The Importance of Pessimism in Fixed-Dataset Policy Optimization

Jacob Buckman (Mila; McGill University)
Carles Gelada (OpenAI)
Marc G. Bellemare (Google Research; Mila; McGill University; CIFAR Fellow)

Abstract

We study worst-case guarantees on the expected return of fixed-dataset policy optimization algorithms. Our core contribution is a unified conceptual and mathematical framework for the study of algorithms in this regime. This analysis reveals that for naive approaches, the possibility of erroneous value overestimation leads to a difficult-to-satisfy requirement: in order to guarantee that we select a policy which is near-optimal, we may need the dataset to be informative of the value of every policy. To avoid this, algorithms can follow the pessimism principle, which states that we should choose the policy which acts optimally in the worst possible world. We show why pessimistic algorithms can achieve good performance even when the dataset is not informative of every policy, and derive families of algorithms which follow this principle. These theoretical findings are validated by experiments on a tabular gridworld, and deep learning experiments on four MinAtar environments.

1 Introduction

We consider fixed-dataset policy optimization (FDPO), in which a dataset of transitions from an environment is used to find a policy with high return.\(^1\) This may be contrasted with the dynamic programming setting \([29]\), in which the algorithm has full knowledge of the true environment, and the reinforcement learning setting \([36]\), in which the algorithm gains information from its interaction with the environment. The FDPO setting is a useful framework when data collection is difficult, expensive, or otherwise constrained. Additionally, since reinforcement learning is concerned with both exploration and exploitation, while FDPO algorithms perform pure exploitation, insights generated from the study of FDPO can have important implications for the more general RL setting.

We compare FDPO algorithms by their worst-case performance, expressed as high-probability guarantees on the suboptimality of the learned policy. It is perhaps obvious that in order to maximize worst-case performance, a good FDPO algorithm should select a policy with high worst-case value. We call this the pessimism principle of exploitation, as it is analogous to the widely-known optimism principle \([22]\) of exploration.\(^2\) Our main contribution is a theoretical justification of the pessimism principle, based on a bound that characterizes the suboptimality incurred by an FDPO algorithm. We further demonstrate how this bound may be used to derive principled algorithms.

We first analyze a family of non-pessimistic naive FDPO algorithms, which estimate the environment from the dataset via maximum likelihood and then apply standard dynamic programming techniques. We prove a bound which shows that the worst-case suboptimality of these algorithms is guaranteed to be small when the dataset contains enough data that we are certain about the value of every possible policy. This is caused by the outsized impact of value overestimation errors on suboptimality, sometimes called the optimizer’s curse \([34]\). It is a fundamental consequence of ignoring the disconnect between the true environment and the picture painted by our limited observations, and not reliant on errors introduced by function approximation.

We contrast these findings with an analysis of pessimistic FDPO algorithms, which select a policy that maximizes some notion of worst-case expected return. We show that these algorithms do not require datasets which inform us about the value of every policy to achieve small suboptimality, due to the critical role that pessimism plays in preventing overestimation. Our analysis naturally leads to two families of principled pessimistic FDPO algorithms. We prove their improved suboptimality guarantees, and confirm our claims with experiments on a gridworld.

Finally, we extend one of our pessimistic algorithms to the deep learning setting. Recently, several deep-learning-based algorithms for fixed-dataset policy optimization have been proposed \([7, 14, 17, 18, 19, 21, 43, 46, 48]\). Our work is complementary to these results. We do not make claims about the novelty or performance of our algorithm; our

\(^{1}\)Correspondence to: jacobbuckman@gmail.com
\(^{2}\)We use the term fixed-dataset policy optimization to emphasize the computational procedure; this setting has also been referred to as batch RL \([5, 20]\) and more recently, offline RL \([23]\).

The optimism principle states that we should select a policy with high best-case value.
primary is goal to theoretically unify existing approaches and motivate the design of pessimistic algorithms more broadly. Using experiments in the MinAtar game suite [47], we provide empirical validation for the predictions of our analysis.

1.1 An Illustrative Example

We begin with a simple example to build intuition. Experienced readers should feel free to skip this section. Consider the following problem setting. We are given an MDP with a single state and some number of actions, each of which return rewards sampled from a Bernoulli distribution on \{0, 1\}. (An MDP with a single state is isomorphic to a multi-armed bandit.) Furthermore, for each action, we are given a dataset containing the outcomes of some number of pulls. We are now given the opportunity to take an action, with the goal of maximizing our expected reward. What strategy should we use?

One obvious strategy is to estimate the expected reward for each action by computing its mean reward in the dataset, and then select the arm with the highest empirical reward. However, in certain problem instances, this “naïve strategy” fails. We can illustrate this with a simple example (visualized in Figure 1). Consider an MDP with a single state and 1000 actions. Let the reward distribution of the first action have mean of 0.99, while the reward distributions of all other actions have means of 0.01. Construct a dataset for this bandit by pulling the first arm 10000 times, and the other arms 1 time each.

Although this problem seems easy, the naïve algorithm achieves close to the worst possible performance. It’s clear that in this problem, the best policy selects the first action. The empirical estimate of the mean of the first action will be less than 1 with probability $1 - 2 \times 10^{-44}$, and there will be at least one other action which has empirical mean of 1 with probability $1 - 4 \times 10^{-5}$. Thus, the first action is almost never selected.

This issue can be resolved by identifying a fundamental failing of the naïve approach: it ignores epistemic uncertainty around the expected return of each action. In order to guarantee good performance on all problem instances, we need to avoid playing actions that we are uncertain about. One way to do this is to construct a high-probability lower bound on the value of each action (for example using concentration inequalities), and select the action with the highest lower bound. If we consider the upper and lower bounds as defining the set of possible “worlds” that we could be in, acting according to the lower bound of every arm means acting as though we are in the worst possible world. In other words: being pessimistic.

The above example may seem somewhat contrived, due to the enormous size of the action space and skewed data collection procedure. However, we argue that it serves as a good analogy for the more common setting of an MDP with many states and a small number of actions at each state. Roughly speaking, selecting an action in a one-state MDP is analogous to selecting a deterministic policy in a multi-state MDP, and the number of policies is exponentially large in the size of the state space. Additionally, it’s very plausible in practical situations that data is collected according to only a small set of similar policies, e.g. expert demonstrations, leading to skewed data coverage.
2 Background

We write vectors using bold lower-case letters, a, and matrices using upper-case letters, A. To refer to individual cells of a vector or rows of a matrix, we use function notation, a(x). We write the identity matrix as I. We use the notation \( \mathbb{E}_p[a] \) to denote the average value of a function under a distribution \( p \), i.e. for any space \( X \), distribution \( p \in \text{Dist}(X) \), and function \( a : X \rightarrow \mathbb{R} \), we have \( \mathbb{E}_p[a] := \mathbb{E}_{x \sim p}[a(x)] \). When applied to vectors or matrices, we use \( \langle \cdot, \cdot \rangle \) to denote element-wise comparison. Similarly, we use \( |\cdot| \) to denote the element-wise absolute value of a vector: \( |a|(x) = |a(x)| \). We use \( |\cdot|_\infty \) to denote the element-wise maximum of a and the zero vector. To denote the total variation distance between two probability distributions, we use \( \text{TV}(p, q) = \frac{1}{2} \| p - q \|_1 \). When \( p \) and \( q \) are conditional probability distributions, we adopt the convention \( \text{TV}_X(p, q) = \frac{1}{2} \| p(x) - q(x) \|_1 : x \in X \), i.e., the vector of total variation distances conditioned on each \( x \in X \).

In this work, several concepts are defined in terms of curried functions, e.g., \( f : X \times Y \rightarrow Z \) represents a function \( f \) which maps from space \( X \) into the space of functions from \( Y \rightarrow Z \). When invoking such functions, we will sometimes write this using the syntax of a single function with multiple arguments, i.e. \( f(x, y) = f(x)(y) \) where \( x \in X, y \in Y \). Also, note that any function \( a : X \rightarrow \mathbb{R} \) mapping from a discrete space \( X \) to the reals can be equivalently represented as a vector \( a \in \mathbb{R}^{|X|} \). Similarly, any function \( A : (X \times Y) \rightarrow \mathbb{R} \) mapping from two discrete spaces \( X, Y \) to the reals can be represented as a matrix \( A \in \mathbb{R}^{|X| \times |Y|} \).

