{ P : \mathcal{S} \times \mathcal{A} \to \Delta^{S} \right\}$ of possible transition functions instead of a single known value P. The solution to an RMDP is the best policy for the worst-case plausible transition function:

$$\max_{\pi \in \Pi} \min_{P \in \hat{\mathcal{P}}} \rho(\pi, P) \ . \qquad (2)$$

The optimization problem in (2) is NP-hard (Nilim and Ghaoui, 2005; Wiesemann et al., 2013) but is tractable for rectangular ambiguity sets which are defined independently for each state and action (Iyengar, 2005; Le Tallec, 2007). We, therefore, restrict our attention to SA-rectangular ambiguity sets defined as p-norm balls around nominal probability distributions for some $w : \mathcal{S} \times \mathcal{A} \to \mathbb{R}_{++}^{S}$ and $\psi : \mathcal{S} \times \mathcal{A} \to \mathbb{R}_{+}$:

$$\mathcal{P}(w, \psi) = \left\{ P \in \mathcal{F} \mid P(s,a) \in \mathcal{P}_{s,a}(w(s,a), \psi(s,a)) \right\},$$

where $\mathcal{F} = (\Delta^{S})^{\mathcal{S} \times \mathcal{A}}$. In the remainder of the paper, we resort to the shorter notation $\boldsymbol{w}_{s,a} = w(s,a)$ and $\psi_{s,a} = \psi(s,a)$ when the meaning is obvious from the context. Note that $\hat{\mathcal{P}}$ refers to a generic ambiguity set, while $\mathcal{P}(w, \psi)$ refers to the specific norm-based one. The ambiguity set $\mathcal{P}_{s,a}(\boldsymbol{w}, \psi)$ for $s \in \mathcal{S}$, $a \in \mathcal{A}$, positive weights $\boldsymbol{w} \in \mathbb{R}_{++}^{S}$, and budget $\psi \in \mathbb{R}_{+}$ is defined as:

$$\mathcal{P}_{s,a}(\boldsymbol{w}, \psi) = \left\{ \boldsymbol{p} \in \Delta^{S} \ : \ \left\| \boldsymbol{p} - \bar{\boldsymbol{p}}_{s,a} \right\|_{\boldsymbol{w}} \leq \psi \right\}, \qquad (3)$$

where $\bar{\boldsymbol{p}}_{s,a} = \mathbb{E}_{\tilde{P}} \left[\tilde{P}(s,a) \right]$ is the mean posterior transition probability. The weighted polynomial norms are defined as $\|\boldsymbol{y}\|_{1,\boldsymbol{w}} = \sum_{i=1}^{S} w_i \cdot |y_i|$ and $\|\boldsymbol{y}\|_{\infty,\boldsymbol{w}} = \max \left\{ w_i \cdot |y_i| \mid i \in \mathcal{S} \right\}$. We use the generic notation $\|\cdot\|_{\boldsymbol{w}}$ in statements that hold for both $\|\cdot\|_{1,\boldsymbol{w}}$ and $\|\cdot\|_{\infty,\boldsymbol{w}}$.

The weights $\boldsymbol{w}$ in (3) determine the shape of the ambiguity set, and the budget ψ determines its size.

Note that the parameter ψ in the definition of $\mathcal{P}_{s,a}(\boldsymbol{w}, \psi)$ is redundant. It can be set to 1 without loss of generality: $\mathcal{P}_{s,a}(\boldsymbol{w}, \psi) = \mathcal{P}_{s,a}(1/\psi \cdot \boldsymbol{w}, 1)$ when $\psi > 0$. In other words, it is possible to change the size of the ambiguity set solely by scaling the weights $\boldsymbol{w}$. To eliminate this redundancy, we assume without loss of generality that the weights of the set are normalized such that $\|\boldsymbol{w}\|_2 = 1$.

In rectangular RMDPs, a unique optimal value function $\hat{\boldsymbol{v}} \in \mathbb{R}^{S}$ exists and is a fixed point of the robust Bellman operator $\mathfrak{L} : \mathbb{R}^{S} \to \mathbb{R}^{S}$ defined for each $s \in \mathcal{S}$ and $\boldsymbol{v} \in \mathbb{R}^{S}$ as (Iyengar, 2005)

$$(\mathfrak{L}\boldsymbol{v})_s = \max_{a \in \mathcal{A}} \min_{\boldsymbol{p} \in \hat{\mathcal{P}}_{s,a}} \left(\boldsymbol{r}_{s,a} + \gamma \cdot \boldsymbol{p}^{\mathsf{T}} \boldsymbol{v} \right) \ . \qquad (4)$$

The optimal robust value function can be computed using value iteration, policy iteration, and other methods (Ho et al., 2020; Iyengar, 2005; Kaufman and Schaefer, 2013). The optimal robust policy $\hat{\pi} : \mathcal{S} \to \mathcal{A}$ is greedy with respect to the optimal robust value function $\hat{\boldsymbol{v}}$, and the robust return can be computed from the value function as (Ho et al., 2020):

$$\hat{\rho} = \max_{\pi \in \Pi} \min_{P \in \hat{\mathcal{P}}} \rho(\pi, P) = \boldsymbol{p}_0^{\mathsf{T}} \hat{\boldsymbol{v}} \ .$$