Markov Decision Processes. We represent the environment with which we are interacting as a Markov Decision Process (MDP), defined in standard fashion: \( M := (S, A, R, P, \gamma, \rho) \). \( S \) and \( A \) denote the state and action space, which we will assume are discrete. We will use \( Z := S \times A \) as the shorthand for the joint state-action space. The reward function \( R : Z \rightarrow \text{Dist}([0, 1]) \) maps state-action pairs to distributions over the unit interval, while the transition function \( P : Z \rightarrow \text{Dist}(S) \) maps state-action pairs to distributions over next states. Finally, \( \rho \in \text{Dist}(S) \) is the distribution over initial states. We use \( r \) to denote the expected reward function, \( r((s, a)) := \mathbb{E}_r \sim \mathcal{R}((s, a))[r] \), which can also be interpreted as a vector \( r \in \mathbb{R}^{|Z|} \). Similarly, note that \( P \) can be described as \( P : (Z \times S) \rightarrow \mathbb{R} \), which can be represented as a stochastic matrix \( P \in \mathbb{R}^{|Z| \times |S|} \). In order to emphasize that these reward and transition functions correspond to the true environment, we will sometimes equivalently denote them as \( r_M, P_M \). To denote the vectors of a constant whose sizes are the state and state-action space, we use a single dot to mean state and two dots to mean state-action, e.g., \( 1 \in \mathbb{R}^{|S|} \) and \( \cdot 1 \in \mathbb{R}^{|Z|} \).

Policies. A policy \( \pi : S \rightarrow \text{Dist}(A) \) defines a distribution over actions, conditioned on a state. We denote the space of all possible policies as \( \Pi \). We define an “activity matrix” for each policy, \( A^\pi \in \mathbb{R}^{|S| \times |S|} \), which encodes the state-conditional state-action distribution of \( \pi \), by letting \( A^\pi(s, \langle s, a \rangle) := \pi(a|s) \) if \( s = \tilde{s} \), otherwise \( A^\pi(s, \langle s, a \rangle) := 0 \). Acting in the MDP according to \( \pi \) can thus be represented by \( A^\pi P \in \mathbb{R}^{|S| \times |S|} \) or \( PA^\pi \in \mathbb{R}^{|Z| \times |Z|} \).

Value functions, returns, and optimal policies. We define a value function as any \( v : \Pi \rightarrow S \rightarrow \mathbb{R} \) or \( q : \Pi \rightarrow Z \rightarrow \mathbb{R} \) whose output is bounded by \( [0, \frac{1}{1-\gamma}] \). Note that this is a slight generalization of the standard definition [36] since it accepts a policy as an input. We use the shorthand \( v^\pi := v(\pi) \) and \( q^\pi := q(\pi) \) to denote the result of applying a value function to a specific policy, which can also be represented as a vector, \( v^\pi \in \mathbb{R}^{|S|} \) and \( q^\pi \in \mathbb{R}^{|Z|} \). To denote the output of an arbitrary value function on an arbitrary policy, we will use unadorned \( v \) and \( q \). One important value function is the expected return of an MDP \( M \), denoted \( v_M \) or \( q_M \) for state-wise and state-action-wise, respectively. The expected return is the discounted sum of rewards acquired when interacting with the environment:

\[
v_M(\pi) := \sum_{t=0}^{\infty} (\gamma A^\pi P)^t A^\pi r \quad q_M(\pi) := \sum_{t=0}^{\infty} (\gamma P A^\pi)^t r
\]

Note that \( v_M^\pi = A^\pi q_M^\pi \). An optimal policy of an MDP, which we will denote \( \pi_M^* \), is a policy for which the expected return \( v_M \) is maximized under the initial state distribution: \( \pi_M^* := \arg \max_{\pi} \mathbb{E}_p[v_M^\pi] \). The statewise expected returns of an optimal policy can be written as \( v_M^\pi \).

Discounted visitations. For any state \( s \), the probability of being in the state \( s^\prime \) after \( t \) time steps when following policy \( \pi \) is \( (A^\pi P)^t(s, s^\prime) \). Furthermore, \( \sum_{t=0}^{\infty} (A^\pi P)^t = (I - \gamma A^\pi P)^{-1} \), since it is a geometric series. We refer to \( (I - \gamma A^\pi P)^{-1} \) as the discounted visitation of \( \pi \). The discounted visitation has several useful properties. Firstly, the discounted visitation has four variants, depending on whether we want to map states to states \((I - \gamma A^\pi P)^{-1} \).
states to state-actions $A^\pi (I - \gamma PA^\pi)^{-1} = (I - \gamma A^\pi P)^{-1} A^\pi$, state-actions to states $(I - \gamma PA^\pi)^{-1} P$, or state-actions to state-actions $(I - \gamma PA^\pi)^{-1}$. Secondly, we can write the expected return as a weighted sum of rewards, where the weights are given by the discounted visitation: $v^\pi_M = (I - \gamma A^\pi P)^{-1} A^\pi r$. Finally, since the discounted visitation is an exponential average of $t$ stochastic matrices, each column sums to $\frac{1}{1 - \gamma}$.

**Value fixed-points.** Of particular interest are value functions whose outputs obey fixed-point relationships, $v^\pi = f(v^\pi)$ for some $f : (S \rightarrow \mathbb{R}) \rightarrow (S \rightarrow \mathbb{R})$. Fixed-points allow us to uniquely identify value vectors with specific properties. For example, one important fixed-point equation is the Bellman consistency equation for a policy $\pi$, $B^\pi_M(x) := A^\pi (r + \gamma P(x))$, which uniquely identifies the vector of expected returns for $\pi$, since $v^\pi_M$ is the only vector for which $v^\pi_M = B^\pi_M(v^\pi_M)$ holds. Throughout this work, we will introduce a variety of useful fixed-point equations.

### 3 Problem Setting

In this section, we introduce basic concepts that are helpful for framing the problem of fixed-dataset policy optimization.

**Datasets.** We define a dataset of $d$ transitions $D := \{(s, a, r, s')\}^d$, and denote the space of all datasets as $D$. In this work, we specifically consider datasets sampled from a data distribution $\Phi : \text{Dist}(Z)$; for example, the distribution of state-actions reached by following some stationary policy. We use $D \sim \Phi_d$ to denote constructing a dataset of $d$ tuples $(s, a, r, s')$, by first sampling each $(s, a) \sim \Phi$, and then sampling $r$ and $s'$ i.i.d. from the environment reward function and transition function respectively, i.e. each $r \sim R(\cdot|s, a)$ and $s' \sim P(\cdot|s, a)$.\(^3\) We will sometimes index $D$ using function notation, using $D(s, a)$ to denote the multiset of all $(r, s')$ such that $(s, a, r, s') \in D$. We use $\tilde{n}_D \in \mathbb{R}[Z]$ to denote the vectors of counts, that is, $\tilde{n}_D(s, a) := |D(s, a)|$. We will sometimes use state-wise versions of these vectors, which we denote with $n_D$.

**Empirical model.** It is further useful to consider the maximum-likelihood reward and transition functions, computed by averaging all rewards and transitions observed in the dataset for each state-action. To this end, we define empirical reward vector $r_D((s, a)) := \frac{1}{|D(s, a)|} \sum_{r, s' \in D((s, a))} I(s' = s')$ and empirical transition matrix $P_D(s'|s, a) := \frac{1}{|D(s, a)|} \sum_{r, s' \in D((s, a))} I(s' = s')$ at all state-actions for which $\tilde{n}_D((s, a)) > 0$. Where with $\tilde{n}_D((s, a)) = 0$, there is no clear way to define the maximum-likelihood estimates of reward and transition, so we do not specify them. All our results hold no matter how these values are chosen, so long as $r_D \in [0, \frac{1}{1 - \gamma}]$ and $P_D$ is stochastic. The empirical policy of a dataset $D$ is defined as $\hat{\pi}_D(a|s) := \frac{|D(s, a)|}{|D(s, \cdot)|}$ except where $\tilde{n}_D((s, a)) = 0$, where it can similarly be any valid action distribution. The empirical visitation distribution of a dataset $D$ is computed in the same way as the visitation distribution, but with $P_D$ replacing $P$, i.e. $(I - \gamma A^\pi P_D)^{-1}$.

**Fixed-dataset policy optimization (FDPO) algorithms.** The primary focus of this work is on the properties of fixed-dataset policy optimization algorithms. These algorithms take the form of a function $\mathcal{O} : D \mapsto \Pi$, which maps from a dataset to a policy.\(^4\) Note that in this work, we consider $D \sim \Phi_d$, so the dataset is a random variable, and therefore $\mathcal{O}(D)$ is also a random variable. The goal of any FDPO algorithm is to output a policy with minimum suboptimality, i.e. maximum return. Suboptimality is a random variable computed by taking the difference between the expected return of an optimal policy and the learned policy under the initial state distribution,

$$\text{SUBOpt}(\mathcal{O}(D)) = \mathbb{E}_\rho[\hat{v}_M] - \mathbb{E}_\rho[v^\mathcal{O}_M].$$

In contrast to algorithms for reinforcement learning, which must trade off between exploration and exploitation, algorithms for the FDPO setting are in essence tasked only with performing exploitation.

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\(^3\)Note that this is in some sense a simplifying assumption. In practice, datasets will typically be collected using a trajectory from a non-stationary policy, rather than i.i.d. sampling from the stationary distribution of a stationary policy. This greatly complicates the analysis, so we do not consider that setting in this work.

\(^4\)This formulation hides a dependency on $\rho$, the start-state distribution of the MDP. In general, $\rho$ can be estimated from the dataset $D$, but this estimation introduces some error that affects the analysis. In this work, we assume for analytical simplicity that $\rho$ is known a priori. Technically, this means that it must be provided as an input to $\mathcal{O}$. We hide this dependency for notational clarity.
Fixed-dataset policy evaluation (FDPE) algorithms. A fixed-dataset policy evaluation algorithm is any function \( \mathcal{E} : \mathcal{D} \to \Pi \to \mathcal{S} \to \mathbb{R} \), which uses a dataset to compute a value function. Fixed-dataset policy evaluation is a well-studied problem setting in its own right, but in this work, we study it mainly in the context of its use as a sub-routine of value-based fixed-dataset policy optimization algorithms (see next paragraph). In particular, we are primarily interested in FDPE algorithms whose output obeys some fixed-point identity.

Value-based FDPO algorithms. In this work, we focus our analysis on a specific type of fixed-dataset policy optimization algorithm. A value-based FDPO algorithm, with FDPE subroutine \( \mathcal{E}_{\text{sub}} \), is any algorithm with the following structure:

\[
\mathcal{O}^{\text{VB}}_{\text{sub}}(D) := \arg \max_{\pi} \mathbb{E}_\rho[E_{\text{sub}}(D, \pi)].
\]

Intuitively, these algorithms use a policy evaluation subroutine to convert a dataset into a value function, and return an optimal policy according to that value function. Importantly, this definition constrains only the objective of the approach, not its actual algorithmic implementation, i.e., it includes algorithms which never actually invoke the FDPE subroutine. This is a very general class of algorithms. For many online model-free reinforcement learning algorithms, including policy iteration, value iteration, and Q-learning, we can construct closely analogous value-based FDPO algorithms; see Appendix B.1. Furthermore, model-based techniques can often be interpreted as using a model to implicitly define a value function, and then optimizing that value function. Thus, although our discussion centers around model-free algorithms, our results also apply to most model-based approaches.

Fixed-point families of algorithms. Using the above concepts, we are able to abstract away the computational details of algorithms, helping us focus instead on the properties of their outputs. We define a fixed-point family of algorithms, sometimes referred to as just a family, in the following way. Any family called family is based on a specific fixed-point identity \( f_{\text{family}} \). We use the notation \( \mathcal{E}_{\text{family}} \) to denote any FDPE algorithm whose output \( v^*_D := \mathcal{E}_{\text{family}}(D, \pi) \) obeys \( v^*_D = f_{\text{family}}(v^*_D) \). Finally, \( \mathcal{O}^{\text{VB}}_{\text{family}} \) refers to any value-based FDPO algorithm whose subroutine is \( \mathcal{E}_{\text{family}} \). We call the set of all algorithms that could implement \( \mathcal{E}_{\text{family}} \) the family of FDPE algorithms, and the set of all algorithms that could implement \( \mathcal{O}^{\text{VB}}_{\text{family}} \) as the family of FDPO algorithms. In this work, all main results apply to entire families of algorithms, and are agnostic to any specific implementation details.

4 Key Ideas

We now begin our analysis of fixed-dataset policy optimization algorithms by introducing the key ideas which underpin our theoretical framework. These objects are both conceptually interesting, in that they are helpful for building intuitions, and also mathematically interesting, in that they can be used to derive and analyze algorithms in this setting.

4.1 Uncertainty

The example given in Section 1.1 illustrated how an intuitive notion of epistemic uncertainty might be used to improve the performance of algorithms. In this section, we propose a concrete notion of uncertainty which is useful in the context of FDPO, and in later sections, we will utilize this concept to construct bounds on suboptimality.

A core insight of our analysis is that the problem of computing uncertainty can be cleanly separated from the problem of decision making. Our approach is to first define a notion of uncertainty as a function with certain properties, then assume that such a function exists, and provide the remainder of our technical results under such an assumption. Separately, we also describe several approaches to computing uncertainty. Thanks to this separation, it is easy for future work to build on our framework: any new technique for computing uncertainty can be easily plugged in to improve the overall bounds. Conversely, we believe that our definition of uncertainty will be a productive abstraction in many other areas in reinforcement learning.
4.1.1 Bellman Uncertainty

We begin by defining a notion of uncertainty which is local to each state. This notion captures the degree to which the outcome of an empirical Bellman update deviates from that of a true Bellman update.

**Definition 1.** A function \( u_{D, \delta}^\pi : S \to \mathbb{R} \) is a Bellman uncertainty function if for a dataset \( D \sim \Phi_d \) and policy \( \pi \), it obeys with probability at least \( 1 - \delta \) for all values \( v \):

\[
u_{D, \delta}^\pi \geq |A^\pi (r_M + \gamma P_M v) - A^\pi (r_D + \gamma P_D v)|\]

We call values returned by a Bellman uncertainty function the **Bellman uncertainty**. Due to the centrality of this concept, we take a moment to briefly discuss its properties.

**How does this definition correspond to our intuitions about uncertainty?** An application of the environment’s true Bellman update can be viewed as updating the value of each state to reflect information about its future. However, no algorithm in the FDPO setting can apply such an update, because the true environment dynamics are unknown. We may use the dataset to estimate what such an update would look like, but since the limited information in the dataset may not fully specify the properties of the environment, this update will be slightly wrong. It is intuitive to say that the uncertainty at each state corresponds to how well the approximate update matches the truth. Our definition of Bellman uncertainty captures precisely this notion.

It is important to notice that in general, some state-actions may have more Bellman uncertainty than others. For example, it is intuitive to see that states which occur more often in the dataset should typically have lower Bellman uncertainty. This is because as more data is collected in a particular state, \( r_D, P_D \) approach \( r_M, P_M \) asymptotically.

**How can we algorithmically implement Bellman uncertainty functions?** In other words, how can we compute a function with the property required for Definition 1, using only the information in the dataset? Bellman uncertainty is an upper-bound to a quantity, and if it is a tighter upper-bound, other results down the line which leverage this quantity will be improved. Therefore, it is worth considering this question carefully.

A vacuous approach is simply \( u_{D, \delta}^\pi (s) = \frac{1}{1-\gamma} \) for all \( s \). But although this is technically a valid Bellman uncertainty function, it is not very useful, because it does not concentrate with data and does not distinguish between certain and uncertain states. It is very loose and so leads to poor guarantees.

In tabular environments, one way to implement a Bellman uncertainty function is to use a concentration inequality. Depending on which concentration inequality is used, many Bellman uncertainty functions are possible. These approaches lead to Bellman uncertainty which is lower at states with more data, typically in proportion to the square root of the count. To illustrate how to do this, we show in Appendix C.1 a basic application of Hoeffding’s inequality; in Appendix C.2, an alternative application of Hoeffding’s which results in a tighter bound; and in Appendix C.3 a discussion of other techniques which may be useful.

When the value function is represented by a neural network, it is not currently known how to implement a Bellman uncertainty function. When an empirical Bellman update is applied to a neural network, the change in value of any given state is impacted by generalization from other states. Therefore, the counts are not meaningful, and concentration inequalities are not applicable. In the neural network literature, many “uncertainty estimation techniques” have been proposed, which capture something analogous to an intuitive notion of uncertainty; however, none are principled enough to be useful in computing Bellman uncertainty.

4.1.2 Value Uncertainty

Although we began by introducing the concept of Bellman uncertainty, the more fundamental form of uncertainty is **value uncertainty**. Value uncertainty functions compute the maximum possible difference between the true value of a policy and its estimated value.