We will find it convenient to use $\hat{\boldsymbol{z}}_{s,a} \in \mathbb{R}^{S}$, $s \in \mathcal{S}, a \in \mathcal{A}$ to denote the vector of values associated with the transitions from the state s and action a:

$$\hat{\boldsymbol{z}}_{s,a} = \boldsymbol{r}_{s,a} + \gamma \cdot \hat{\boldsymbol{v}} \ . \qquad (5)$$

In the remainder of the paper, we use $\hat{\mathcal{P}}$ to denote a generic RMDP ambiguity set and use $\mathcal{P}(w, \psi)$ to denote an ambiguity set defined in terms of a weighted norm ball.

3 RMDPs for Percentile Optimization

This section describes the general algorithm for constructing RMDP ambiguity sets for optimizing the percentile criterion. We derive new bounds on the safety and optimality of the RMDP solution and propose a new algorithm that optimizes them. The bounds and algorithms in this section are general and are not restricted to norm-based ambiguity sets.

An important assumption, which is used throughout this paper, is that the ambiguity set in the RMDP is constructed to guarantee that it contains the unknown transition probabilities $\tilde{P}$ with a high probability as formalized next.

Assumption 1. *The RMDP ambiguity set* $\hat{\mathcal{P}} \subseteq \left\{ P : \mathcal{S} \times \mathcal{A} \to \Delta^{S} \right\}$ *satisfies that:*

$$\mathbb{P}_{\tilde{P}} \left[\tilde{P} \in \hat{\mathcal{P}} \right] \geq 1 - \delta \ .$$

Assumption 1 is common when constructing RMDPs for optimizing the percentile criterion (Delage and Mannor, 2010; Petrik and Russel, 2019). The following theorem shows that Assumption 1 is a sufficient condition for $\hat{\rho}$ to be a lower bound on the true return of the robust policy $\hat{\pi}$. We state the result in terms of a generic ambiguity set $\hat{\mathcal{P}}$.

Theorem 3.1. *If Assumption 1 holds, then the following inequality is satisfied with probability $1 - \delta$:*

$$\hat{\rho} \leq \rho(\hat{\pi}, \tilde{P}) \ .$$

Please see Appendix A.1 for the proof.

Theorem 3.1 generalizes Theorem 4.2 in (Petrik and Russel, 2019) by relaxing its assumptions. In particular, Assumption 1 allows for non-rectangular ambiguity sets $\hat{\mathcal{P}}$ and does not require the use of a union bound in its construction.

Next, we bound the performance loss of the RMDP policy $\hat{\pi}$ with respect to the optimal percentile criterion guarantee in (1). As we show, the quality of the RMDP policy depends not simply on the absolute size of the ambiguity set ψ, but on its span along a specific direction. The *span* $\beta_{\boldsymbol{z}}^{s,a}(\boldsymbol{w}, \psi)$ of an ambiguity set $\mathcal{P}_{s,a}(\boldsymbol{w}, \psi)$ along a vector $\boldsymbol{z} \in \mathbb{R}^S$ for $s \in \mathcal{S}$ and $a \in \mathcal{A}$ is defined as:

$$\beta_{\boldsymbol{z}}^{s,a}(\boldsymbol{w}, \psi) = \max_{\boldsymbol{p}_1, \boldsymbol{p}_2} \left\{ (\boldsymbol{p}_1 - \boldsymbol{p}_2)^\mathsf{T} \boldsymbol{z} \mid \boldsymbol{p}_1, \boldsymbol{p}_2 \in \mathcal{P}_{s,a}(\boldsymbol{w}, \psi) \right\}.$$

The following theorem bounds the performance loss of the RMDP solution when using norm-bounded ambiguity sets. Note that Theorem 3.1 implies that, under Assumption 1, the RMDP return $\hat{\rho}$ bounds the true return with high confidence and therefore must be a lower bound on the optimal $y^\star$ in (1).

Theorem 3.2. *When Assumption 1 holds for $\hat{\mathcal{P}} = \mathcal{P}(w, \psi)$, $w : \mathcal{S} \times \mathcal{A} \to \mathbb{R}_{++}^S$, $\psi : \mathcal{S} \times \mathcal{A} \to \mathbb{R}_+$, then the performance loss with respect to $y^\star$ optimal in (1) is:*

$$0 \leq y^\star - \hat{\rho} \leq \frac{1}{1 - \gamma} \cdot \max_{s \in \mathcal{S}} \max_{a \in \mathcal{A}} \beta_{\hat{\boldsymbol{z}}_{s,a}}^{s,a}(\boldsymbol{w}, \psi) \ ,$$

where $\hat{\rho}$ is a function of w and ψ.

The proof can be found in Appendix A.1.