**Definition 2.** A function \( \mu_{D, \delta}^\pi : S \to \mathbb{R} \) is a value uncertainty function if for a dataset \( D \sim \Phi_d \) and policy \( \pi \), it
obeys with probability at least $1 - \delta$ for all values $v$:

$$\mu_{D,\delta} \geq \sum_{t=0}^{\infty} (\gamma A^\pi P_D)^t |A^\pi (r_M + \gamma P_M v) - A^\pi (r_D + \gamma P_D v)|$$

Value uncertainty refers to the values returned by a value uncertainty function. Value uncertainty is equivalent to summing the discounted Bellman uncertainty over all future timesteps. This property makes implementing value uncertainty simple. Any implementation of a Bellman uncertainty function can be seamlessly converted into an implementation of a value uncertainty function, by taking a weighted sum using the empirical visitation distribution. In fact, since value uncertainty is the more fundamental quantity, Bellman uncertainty functions are best viewed as a convenient tool which emerges from a particular decomposition of value uncertainty functions.

### 4.2 Over/Under Decomposition of Suboptimality

The second core insight is a simple but informative bound on the suboptimality of any value-based FDPO algorithm. This bound is abstract; next, in Section 5, we will make this more concrete by defining the family of naïve algorithms and invoking this bound. This bound is insightful because it distinguishes the impact of errors of value overestimation from errors of value underestimation. We define these quantities in the following way.

**Definition 3.** Consider any fixed-dataset policy evaluation algorithm $E$ on any dataset $D$ and any policy $\pi$. Denote $v_D^\pi := E(D, \pi)$. We define the underestimation error as $E_{\rho}[v_M^\pi - v_M^D]$ and overestimation error as $E_{\rho}[v_D^\pi - v_M^D]$.

The following lemma shows how these quantities can be used to bound suboptimality.

**Lemma 1 (Value-based FDPO suboptimality bound).** Consider any value-based fixed-dataset policy optimization algorithm $O^{VB}$, with fixed-dataset policy evaluation subroutine $E$. For any policy $\pi$ and dataset $D$, denote $v_D^\pi := E(D, \pi)$, and $\pi_D^* := O^{VB}(D)$. The suboptimality of $O^{VB}$ is bounded by

$$\text{SubOpt}(O^{VB}(D)) \leq \inf_{\pi} \left( E_{\rho}[v_M^\pi - v_M^D] + E_{\rho}[v_M^\pi - v_D^\pi] \right) + \sup_{\pi} \left( E_{\rho}[v_D^\pi - v_M^\pi] \right)$$

**Proof.** Starting from the definition of suboptimality, we see

$$\text{SubOpt}(O^{VB}(D)) = E_{\rho}[v_M^\pi - v_D^\pi]$$

$$= E_{\rho}[v_M^\pi + (-v_D^\pi + v_D^\pi) + (-v_D^\pi + v_D^\pi) - v_M^\pi]$$

$$\leq E_{\rho}[v_M^\pi - v_D^\pi] + E_{\rho}[v_D^\pi - v_M^\pi]$$

(valid for any $\pi$)

(using $E_{\rho}[v_D^\pi - v_M^\pi] \leq 0$)

Since the above holds for all $\pi$,

$$\text{SubOpt}(O^{VB}(D)) \leq \inf_{\pi} \left( E_{\rho}[v_M^\pi - v_D^\pi] \right) + \sup_{\pi} \left( E_{\rho}[v_D^\pi - v_M^\pi] \right)$$

$$\leq \inf_{\pi} \left( E_{\rho}[v_M^\pi - v_D^\pi] \right) + \sup_{\pi} \left( E_{\rho}[v_D^\pi - v_M^\pi] \right)$$

$$= \inf_{\pi} \left( E_{\rho}[v_M^\pi - v_D^\pi] + E_{\rho}[v_M^\pi - v_M^D] \right) + \sup_{\pi} \left( E_{\rho}[v_D^\pi - v_M^\pi] \right)$$

This bound is tight; see Appendix A.1. The bound highlights the potentially outsized impact of overestimation on the suboptimality of a FDPO algorithm. To see this, we consider each of its terms in isolation:

$$\text{SubOpt}(O^{VB}(D)) \leq \inf_{\pi} \left( E_{\rho}[v_M^\pi - v_D^\pi] + E_{\rho}[v_M^\pi - v_M^D] \right) + \sup_{\pi} \left( E_{\rho}[v_D^\pi - v_M^\pi] \right)$$
The term labeled (A) reflects the degree to which the dataset informs us of a near-optimal policy. For any policy \( \pi \), (A1) captures the suboptimality of that policy, and (A2) captures its underestimation error. Since (A) takes an infimum, this term will be small whenever there is at least one reasonable policy whose value is not very underestimated.

On the other hand, the term labeled (n) corresponds to the largest overestimation error on any policy. Because it consists of a supremum over all policies, it will be small only when no policies are overestimated at all. Even a single overestimation can lead to significant suboptimality.

We see from these two terms that errors of overestimation and underestimation have differing impacts on suboptimality, suggesting that algorithms should be designed with this asymmetry in mind. We will see in Section 6 how this may be done. But first, let us further understand why this is necessary by studying in more depth a family of algorithms which treats its errors of overestimation and underestimation equivalently.

5 Naïve Algorithms

The goal of this section is to paint a high-level picture of the worst-case suboptimality guarantees of a specific family of non-pessimistic approaches, which we call naïve FDPO algorithms. Informally, the naïve approach is to take the limited dataset of observations at face value, treating it as though it paints a fully accurate picture of the environment. Naïve algorithms construct a maximum-likelihood MDP from the dataset, and then use standard dynamic programming approaches on this empirical MDP.

There are two main reasons why this is an important family of algorithms to study. Firstly, this will provide a valuable point of comparison for our subsequent analysis of pessimistic approaches (Section 6); our conclusions emerge from the juxtaposition of these two results. Secondly, naïve algorithms are so-called due to their simplicity, and therefore appear in many places in the literature. By studying this class of algorithms, we extend our understanding of some universal phenomena within RL and FDPO. For example, our analysis will show mathematically why overestimating values seems to be more of an issue than underestimating them. (By overestimating and underestimating, we mean that an FDPE algorithm incorrectly outputs values that are too high or low, respectively.)

The family of naïve algorithms is derived from the following fixed-point identity.

**Definition 4** (Naïve algorithms). A naïve algorithm is any algorithm in the family defined by the fixed-point function

\[ f_{\text{naïve}}(v_\pi) := A_\pi (r_D + \gamma P_D v_\pi). \]

Various FDPE and FDPO algorithms from this family could be described, primarily by modifying algorithms for the dynamic programming setting to use the empirical MDP defined by \( \langle S, A, r_D, P_D, \gamma \rangle \). In this work, we do not study these implementations in detail, although we do give pseudocode for some implementations in Appendix B.1.

One example of a naïve FDPO algorithm which can be found in the literature is certainty equivalence [15]. The core ideas behind naïve algorithms can also be found in the function approximation literature, for example in FQI [5, 16].\(^3\) Additionally, when available data is held fixed, nearly all deep reinforcement algorithms are transformed into naïve value-based FDPO algorithms. For example, DQN [25] with a fixed replay buffer is a naïve value-based FDPO algorithm.

5.1 Naïve FDPE Error Bound

We first show how the error of naïve FDPE algorithms is bounded by the value uncertainty of state-actions visited by the policy under evaluation. Next, in Section 5.2, we will use this bound to derive a suboptimality guarantee for naïve FDPO.

\(^3\)Note that our definition of a fixed-point family is not quite adequate once function approximation is introduced, since algorithms will not choose the exact fixed-point function when it is not in the class of available functions. In such cases, they will instead select a projected fixed-point, and our current bounds do not immediately apply. Further work is needed to rigorously extend our results to the function approximation setting.
Lemma 2 (Naïve FDPE error bound). Consider any naïve fixed-dataset policy evaluation algorithm \(E_{\text{naïve}}\). For any policy \(\pi\) and dataset \(D\), denote \(v_D^{\pi} := E_{\text{naïve}}(D, \pi)\). Let \(\mu_{D,\delta}^{\pi}\) be any value uncertainty function. The following component-wise bound holds with probability at least \(1 - \delta\):

\[ |v_M^{\pi} - v_D^{\pi}| \leq \mu_{D,\delta}^{\pi} \]

Proof. See Appendix A.3.

Thus, reducing value uncertainty improves our guarantees on evaluation error. For any fixed policy, value uncertainty can be reduced by reducing the Bellman uncertainty on states visited by that policy. In the tabular setting this means observing more interactions from the state-actions that that policy visits frequently. Conversely, for any fixed dataset, we will have a certain Bellman uncertainty in each state, and policies mostly visit low-Bellman-uncertainty states can be evaluated with lower error.\(^6\)

Our bound differs from prior work \([8, 15]\) in that it is significantly more fine-grained. We provide a component-wise bound on error, whereas previous results bound the \(l_\infty\) norm. Furthermore, our bounds are sensitive to the Bellman uncertainty in each individual reward and transition, rather than only relying on the most-uncertain. As a result, our bound does not require all states to have the same number of samples, and is non-vacuous even in the case where some state-actions have no data.

Our bound can also be viewed as an extension of work on approximate dynamic programming. In that setting, the literature contains fine-grained results on the accumulation of local errors \([26]\). However, those results are typically understood as applying to errors induced by approximation via some limited function class. Our bound can be seen as an application of those ideas to the case where errors are induced by limited observations.

5.2 Naïve FDPO Suboptimality Bound

We now use our previous results to derive a guarantee for the suboptimality of naïve value-based FDPO algorithms. Value uncertainty bounds absolute error, and thus, bounds both overestimation and underestimation error, transforming our decomposition lemma into a concrete bound.

Theorem 1 (Naïve FDPO suboptimality bound). Consider any naïve value-based fixed-dataset policy optimization algorithm \(O_{\text{naïve}}^{\text{VB}}\). Let \(u_{D,\delta}^{\pi}\) be any Bellman uncertainty function. For any dataset \(D\), denote \(\pi_{D}^{*} := O_{\text{naïve}}^{\text{VB}}(D)\). With probability at least \(1 - \delta\), the suboptimality of \(O_{\text{naïve}}^{\text{VB}}\) is bounded with probability at least \(1 - \delta\) by

\[ \text{SubOrr}(O_{\text{naïve}}^{\text{VB}}(D)) \leq \inf_{\pi} \left( \mathbb{E}_\rho[|v_M^{\pi} - v_M^{\pi_D}|] + \mathbb{E}_\rho[\mu_{D,\delta}^{\pi}] \right) + \sup_{\pi} \mathbb{E}_\rho[\mu_{D,\delta}^{\pi}] \]

Proof. This result follows directly from Lemma 1 and Lemma 2.

The conclusions discussed in Section 4.2 regarding overestimation and underestimation can now be restated in terms of value uncertainty. The infimum term is small whenever there is some reasonably good policy with low value uncertainty. In practice, this condition can typically be satisfied, for example by including expert demonstrations in the dataset. On the other hand, the supremum term will only be small if we have low value uncertainty for all policies – a much more challenging requirement.\(^7\)

This explains the behavior of pathological examples, e.g. in Section 1.1, where performance is poor despite access to virtually unlimited amounts of data from a near-optimal policy. Such a dataset ensures that the first term will be small by reducing value uncertainty of the near-optimal data collection policy, but does little to reduce the uncertainty.

\(^6\)In the function approximation setting, we do not necessarily need to observe an interaction with a particular state-action to reduce our Bellman uncertainty on it. This is because observing other state-actions may allow us to reduce Bellman uncertainty through generalization. Similarly, the most-certain policy for a fixed dataset may not be the policy for which we have the most data, but rather, the policy which our dataset informs us about the most.

\(^7\)One can restrict this to all deterministic policies by a value polytope argument \([4]\). However, even with this restriction, the number of policies is still exponential in the size of the state space.
value uncertainty of any other policy, leading the second term to be large. Thus, the overall suboptimality is quite large.

However, although pathological examples exist, it is clear that this bound will not be tight on all environments. It is reasonable to ask: is it likely that this bound will be tight on real-world examples? We identify two properties that most real-world tasks share: (1) The set of policies is pyramidal: there are an enormous number of bad policies, many mediocre policies, a few good policies, etc. (2) Due to the size of the policy space and cost of data collection, most policies have high value uncertainty.

Given that these assumptions hold, naïve algorithms will perform as poorly on most real-world environments as they do on pathological examples. Consider: there are many more policies than there is data, so there will be many policies with high value uncertainty; naïve algorithms will likely overestimate several of these policies, and erroneously select one; since good policies are rare, the selected policy will likely be bad. It follows that running naïve algorithms on real-world problems will typically yield suboptimality close to our worst-case bound. And, indeed, on deep RL benchmarks, which are selected due to their similarity to real-world settings, overestimation has been widely observed, and is often identified as a cause of poor performance \([2, 7, 42]\).

### 6 The Pessimism Principle

"Choose the policy which behaves optimally in the worst possible world." The pessimism principle tells us how to exploit our current knowledge to find the stationary policy with the best worst-case guarantee on expected return.

We begin by proving a simple corollary which highlights why pessimism leads to improved suboptimality guarantees. We then consider two specific families, the uncertainty-aware pessimistic algorithms and proximal pessimistic algorithms, and bound the worst-case suboptimality of each.

#### 6.1 Pessimism Addresses Overestimation

We begin with a simple corollary to Lemma 1. Consider any value-based FDPO algorithm whose value function is guaranteed to always return values which underestimate the expected return with high probability. This property is not the only way to implement pessimism, but it is useful and illustrative.

**Corollary 1** (Value-lower-bound-based FDPO suboptimality bound). Consider any value-based fixed-dataset policy optimization algorithm \(O_{\text{VF}}\), with internal fixed-dataset policy evaluation subroutine \(\hat{E}\), which has the lower-bound guarantee that \(\hat{E}(D, \pi) \leq v^\pi_M\) with probability at least \(1 - \delta\). For any policy \(\pi\), dataset \(D\), denote \(v^\pi_D := \hat{E}(D, \pi)\).

With probability at least \(1 - \delta\), the suboptimality of \(O_{\text{VF}}\) is bounded by

\[
\text{SubOpt}(O_{\text{VF}}(D)) \leq \inf_{\pi} \left( E_{\pi}[v^\pi_M - v^\pi] + E_{\pi}[v^\pi_M - v^\pi_D] \right)
\]

**Proof.** This result follows directly from Lemma 1, using the fact that \(v^\pi_D - v^\pi_M \leq 0\).

This bound is identical to the term labeled (a) from Lemma 1. The term labeled (b), which contained a supremum over policies, has vanished, leaving only the term containing an infimum. Where the bound of Lemma 1 demands that some condition hold for all policies, we now only require that there exists any single suitable policy. It is clear that this condition is much easier to satisfy, and thus, this suboptimality bound will typically be much smaller.

A value lower-bound algorithm is in some sense the most extreme example of a pessimistic approach. Any algorithm which penalizes its predictions to decrease overestimation can be described as pessimistic. In such cases, (b) will be decreased, rather than removed entirely. Still, any amount of pessimism reduces dependence on a global condition, decreasing overall suboptimality.

Furthermore, blind pessimism is not helpful. For example, one could trivially construct a value lower-bound algorithm from a naïve algorithm by simply subtracting a large constant from the naïve value estimate of every policy.
But this would achieve nothing, as the infimum term would immediately increase by this same amount. To yield a productive change in policy, pessimism must instead vary across states in an intelligent way.

### 6.2 Uncertainty-Aware Pessimistic Algorithms

We now introduce our first family of pessimistic algorithms, which we call the uncertainty-aware (UA) pessimistic algorithms. As the name suggests, this family of algorithms estimates the Bellman uncertainty of each transition and penalizes policies accordingly, leading to a pessimistic value estimate and a preference for policies with low value uncertainty.

**Definition 5** (Uncertainty-aware pessimistic algorithms). An uncertainty-aware pessimistic algorithm, with a Bellman uncertainty function $u_{D,\delta}^{\pi}$ and pessimism hyperparameter $\alpha \in [0, 1]$, is any algorithm in the family defined by the fixed-point function

$$f_{ua}(v^{\pi}) = A^{\pi}(r_{D} + \gamma P_{D}v^{\pi}) - \alpha u_{D,\delta}^{\pi}$$

This fixed-point function is simply the naïve fixed-point function penalized by the Bellman uncertainty. This can be interpreted as being pessimistic about the outcome of every action. Note that this definition is still somewhat general, as it remains to specify a technique to compute the Bellman uncertainty function, e.g. Appendix C, in order to get a concrete algorithm.