The following illustrates how the span along $\hat{\boldsymbol{z}}$ impacts the performance loss of the RMDP policy.

Example 3.3. *Consider an MDP with states $\{0, 1, 2, 3\}$ and a single action $\{1\}$. The state 0 is initial, and the states $1, 2, 3$ are terminal with $P(i, 1, i) = 1, i = 1, 2, 3$ with zero rewards. To keep the notation simple, we assume that it is only possible to transition from state 0 to states $1, 2, 3$. The transition probability $\tilde{\boldsymbol{p}}_{0,1}$ is uncertain and distributed as $\tilde{\boldsymbol{p}}_{0,1} \sim$*
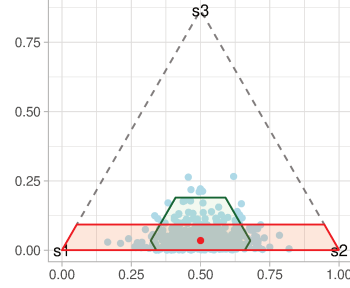

Figure 1: Posterior samples of $\tilde{\boldsymbol{p}}$ (blue) and ambiguity sets $\mathcal{P}^{\mathrm{std}}$ (green) and $\mathcal{P}^{\mathrm{opt}}$ (red) from Example 3.3.

Dirichlet$(10, 10, 1)$ with $\mathbb{E}[\tilde{\boldsymbol{p}}_{0,1}] = [0.48, 0.48, 0.04]$. The rewards are $\boldsymbol{r}_{0,1} = [0.25, 0.25, -1]$. The goal is to maximize the percentile criterion with $\delta = 0.2$.

Take the MDP from Example 3.3 and construct RMDPs with the following two ambiguity sets depicted in Figure 1. Let $\mathcal{P}^{\mathrm{std}} = \mathcal{P}_{1,1}(1/\sqrt{3} \cdot \mathbf{1}, 0.1)$ be the standard ambiguity set with uniform weights, and let $\mathcal{P}^{\mathrm{opt}} = \mathcal{P}_{1,1}(1/\sqrt{1.12} \cdot [0.25, 0.25, 1], 0.1)$ be an ambiguity set with optimized weights $\boldsymbol{w} = 1/\sqrt{1.12} \cdot [0.25, 0.25, 1]$. The budgets for both ambiguity sets are minimally sufficient to satisfy Assumption 1. Intuitively, this means that at least 80% of the posterior samples of $\tilde{\boldsymbol{p}}_{0,1}$ (blue dots in Figure 1) must be contained inside of each ambiguity set. Now, with 80% confidence, the RMDP with $\mathcal{P}^{\mathrm{opt}}$ guarantees return $\hat{\rho}^{\mathrm{opt}} = 0.16$, while the RMDP with $\mathcal{P}^{\mathrm{std}}$ guarantees only $\hat{\rho}^{\mathrm{std}} = -0.06$. Although the volumes of $\mathcal{P}^{\mathrm{std}}$ and $\mathcal{P}^{\mathrm{opt}}$ are approximately equal, the span along the dimension $\boldsymbol{z} = [0.25, 0.25, -1]$ of $\mathcal{P}^{\mathrm{opt}}$ is half of the span of $\mathcal{P}^{\mathrm{std}}$.

Armed with the safety and performance loss guarantees in Theorems 3.1 and 3.2, we propose a new heuristic algorithm in Algorithm 1 which iteratively optimizes the shape of the ambiguity set in order to improve the guaranteed percentile. It constructs ambiguity sets that minimize the span of the ambiguity set. The algorithm may not construct the optimal ambiguity set because it first uses the nominal value function $\boldsymbol{v}'$. However, the algorithm provides guarantees on the quality of the policy that it computes from Assumption 1 and Theorems 3.1 and 3.2.

4 Minimizing Ambiguity Spans

This section describes tractable algorithms that optimize the weights $\boldsymbol{w}$ to minimize that span $\beta_{\boldsymbol{z}}^{s,a}$ for some fixed state $s \in \mathcal{S}$, action $a \in \mathcal{A}$, a vector $\boldsymbol{z} \in \mathbb{R}^S$, and a budget $\psi \in \mathbb{R}_+$. We describe an analytical solution and a conic formulation that minimize an upper bound on the span for weighted L_1 and L_∞ sets. The budget

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Algorithm 1: Ambiguity shape optimization scheme.

Input: Confidence $1 - \delta$, posterior distribution f over $\tilde{P}$
Output: Ambiguity set $\mathcal{P}(\boldsymbol{w}, \psi)$

1   Compute $\boldsymbol{v}' \in \mathbb{R}^S$ by solving $\max_\pi \rho\big(\pi, \mathbb{E}[\tilde{P}]\big)$ and let $\boldsymbol{z}'_{s,a} \leftarrow \boldsymbol{r}_{s,a} + \gamma \cdot \boldsymbol{v}'$, $s \in \mathcal{S}, a \in \mathcal{A}$;

2   Compute minimal $\psi' : \mathcal{S} \times \mathcal{A} \to \mathbb{R}_+$ such that Assumption 1 holds for $\mathcal{P}(1/\sqrt{s} \cdot \mathbf{1}, \psi')$;   // Algorithm 3

3   Compute $\boldsymbol{w}_{s,a} \leftarrow \min_{\boldsymbol{w} \in \mathbb{R}_+^S} \{\beta_{\boldsymbol{z}'}^{s,a}(\boldsymbol{w}, \psi') \mid \|\boldsymbol{w}\|_2 = 1\}$ for each $s \in \mathcal{S}, a \in \mathcal{A}$;   // Algorithm 2

4   Compute minimal $\psi : \mathcal{S} \times \mathcal{A} \to \mathbb{R}_+$ such that Assumption 1 holds for $\mathcal{P}(\boldsymbol{w}, \psi)$;   // Algorithm 3

5   **return** *Ambiguity set* $\mathcal{P}(\boldsymbol{w}, \psi)$

ψ is fixed throughout this section; Section 5 describes how to optimize it.

The goal of computing the weights $\boldsymbol{w}$ that minimize the span of the ambiguity set for a fixed budget ψ can be formalized as the following optimization problem:

$$\min_{\boldsymbol{w} \in \mathbb{R}_+^S} \left\{ \beta_{\boldsymbol{z}}^{s,a}(\boldsymbol{w}, \psi) \mid \|\boldsymbol{w}\|_2 = 1 \right\}. \tag{6}$$

The optimization in (6) is not obviously convex, but we propose methods that minimize an *upper* bound on $\beta_{\boldsymbol{z}}^{s,a}(\boldsymbol{w}, \psi)$. Note that minimizing this upper bound also minimizes an upper bound on Theorem 3.2.

We first describe two analytical solutions and then describe a more precise but also more computationally intensive method based on second order conic approximation. The following lemma provides a bound that enables efficient optimization.

Lemma 4.1. *The span $\beta_{\boldsymbol{z}}^{s,a}$ of the ambiguity set $\mathcal{P}_{s,a}(\boldsymbol{w}, \psi)$ is bounded for any $\lambda \in \mathbb{R}$ as:*

$$\beta_{\boldsymbol{z}}^{s,a}(\boldsymbol{w}, \psi) \le 2 \cdot \psi \cdot \|\boldsymbol{z} - \lambda \cdot \mathbf{1}\|_\star , \tag{7}$$

where $\|\cdot\|_\star$ is the norm dual to $\|\cdot\|_{\boldsymbol{w}}$.

The proof is deferred to Appendix A.2. Recall that the *dual norm* is defined as $\|\boldsymbol{c}\|_\star = \max_{\boldsymbol{x} \in \mathbb{R}^S} \{\boldsymbol{c}^\mathsf{T}\boldsymbol{x} \mid \|\boldsymbol{x}\| \le 1\}$.

In order to use the bound in Lemma 4.1, we need to derive the dual norms to the weighted L_1 and weighted L_∞ norms. For unweighted p-norms, it is well known that L_1 and L_∞ norms are dual of each other, but we are not aware of a similar result for their weighted variants. The following lemma establishes that weighted L_1 and L_∞ norms are dual as long as their weights are inverse elementwise.

Lemma 4.2. *Suppose that $\boldsymbol{w} \in \mathbb{R}^S$ and $\boldsymbol{w}' \in \mathbb{R}^S$ are positive $w_i > 0, w_i' > 0$ and satisfy that $w_i' = 1/w_i$ for all $i \in \mathcal{S}$. Then:*

$$\|\boldsymbol{z}\|_{\infty, \boldsymbol{w}'} = \max_{\boldsymbol{x} \in \mathbb{R}^S} \left\{ \boldsymbol{z}^\mathsf{T}\boldsymbol{x} \mid \|\boldsymbol{x}\|_{1, \boldsymbol{w}} = 1 \right\}.$$

The proof of the lemma can be found in Appendix A.2.

Algorithm 2: Weight optimization.

Input: Norm $q \in \{1, \infty\}$, parameter $\lambda \in \mathbb{R}$
Output: Weights $\boldsymbol{w}^\star \in \mathbb{R}_+^S$ that minimize (7)

1   **if** $q = 1$ **then**

2     $\Big| \quad w_i^\star \leftarrow \dfrac{|z_i - \lambda|^{1/3}}{\sqrt{\sum_{j=1}^S |z_j - \lambda|^{2/3}}}, \forall i \in \mathcal{S}$;

3   **else if** $q = \infty$ **then**

4     $\Big| \quad w_i^\star \leftarrow \dfrac{|z_i - \lambda|}{\sqrt{\sum_{j=1}^S |z_j - \lambda|^2}}, \forall i \in \mathcal{S}$;

5   **end**

6   **return** $\boldsymbol{w}^\star$;

Based on the results above, Algorithm 2 summarizes our algorithms for computing weights $\boldsymbol{w}$ that minimize the upper bound on the performance loss in Theorem 3.2. The algorithm runs in linear time. Note that the algorithm assumes that a value of λ is given. Although it would be possible to optimize for the best value of λ, our preliminary experimental results suggest that this is not worthwhile because it does not lead to a significant improvement. Instead, we use $\lambda = (\max_i z_i + \min_i z_i)/2$ and $\lambda = \mathrm{median}(\boldsymbol{z})$ for L_∞ and L_1 norms respectively. These are the optimal values (values for which the upper bound is smallest) for the uniform weight version of (7). The following proposition states the correctness of this algorithm.