It is straightforward to construct algorithms from this family by modifying naïve algorithms to subtract the penalty term. Similar algorithms have been explored in the safe RL literature [8, 21] and the robust MDP literature [9], where algorithms with high-probability performance guarantees are useful in the context of ensuring safety.

**Theorem 2** (Uncertainty-aware pessimistic FDPO suboptimality bound). Consider an uncertainty-aware pessimistic value-based fixed-dataset policy optimization algorithm $O_{VB}^{ua}$. Let $u_{D,\delta}^{\pi}$ be any Bellman uncertainty function, $\mu_{D,\delta}^{\pi}$ be a corresponding value uncertainty function, and $\alpha \in [0, 1]$ be any pessimism hyperparameter. The suboptimality of $O_{ua}^{VB}$ is bounded with probability at least $1 - \delta$ by

$$\text{SubOpt}(O_{ua}^{VB}(D)) \leq \inf_{\pi} \left( E_{\rho}[\nu_{M}^{\pi} - \nu_{M}] + (1 + \alpha) \cdot E_{\rho}[\mu_{D,\delta}^{\pi}] \right) + \sup_{\pi} (1 - \alpha) \cdot E_{\rho}[\mu_{D,\delta}^{\pi}]$$

**Proof.** See Appendix A.6. \qed

This bound should be contrasted with our result from Theorem 1. With $\alpha = 0$, the family of pessimistic algorithms reduces to the family of naïve algorithms, so the bound is correspondingly identical. We can add pessimism by increasing $\alpha$, and this corresponds to a decrease in the magnitude of the supremum term. When $\alpha = 1$, we have a value lower-bound, and there is no supremum term at all.

The infimum term is small under the condition previously discussed: when there exists any policy with high expected return and low value uncertainty. Increasing pessimism increases underestimation, making this term somewhat larger; however, this term is much smaller to begin with, so the increase does not have much of an impact on the overall suboptimality. We see that for the task given in Section 1.1, and for real-world tasks with similar attributes, sufficiently pessimistic algorithms will have low suboptimality, in contrast to naïve algorithms.

To further understand the power of this approach, it is illustrative to compare it to imitation learning. Consider the case where the dataset contains a small number of expert trajectories but also a large number of interactions from a random policy, i.e. when learning from suboptimal demonstrations [3]. If the dataset contained only a small amount of expert data, then both an UA pessimistic FDPO algorithm and an imitation learning algorithm would return a high-value policy. However, the injection of sufficiently many random interactions would degrade the performance of imitation learning algorithms, whereas UA pessimistic algorithms would continue to behave similarly to the expert data.
6.3 Proximal Pessimistic Algorithms

The next family of algorithms we study are the proximal pessimistic algorithms, which implement pessimism by penalizing policies that deviate from the empirical policy. The name proximal was chosen to reflect the idea that these algorithms prefer policies which stay "nearby" to the empirical policy.

Proximal pessimistic algorithms are strictly less powerful than uncertainty-aware algorithms, but are useful in the context of deep learning. This is because we do not currently know how to compute non-vacuous local dynamics uncertainties for neural networks, and proximal pessimistic algorithms can be implemented without implementing any Bellman uncertainty function. Many FDPO algorithms in the literature, and in particular several recently-proposed deep learning algorithms \[7, 14, 18, 21, 46\], resemble members of the family of proximal pessimistic algorithms; see Appendix D.

**Definition 6 (Proximal pessimistic algorithms).** A proximal pessimistic algorithm with pessimism hyperparameter \(\alpha \in [0, 1]\) is any algorithm in the family defined by the fixed-point function

\[
f_{\text{proximal}}(v^\pi) = A^\pi(r_D + \gamma P_D v^\pi) - \alpha \left( \frac{\gamma TV_S(\pi, \hat{\pi}_D)}{(1 - \gamma)^2} \right)
\]

The proximal pessimistic fixed-point function also takes the form of a penalized version of the naive fixed-point function, except the penalty now corresponds to the local similarity to the empirical policy. Once again, we can find the optimal policy using a penalized version of any dynamic programming algorithm, e.g. policy iteration or value iteration.

**Theorem 3 (Proximal pessimistic FDPO suboptimality bound).** Consider any proximal pessimistic value-based fixed-dataset policy optimization algorithm \(O_{\text{proximal}}\). Let \(\mu\) be any value uncertainty function, and \(\alpha \in [0, 1]\) be a pessimism hyperparameter. For any dataset \(D\), the suboptimality of \(O_{\text{proximal}}\) is bounded with probability at least \(1 - \delta\) by

\[
\text{SUBOPT}(O_{\text{proximal}}(D)) \leq (1 - \alpha) \cdot \mathbb{E}_\rho[\mu_{D,\delta}] + \inf_\pi \left( \mathbb{E}_\rho[v_{_{\pi M}} - v_{_{\hat{\pi} M}}] + (1 + \alpha) \cdot \mathbb{E}_\rho \left[ (I - \gamma A^\pi P_D)^{-1} \frac{\gamma TV_S(\pi, \hat{\pi}_D)}{(1 - \gamma)^2} \right] \right) + \sup_\pi \left( (1 - \alpha) \cdot \mathbb{E}_\rho \left[ (I - \gamma A^\pi P_D)^{-1} \frac{\gamma TV_S(\pi, \hat{\pi}_D)}{(1 - \gamma)^2} \right] \right)
\]

**Proof.** See Appendix A.7.

This bound indicates that the performance of the algorithm is dependent on three things. Firstly, the value uncertainty of empirical policy itself. Secondly, the existence of a near-optimal policy that is similar to the empirical policy. Finally, the non-existence of any policies which are dissimilar to the empirical policy. Once again, we see that as \(\alpha\) grows, the supremum term shrinks, leading to a suboptimality bound that is not reliant on satisfying a global condition.

The primary limitation of the proximal approach is the looseness of the value lower-bound. Intuitively, this algorithm can be understood as performing imitation learning, but permitting minor deviations. Constraining the policy to be near in distribution to the empirical policy can fail to take advantage of highly-visited states which are reached via many trajectories. In fact, in contrast to both the naive approach and the UA pessimistic approach, in the limit of infinite data this approach is not guaranteed to converge to the optimal policy. Also, note that when \(\alpha \geq \frac{1 - \gamma}{\gamma}\), this algorithm is identical to imitation learning. This can be seen by solving for the locally optimal policy at any state, and noting that it will be equal to the empirical policy under this condition.

7 Experiments

We implement algorithms from each family to empirically investigate whether their performance follows the predictions of our bounds. Below, we summarize the key predictions made by our theory.
(a) Performance of FDPO algorithms on a dataset of 2000 transitions, as the data collection policy is interpolated from random to optimal.

(b) Performance of FDPO algorithms as dataset size increases. Data is collected with an optimal \(\epsilon\)-greedy policy, with \(\epsilon = 50\%\).

Figure 2: Tabular gridworld experiments.

- **Imitation.** This algorithm simply learns to copy the empirical policy. We expect it to perform well if and only if the data collection policy performs well.

- **Naïve.** We expect this algorithm to perform well only when almost no policies have high value uncertainty. This means that when the data is collected from any mostly-deterministic policy, performance of this algorithm will be poor, since many states will be missing data. Stochastic data collection will improve performance. As the size of the dataset grows, we expect this algorithm to approach optimality.

- **Proximal.** We expect this algorithm to roughly mirror the performance of the imitation approach, but improve upon it. As the size of the dataset grows, we do not expect this algorithm to approach optimality.

- **Uncertainty-aware.** We expect this algorithm to perform well when there is data on states visited by near-optimal policies. This is the case when a small amount of data has been collected from a near-optimal policy, or a large amount of data has been collected from a worse policy. As the size of the dataset grows, we expect this algorithm to approach optimality. We expect this approach to outperform all other approaches.

See Appendix B for pseudocode of all algorithms. Since the algorithms can be computed exactly in tabular environments, we begin by comparing their performance on a simple gridworld. Then, we demonstrate the relevance of our results to neural FDPO by extending some algorithms to the deep learning setting, and evaluate them using the MinAtar environments [47]. In this document, we provide only a high-level overview of the experiments. For an open-source implementation, including full details suitable for replication, please refer to the code in the accompanying GitHub repository: github.com/jbuckman/tiopifdpo.