Proposition 4.3. *Fix an arbitrary $\lambda \in \mathbb{R}$ and let $\boldsymbol{w}^\star \in \mathbb{R}_+^S$ the return from Algorithm 2. Then $\boldsymbol{w}^\star$ is an optimal solution to (7) weighted L_1 and L_∞ norms.*

Please see Appendix A.2 for the proof.

It is important to recognize that even though Algorithm 2 effectively minimizes the value $\beta_{\boldsymbol{z}}^{s,a}$, it may, in the process, violate Assumption 1. This is because scaling weights may reduce the probability that $\tilde{P} \in \mathcal{P}$. We are not aware of a tractable algorithm that can optimize the weights $\boldsymbol{w}$ directly while enforcing the constraint of Assumption 1. Instead, the constraint $\|\boldsymbol{w}\|_2 = \psi$ serves as a proxy to prevent the ambiguity from shrinking. This is why it is necessary to re-optimize the budget ψ in Algorithm 1 after the weights are optimized.

As an alternative to the analytical algorithms in Algorithm 2, we also examine a Second-Order Conic Program (SOCP) formulation. This formulation optimizes a tighter upper bound on $\beta_{\mathbf{z}}^{s,a}$ but is more computationally intensive. For any fixed state s and action a, the following SOCP minimizes the bound (7) on $\beta_{\mathbf{z}}^{s,a}(\boldsymbol{w}, \psi)$ for the L_1 norm:

$$\begin{aligned} \underset{\boldsymbol{g}, c, \lambda}{\text{minimize}} \quad & \psi \cdot c \\ \text{subject to} \quad & \boldsymbol{g} \geq \max\{\boldsymbol{z} - \lambda \cdot \mathbf{1}, -\boldsymbol{z} + \lambda \cdot \mathbf{1}\} \quad (8) \\ & \boldsymbol{g}^{\mathsf{T}} \boldsymbol{g} \leq c^2, \quad \boldsymbol{g} \geq \mathbf{0} . \end{aligned}$$

The SOCP formulation follows from Lemma 4.2 and variable substitution $\boldsymbol{g} = \boldsymbol{w} \cdot c$.

Remark 4.4 (Unreachable states). We assume that the prior can specify some transitions as impossible, or unreachable: that is $P(s, a, s') = 0$. This information is used as an additional pre-processing step in optimizing the weights. In particular, if the transition from state s after taking action a to state s' is not possible, then we set $(\boldsymbol{w}_{s,a})_{s'} = \infty$. Or, in other words, each $\boldsymbol{p} \in \mathcal{P}_{s,a}(\boldsymbol{w}, \psi)$ satisfies $p_{s'} = 0$.

5 Minimizing Ambiguity Budgets

This section describes how to determine the size of the ambiguity set in the Bayesian setting in order to minimize the performance loss in Theorem 3.2 of the RMDP policy while satisfying Assumption 1. We assume that the weights $\boldsymbol{w}_{s,a}, s \in \mathcal{S}, a \in \mathcal{A}$ are arbitrary but fixed and aim to construct $\psi_{s,a}, s \in \mathcal{S}, a \in \mathcal{A}$ to minimize the performance loss.

Before describing the algorithm, we state a simple observation that motivates its construction. The following lemma implies that the smaller the ambiguity budget is, the better $\hat{\rho}$ approximates the percentile criterion. Of course, this is only true as long as the budget is sufficiently large for Assumption 1 to hold. The following proposition follows from the definition of $\beta_{\mathbf{z}}^{s,a}$ by algebraic manipulation.

Lemma 5.1. *The function* $\psi \mapsto \beta_{\mathbf{z}}^{s,a}(\boldsymbol{w}_{s,a}, \psi)$ *is non-decreasing.*

We are now ready to describe our method as outlined in Algorithm 3. The algorithm follows the well-known sample average approximation (SAA) approach common in stochastic programming (Shapiro et al., 2014). It constructs ambiguity sets as *credible regions* for the posterior distribution over $\tilde{P}$ similarly to prior work (Petrik and Russel, 2019). The next proposition states the correctness of Algorithm 3.

Proposition 5.2. *Suppose that* $\psi_{s,a}$ *are computed by Algorithm 3 for some* $\boldsymbol{w}_{s,a}$ *for each* $s \in \mathcal{S}$ *and* $a \in \mathcal{A}$.

Algorithm 3: Budget optimization.

> **Input:** Posterior samples $P_1, \ldots, P_n$ from $\tilde{P}$, weights $\boldsymbol{w}_{s,a}$, norm $q \in \{1, \infty\}$
> **Output:** Nominal $\bar{\boldsymbol{p}}_{s,a}$ and budget $\psi_{s,a}$

1 Compute nominal $\bar{\boldsymbol{p}}_{s,a} \leftarrow (1/n) \sum_{i=1}^{n} P_i(s, a)$;
2 Compute distance $d_i \leftarrow \left\| P_i(s,a) - \bar{\boldsymbol{p}}_{s,a} \right\|_{q, \boldsymbol{w}_{s,a}}$;
3 Ascending sort: $d_{(j)} \leq d_{(j+1)}, j = 1, \ldots, n$;
4 Compute the quantile $\psi_{s,a} \leftarrow d_{(\lceil (1-\delta/(S \cdot A)) \cdot n \rceil)}$;
5 **return** $\bar{\boldsymbol{p}}_{s,a}$ *and* $\psi_{s,a}$

Also let $w : (s, a) \mapsto \boldsymbol{w}_{s,a}$ *and* $\psi : (s, a) \mapsto \psi_{s,a}$. *Then* $\mathcal{P}(w, \psi)$ *satisfies Assumption 1 with high probability when a sufficient number of samples from* $\tilde{P}$ *are used.*

Please see Appendix A.3 for the proof.

Algorithm 3 constructs credible regions for each state and action separately (Murphy, 2012). A notable limitation of Algorithm 3 is that it constructs the credible regions independently for each state and action. Although this is convenient computationally, it also means that the confidence region needs to rely on the union bound which makes it the impractical when the number of states and actions is large. Although, Assumption 1 allows for a construction that avoids the union-bound-based construction.

While Proposition 5.2 provides asymptotic convergence guarantees, it is possible to obtain finite sample guarantee by using more careful analysis (Luedtke and Ahmed, 2008) or by adapting Algorithm 3 as suggested in (Hong et al., 2020). We leave this finite-sample analysis for future work.

6 Frequentist Guarantees

In this section, we extend the analysis above to outline how our results apply to frequentist guarantees. The advantage of the frequentist setup is that it provides guarantees even without needing access to a prior distribution. The disadvantage is that, without good priors, frequentist settings may need an excessive amount of data to provide reasonable guarantees. The main contribution in this section are new sampling bounds for weighted L_1 and L_∞ ambiguity sets.

The frequentist perspective on the percentile criterion (Delage and Mannor, 2010) represents a viable alternative to the Bayesian perspective when it is difficult to construct a good prior distribution. The frequentist view assumes that the true model $P^\star$ is known. The analysis considers the uncertainty over datasets. To define the criterion, let $\mathcal{D}$ represent the set of all possible datasets D. Then the pair of algorithms $F : \mathcal{D} \to \Pi$, which computes the policy for a

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dataset, and $G : \mathcal{D} \to \mathbb{R}$, which estimates the return of the policy, solves the percentile criterion if:

$$\mathbb{P}_{D \sim P^\star} [\rho(F(D), P^\star) \geq G(D)] \geq 1 - \delta . \quad (9)$$

A frequentist modeler assumes that $P^\star_{s,a}$ is fixed and the probability statements are qualified over sampled data sets $(s_t, a_t, s'_t)_{t=1,\ldots,T}$ generated from the true transition probabilities $s'_t \sim \boldsymbol{p}^\star_{s_t, a_t}$.

To construct an RMDP that solves the frequentist percentile criterion, we make very similar assumptions to the Bayesian setting. The next assumption restates Assumption 1 in the frequentist setting; note the change in random variables.

Assumption 2. *The data-dependent ambiguity set $\hat{\mathcal{P}}$ satisfies:*

$$\mathbb{P}_{D \sim P^\star} [P^\star \in \hat{\mathcal{P}}] \geq 1 - \delta ,$$

where $\hat{\mathcal{P}}$ is a function of D.

Recall that Theorem 3.1 establishes that an RMDP that satisfies Assumption 1 computes a high-confidence lower bound on the return. The proof of Theorem 3.1 easily extends to the frequentist setup. Therefore, Assumption 2 implies that $\mathbb{P}_D [\hat{\rho} \leq \rho(\hat{\pi}, P)] \geq 1 - \delta$ where $\hat{\rho}$ and $\hat{\pi}$ are the return and policy to the RMDP. In other words, the RMDP algorithm (joint policy and return estimate computation) solves the frequentist percentile criterion in (9) when Assumption 2 holds.

Because the optimization methods described in Section 4 make no probabilistic assumptions, they can be applied to the frequentist setup with no change. The optimization of ψ described in Section 5 assumes that samples from the posterior over transition functions are available and cannot be readily used to satisfy Assumption 2. Instead, we present two new finite-sample bounds that can be used to construct frequentist ambiguity sets. Since prior work has been limited to the ambiguity sets defined in terms L_1 ambiguity sets with uniform weights (Auer et al., 2010; Dietterich et al., 2013; Petrik and Russel, 2019; Weissman et al., 2003), we derive new high-confidence bounds for ambiguity sets defined using *weighted* L_1 and L_∞ norms. To state our new results, let the nominal point $\bar{\boldsymbol{p}}_{s,a} \in \Delta^S$ in (3) be the empirical estimate of the transition probability computed from $n_{s,a} \in \mathbb{N}$ transition samples for each state $s \in \mathcal{S}$ and action $a \in \mathcal{A}$.