### 7.1 Tabular

The first set of experiments utilize a simple tabular gridworld. The state space is 8x8, and the action space is \{Up, Down, Left, Right\}. Rewards are Bernoulli-distributed, with the mean reward for each state-action sampled from Beta(3,1); transitions are stochastic, moving in a random direction with probability 0.2; the discount is .99. This environment was selected to be simple and generic. We compare the performance of four approaches: imitation, naïve, uncertainty-aware pessimistic, and proximal pessimistic. The imitation algorithm simply returns the policy which takes actions in proportion to their observed frequencies in the dataset. For the UA pessimistic algorithm, we use the technique described in Appendix C.1 to implement Bellman uncertainty functions. For both pessimistic algorithms, we absorb all constants into the hyperparameter \(\alpha\), which we selected to be \(\alpha = 1\) for both algorithms.
of -greedy data collection policy

Figure 3: Performance of deep FDPO algorithms on a dataset of 500000 transitions, as the data collection policy is interpolated from near-optimal to random. Note that here, the only pessimistic algorithm evaluated is proximal.

by a simple manual search. For state-actions with no observations, we select \( r_D \) uniformly at random in \([0, 1]\), \( P_D \) transitions uniformly at random, and \( \hat{\pi}_D \) acts uniformly at random. We report the average of 1000 trials. The shaded region represents a 95% confidence interval.

The first experiment, whose results are shown in Figure 2(a), compares the performance of the algorithms as the policy used to collect the dataset is interpolated from the uniform random policy to an optimal policy using \( \epsilon \)-greedy. The second experiment, whose results are shown in Figure 2(b), compares the performance of the algorithms as we increase the size of the dataset from 1 sample to 200000 samples. In both experiments, we notice a qualitative difference between the trends of the various algorithms, which aligns with the predictions of our theory.

7.2 Deep Learning

The second setting we evaluate on consists of four environments from the MinAtar suite \([47]\). In order to derive a near-optimal policy on each environment, we run DQN to convergence and save the resulting policy. We report the average of 3 trials. The shaded area represents the range between the maximum and minimum values.

We implement deep learning versions of the above algorithms in the style of Neural Fitted Q-Iteration \([30]\). In this setting, we implement only proximal pessimistic algorithms. To compute the penalty term, we must approximate \( \hat{\pi}_D \); this can be done by training a policy network on the dataset to predict actions via maximum likelihood. Just as in the tabular setting, we absorb all constant coefficients into our pessimism hyperparameter, here setting \( \alpha = .25 \).

The results of these experiments can be seen in Figure 3. Similarly to the tabular experiments, we see that the naïve approach performs well when data is fully exploratory, and poorly when data is collected via an optimal policy; the pure imitation approach performs better when the data collection policy is closer to optimal. The pessimistic approach achieves the best of both worlds: it learns a good policy from an exploratory policy, but also correctly imitates a near-optimal policy. In many cases, it is able to improve on both.\(^8\) One notable exception is in Freeway, where the performance of the pessimistic approach closely mirrors the imitation policy, despite the naïve approach performing near-optimally for intermediate values of \( \epsilon \).

All experiments used identical hyperparameters. Hyperparameter tuning was done on just two experimental setups: Breakout using \( \epsilon = 0 \), and Breakout using \( \epsilon = 1 \). Tuning was very minimal, and done via a small manual search.

7.2.1 Practical Considerations

Through the process of running experiments in the deep learning setting, the authors noted that several aspects of the experimental setup, which have not been addressed in previous work, had surprisingly large impacts on the results. In this section, we informally report some of our findings, which future researchers may find useful. Additionally, we hope these effects will be studied more rigorously in future work.

\(^8\)By adjusting the hyperparameter controlling the amount of pessimism, we can in fact interpolate from being exactly naïve to exactly imitation. By selecting a hyperparameter that is in between, we get this best-of-both-worlds behavior.
The first consideration is that performance is highly nonmonotonic with respect to training time. In almost all experiments, it was observed that with every target-network update, the performance of the policy would oscillate wildly. Even after performing many Bellman updates, few experiments showed anything resembling convergence. It is therefore important that the total number of steps be selected beforehand, to avoid unintentional cherry-picking of results. Additionally, one common trend was for algorithms to have high performance early on, and then eventually crash. For this reason, it is important that algorithms be run for a long duration, in order to be certain that the conclusions drawn are valid.

The second consideration is the degree to which the inner-loop optimization process succeeds. If throughout training, whenever we update the target network, its error is low, convergence near to the fixed point is guaranteed [1]. However, computational restrictions force us to make tradeoffs about the degree to which this condition is satisfied. Experimentally, we found this property to be very important: when the error was not properly minimized, performance was negatively impacted, sometimes even leading to divergence. There are three notable algorithmic decisions which we found were required to ensure that the error was adequately minimized.

The size of the network. It is important to ensure that the network is large enough to reasonably fit the values at all points throughout training. Most prior works [7, 18, 19] utilize the same network architecture as the original DQN [25], which is fairly small by modern standards. We found that this size of network was adequate to fit MinAtar environments, but that decreasing the size of the network further led to significant performance degradation. Preliminary experiments indicated that since the full Atari environment is much more complex than MinAtar, a larger network may be required.

The amount of training steps in the inner loop of Neural Fitted Q-Iteration. If the number of steps is too small, error will not be adequately minimized. In our experiments, approximately 250,000 gradient steps per target update were required to consistently minimize error enough to avoid divergence. We note that many prior works [7, 18, 19] do not adjust this hyperparameter; typical results in the literature use fewer than 10,000 gradient steps per update.

The per-update initialization of the network. When changing the target network, we are in essence beginning a new supervised learning problem. Thus, to ensure that we could reliably find a good solution, we found that we needed to fully reinitialize the neural network whenever we updated the target network. The dynamics of training neural networks via gradient descent are still not fully understood, but it is well known that the initialization is of great importance [11]. It has been observed that certain initializations can seriously impact training: for example, if the final parameters of a classifier trained on randomly-relabeled CIFAR classifier are used as the initialization for the regular CIFAR classification task, the trained network will have worse test-set performance.\(^9\)

8 Discussion

We described two families of pessimistic algorithms, uncertainty-aware and proximal. We see theoretically that both of these approaches have advantages over the naïve approach, and observed these advantages empirically. Comparing these two families of pessimistic algorithms, we see theoretically that uncertainty-aware algorithms are strictly better than proximal algorithms, and that proximal algorithms may not yield the optimal policy, even with infinite data.\(^{10}\) This, too, was observed in our experiments.

Current deep learning approaches to fixed-dataset policy optimization are most similar to the proximal approach, in that they utilize some form of policy constraint or penalty to keep the learned policy similar to the empirical policy [7, 18, 21]. This is due to the fact that the UA approach requires estimating the uncertainties of our neural networks, which is still an unsolved problem. Further research into uncertainty estimation with neural networks will enable the development of deep learning algorithms in the family of uncertainty-aware algorithms. As is evidenced by our tabular results, we expect these approaches to yield dramatic performance improvements.

One surprising property of pessimistic algorithms is that the optimal policy is often stochastic. This is because

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\(^9\) Chelsea Finn, Suraj Nair, Henrik Marklund; personal communication.

\(^{10}\) With adequate tuning, for any particular problem, it is generally possible to select a pessimism hyperparameter that allows us to converge. However, doing the tuning requires evaluating each policy in the environment, which means gaining information by interacting with the environment; this is not permitted by the problem setting. Also, one might imagine a variety of algorithmic schemes to address this issue, e.g. an adaptive pessimism hyperparameter which decays with data. However, most such modifications are not useful, because they implicitly utilize a Bellman uncertainty function. If a Bellman uncertainty function is available, we can simply use a UA approach instead of a proximal approach.
the penalty term included in their fixed-point objective is often minimized by stochastic policies. For the penalty of proximal pessimistic algorithms, it is easy to see that this will be the case for any non-deterministic empirical policy; for UA pessimistic algorithms, it is dependent on the choice of Bellman uncertainty function, but often still holds (see Appendix C.2 for the derivation of a Bellman uncertainty function with this property). This observation lends mathematical rigor to the intuition that agents should ‘hedge their bets’ in the face of epistemic uncertainty. This property also means that the simple approach of selecting the argmax action is no longer adequate for policy improvement. In Appendix B.2.2 we discuss a policy improvement procedure that takes into account the proximal penalty to find the stochastic optimal policy.

The problem of fixed-dataset policy optimization is closely related to the problem of reinforcement learning, and as such, there is a large body of work which contains ideas related to those discussed in this paper. We discuss these works in detail in Appendix D.