Theorem 6.1 (L_∞ norm). *Suppose that $\mathcal{P}(\boldsymbol{w}, \psi)$ is defined in terms of the $\boldsymbol{w}_{s,a}$-weighted L_∞ norm. Then Assumption 2 is satisfied if $\psi_{s,a} \in \mathbb{R}_+$ for each $s \in \mathcal{S}$ and $a \in \mathcal{A}$ satisfies the following inequality:*

$$\delta \leq 2 \cdot SA \cdot \sum_{i=1}^{S} \exp \left(-2 \frac{\psi^2_{s,a} \cdot n_{s,a}}{(\boldsymbol{w}_{sa})^2_i} \right) . \quad (10)$$

Theorem 6.2 (L_1 norm). *Suppose that $\mathcal{P}(\boldsymbol{w}, \psi)$ is defined in terms of the $\boldsymbol{w}_{s,a}$-weighted L_1 norm. Then Assumption 2 is satisfied if $\psi_{s,a} \in \mathbb{R}_+$ for each $s \in \mathcal{S}$ and $a \in \mathcal{A}$ satisfies the following inequality:*

$$\delta \leq 2 \cdot SA \cdot \sum_{i=1}^{S-1} 2^{S-i} \cdot \exp \left(-\frac{\psi^2_{s,a} \cdot n_{s,a}}{2 \cdot (\boldsymbol{w}_{sa})^2_i} \right) , \quad (11)$$

where positive weights $\boldsymbol{w}_{s,a} \in \mathbb{R}^S_{++}, s \in \mathcal{S}, a \in \mathcal{A}$ are assumed to be sorted in a non-increasing order $(\boldsymbol{w}_{s,a})_i \geq (\boldsymbol{w}_{s,a})_{i+1}$ for $i = 1, \ldots, S-1$.

The proofs of the theorems are in Appendix A.4. They follow by standard techniques combining the Hoeffding and union bounds.

A natural question is how to construct $\psi_{s,a}$ that satisfies Theorems 6.1 and 6.2. Although the theorems do not provide us with an analytical solution, the value of $\psi_{s,a}$ can be computed efficiently using the standard bisection method (Boyd and Vandenberghe, 2004). This is because right-hand side functions in (10) and (11) are monotonically decreasing in $\psi_{s,a}, s \in \mathcal{S}, a \in \mathcal{A}$. Theorem A.3 further tightens the error bounds using Bernstein's inequality.

Theorems 6.1 and 6.2 also provide new insights into which ambiguity set may be a better fit for a particular problem. Simple algebraic manipulation and (7) show that the L_1 norm is preferable to the L_∞ norm when $\|\boldsymbol{v} - \bar{v} \cdot \boldsymbol{1}\|_1 > \sqrt{S} \cdot \|\boldsymbol{v} - \tilde{v} \cdot \boldsymbol{1}\|_\infty$. Here, $\boldsymbol{v} \in \mathbb{R}^S$ is the optimal value function, $\bar{v} = \boldsymbol{1}^\mathsf{T} \boldsymbol{v} / S$ is the mean value, and $\tilde{v}$ is the median value of $\boldsymbol{v}$.

In terms of their tightness, Theorems 6.1 and 6.2 are similar to the most well-known bounds on the uniformly-weighted norms. Theorem 6.2 recovers the equivalent best-known (Hoeffding-based) result for uniformly-weighted norm within a factor of 2. We are not aware of comparable prior results for ambiguity sets defined in terms of L_∞ norms. Unfortunately, frequentist bounds on probability distributions are generally useful only when the number of samples $n_{s,a}$ is quite large. We also investigated Bernstein-based versions of the bounds, but they show little difference in our experimental results.

Finally, it is important to note that Theorems 6.1 and 6.2 require that the weights $\boldsymbol{w}$ are independent of data. Therefore, the weights $\boldsymbol{w}$ should be optimized using a dataset different from the one used to estimate ψ. However, in our experiment, we found that reusing the same dataset to optimize both $\boldsymbol{w}$ and ψ empirically does compromise the percentile guarantees.

7 Empirical Evaluation

In this section, we evaluate Algorithm 1 empirically using five standard reinforcement domains that have

been previously used to evaluate robustness.

Tables 1 and 2 summarize the results for the Bayesian and frequentist setups respectively. The results compare our algorithms (rows) against baselines (rows) for fixed datasets D for all domains (column). The method names indicate how the weights are computed and which norm is used to defined the ambiguity set. Methods denoted as "Uniform" represent $\boldsymbol{w} = \boldsymbol{1}$ and "Optimized" represent $\boldsymbol{w}$ computed using Algorithms 1 and 2. Please see Appendix B for a complete report of the statistics and methods (including the SOCP formulation).

As the main metric, we compare the computed return guarantees $\hat{\rho}$ (the return of the RMDP). Because all methods use ambiguity sets that satisfy Assumptions 1 and 2, $\hat{\rho}$ lower bounds $\rho(\hat{\pi}, \tilde{P})$ with probability $1 - \delta$. In order to enable the comparison of the results among different domains, we normalize the guarantee by the maximal nominal return $\bar{\rho} = \max_{\pi \in \Pi} \rho(\pi, \mathbb{E}[\tilde{P}])$. We use $\bar{\rho}$ instead of the unknown $y^\star$.

As a baseline, we compare our results with the standard RMDPs construction (Delage and Mannor, 2010; Petrik and Russel, 2019), which uses uniformly-weighted L_1 and L_∞ norms. We do not compare to policy-gradient-style methods in (Delage and Mannor, 2010) because they cannot be used with general posterior distributions over $\tilde{P}$ in our domains. We note that various modifications to probability norms have been proposed in the RL context (e.g., (Maillard et al., 2014; Taleghan et al., 2015)), but it is unclear how to use them in the context of the percentile criterion.

The results in Tables 1 and 2 show that optimizing the weights in RMDP ambiguity sets decreases the guaranteed performance loss dramatically in Bayesian settings (geometric mean 2.8×) and reliably in frequentist settings (geometric mean 1.6×). The guarantees improve because the RMDPs with optimized sets simultaneously compute a better policy and a tighter bound on its return. Note that zero losses in the tables may be unachievable ($\bar{\rho} > y^\star$), and losses greater than one are possible (when $\bar{\rho} < 0$). The total computational complexity of Algorithms 1 and 2 is small and reported in Appendix B.

We now briefly summarize the domains used; please consult Appendix B for more details.

RiverSwim (RS) is a simple and standard benchmark (Strehl and Littman, 2008), which is an MDP consisting of six states and two actions. The process follows by sampling synthetic datasets from the true model and then computing the guaranteed robust returns for different methods. The prior is a uniform Dirichlet distribution over reachable states.

	RS	MR	PG	IM	CP
Uniform L_1	0.60	1.56	5.24	0.97	0.77
Uniform L_∞	0.60	1.56	5.50	0.98	0.76
Optimized L_1	0.25	0.41	1.84	0.90	0.12
Optimized L_∞	0.31	0.39	3.10	0.87	0.19

Table 1: Normalized *Bayesian* performance loss $(\bar{\rho} - \hat{\rho})/|\bar{\rho}|$ for $\delta = 0.05$. (Smaller value is better).

	RS	MR	PG	IM	CP
Uniform L_1	0.80	5.83	5.66	1.05	0.78
Uniform L_∞	0.76	3.45	5.65	1.05	0.78
Optimized L_1	0.53	1.05	5.55	0.99	0.77
Optimized L_∞	0.43	0.94	5.56	0.96	0.69

Table 2: Normalized *frequentist* performance loss $(\bar{\rho} - \hat{\rho})/|\bar{\rho}|$ for $\delta = 0.05$. (Smaller value is better).

Machine Replacement (MR) is a small benchmark MDP problem with $S = 10$ states that models progressive deterioration of a mechanical device (Delage and Mannor, 2010). Two repair actions $A = 2$ are available and restore the machine's state. Uses a Dirichlet prior.

Population Growth Model (PG) is an exponential population growth model (Kéry and Schaub, 2011), which constitutes a simple state-space $0, \ldots, S = 50$ with exponential dynamics. At each time step, the land manager has to decide whether to apply a control measure to reduce the species' growth rate. We refer to (Tirinzoni et al., 2018) for more details of the model.

Inventory Management (IM) is a classic inventory management problem (Zipkin, 2000), with discrete inventory levels $0, \ldots, S = 30$. The purchase cost, sale price, and holding cost are $2.49, 3.99$, and 0.03, respectively. The demand is sampled from a normal distribution with a mean $S/4$ and a standard deviation of $S/6$. It also uses a Dirichlet prior.

Cart-Pole (CP) is the standard RL benchmark problem (Brockman et al., 2016; Sutton and Barto, 2018). We collect samples of 100 episodes from the true dynamics. We fit a linear model with that dataset to generate synthetic samples and aggregate close states to a 200-cell grid ($S = 200$) using the k-nearest neighbor strategy and assume a uniform Dirichlet prior.

8   Conclusion

We proposed a new approach for optimizing the percentile criterion using RMDPs that goes beyond the conventional ambiguity sets. At the heart of our method are new bounds on the performance loss of

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the RMDPs with respect to the optimal percentile criterion. These bounds show that the quality of the RMDP is driven by the span of its ambiguity sets along a specific direction. We proposed a linear-time algorithm that minimizes the span of the ambiguity sets and also derived new sampling guarantees. Our experimental results show that this simple RMDP improvement can lead to much better return guarantees. Future work needs to focus on scaling the method to a large state-space using value function approximation or other techniques.

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