Finally, due to the close connection between the FDPO and RL settings, this work has implications for deep reinforcement learning. Many popular deep RL algorithms utilize a replay buffer to break the correlation between samples in each minibatch [25]. However, since these algorithms typically alternate between collecting data and training the network, the replay buffer can also be viewed as a ‘temporarily fixed’ dataset during the training phase. These algorithms are often very sensitive to hyperparameters; in particular, they perform poorly when the number of learning steps per interaction is large [6]. This effect can partially be explained by our results: additional steps of learning cause the policy to approach its naïve FDPO fixed-point, which has poor worst-case suboptimality. A pessimistic algorithm with a better fixed-point could therefore allow us to train more per interaction, improving sample efficiency. A potential direction of future work is therefore to incorporate pessimism into deep RL.

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A Proofs

A.1 Tightness of Over/Under Decomposition

We show that the bound given in Lemma 1 is tight via a simple example.

Proof. Consider a bandit-structured MDP with a single state and two actions, A and B, with rewards of 0 and 1 respectively, which both lead to terminal states.

First, consider the left-hand side. If an FDPE subroutine estimates the value of both arms to be 1, then the policy which always selects arm A is an optimal policy of the corresponding FDPO algorithm. In this case, the suboptimality is clearly equal to 1. This is clearly the worst-case suboptimality, since it is the largest possible suboptimality in the environment.

On the right-hand side, note that term (a) is 0 when π is the policy that always picks B, while term (b) is 1 when π is the policy that always picks A. Thus, the left-hand and right-hand sides are equal, and the bound is tight. □

A.2 Residual Visitation Lemma

We prove a basic lemma showing that the error of any value function is equal to its one-step Bellman residual, summed over its visitation distribution. Though this result is well-known, it is not clearly stated elsewhere in the literature, so we prove it here for clarity.

Lemma 3. For any MDP ξ and policy π, consider the Bellman fixed-point equation given by, let \( v_\xi^\pi \) be defined as the unique value vector such that \( v_\xi^\pi = A^\pi (r_\xi + \gamma P_\xi v_\xi^\pi) \), and let \( v \) be any other value vector. We have

\[
\begin{align*}
|v_\xi^\pi - v| &= (I - \gamma A^\pi P_\xi)^{-1}(A^\pi (r_\xi + \gamma P_\xi v) - v) \\
|v_\xi^\pi - v| &= (I - \gamma A^\pi P_\xi)^{-1}(v - A^\pi (r_\xi + \gamma P_\xi v)) \\
|v_\xi^\pi - v| &= (I - \gamma A^\pi P_\xi)(v_\xi^\pi - v)
\end{align*}
\]

Proof.

\[
\begin{align*}
A^\pi (r_\xi + \gamma P_\xi v) - v &= A^\pi (r_\xi + \gamma P_\xi v) - v_\xi^\pi + v_\xi^\pi - v \\
&= A^\pi (r_\xi + \gamma P_\xi v) - A^\pi (r_\xi + \gamma P_\xi v_\xi^\pi) + v_\xi^\pi - v \\
&= \gamma A^\pi P_\xi (v - v_\xi^\pi) + (v_\xi^\pi - v) \\
&= (v_\xi^\pi - v) - \gamma A^\pi P_\xi (v_\xi^\pi - v) \\
&= (I - \gamma A^\pi P_\xi)(v_\xi^\pi - v)
\end{align*}
\]

Thus, we see \((I - \gamma A^\pi P_\xi)^{-1}(A^\pi (r_\xi + \gamma P_\xi v) - v) = v_\xi^\pi - v.\) An identical proof can be completed starting with \(v - A^\pi (r_\xi + \gamma P_\xi v)\), leading to the desired result. □

A.3 Naïve FDPE Error Bound

Notice that the naïve fixed-point function is equivalent to the Bellman fixed-point equation for a specific MDP: the empirical MDP defined by \((\mathcal{S}, \mathcal{A}, r_D, P_D, \gamma, \rho)\). Thus, invoking Lemma 3, for any values \( v \) we have

\[
|v_D^\pi - v| = (I - \gamma A^\pi P_D)^{-1}|A^\pi (r_D + \gamma P_D v) - v|.
\]

Since \(v_M^\pi\) is a value vector, this immediately implies that

\[
|v_D^\pi - v_M^\pi| = (I - \gamma A^\pi P_D)^{-1}|A^\pi (r_D + \gamma P_D v_M^\pi) - v_M^\pi|.
\]
Since $v^*_M$ is the solution to the Bellman consistency fixed-point,

$$|v^*_D - v^*_M| = (I - \gamma A^\pi P_D)^{-1}|A^\pi (r_D + \gamma P_D v^*_M) - A^\pi (r_M + \gamma P_M v^*_M)|.$$  

Finally, using the definition of a value uncertainty function $\mu^\pi_{D,\delta}$, we arrive at

$$|v^*_D - v^*_M| \leq \mu^\pi_{D,\delta}$$

completing the proof.

### A.4 Relative Value Uncertainty

The key to the construction of proximal pessimistic algorithms is a bound on the error of a naïve FDPE algorithm when evaluating some policy $\pi$, in terms of the value uncertainty of some other policy $\pi'$, as well as the similarity between $\pi$ and $\pi'$.

**Lemma 4** (Relative value uncertainty). For any two policies $\pi, \pi'$, and any value uncertainty $u$, we have

$$\mu^\pi_{D,\delta} = \mu'^\pi_{D,\delta} + (I - \gamma A^\pi P_D)^{-1}(\gamma)(A^\pi - A'^\pi)P_D \mu'^\pi_{D,\delta}$$

**Proof.** Firstly, we express the value uncertainty for $\pi$ (without loss of generality) in a Bellman-like form.

$$\mu^\pi_{D,\delta} = (I - \gamma A^\pi P_D)^{-1} u^\pi_{D,\delta}$$

$$\mu^\pi_{D,\delta} - \gamma P_D A^\pi u^\pi_{D,\delta} = u^\pi_{D,\delta}$$

$$\mu^\pi_{D,\delta} = u^\pi_{D,\delta} + \gamma A^\pi P_D \mu^\pi_{D,\delta}$$

Next, we bound the difference between the value uncertainty of $\pi$ and $\pi'$.

$$\mu^\pi_{D,\delta} - \mu'^\pi_{D,\delta} = (u^\pi_{D,\delta} + \gamma A^\pi P_D \mu^\pi_{D,\delta}) - (u'^\pi_{D,\delta} + \gamma A'^\pi P_D \mu'^\pi_{D,\delta})$$

$$= \gamma A^\pi P_D \mu^\pi_{D,\delta} - \gamma A'^\pi P_D \mu'^\pi_{D,\delta}$$

$$= \gamma A^\pi P_D (\mu^\pi_{D,\delta} - \mu'^\pi_{D,\delta}) + \gamma (A^\pi - A'^\pi)P_D \mu'^\pi_{D,\delta}$$

This is a geometric series, so $(I - \gamma A^\pi P_D) (\mu^\pi_{D,\delta} - \mu'^\pi_{D,\delta}) = \gamma (A^\pi - A'^\pi)P_D \mu'^\pi_{D,\delta}$. Left-multiplying by $(I - \gamma A^\pi P_D)^{-1}$ we see

$$\left(\mu^\pi_{D,\delta} - \mu'^\pi_{D,\delta}\right) = (I - \gamma A^\pi P_D)^{-1}(\gamma)(A^\pi - A'^\pi)P_D \mu'^\pi_{D,\delta}$$

$$\mu^\pi_{D,\delta} = \mu'^\pi_{D,\delta} + (I - \gamma A^\pi P_D)^{-1}(\gamma)(A^\pi - A'^\pi)P_D \mu'^\pi_{D,\delta}$$

Looking at this result, we see that we can write the value uncertainty of $\pi$ in terms of the value uncertainty of any other policy $\pi'$. Since the two policies are different, there is a corrective term which scales up the bound by the magnitude of the difference.

### A.5 Naïve FDPE Relative Error Bound

**Lemma 5** (Naïve FDPE relative error bound). Consider any naïve fixed-dataset policy evaluation algorithm $\mathcal{E}_{\text{naïve}}$. For any policy $\pi$ and dataset $D$, denote $v^\pi_D := \mathcal{E}_{\text{naïve}}(D, \pi)$. Then, for any other policy $\pi'$, the following bound holds with probability at least $1 - \delta$:

$$|v^\pi_D - v^\pi_M| \leq \mu^\pi_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{1 - \gamma^2}\right) \text{TV}_S(\pi, \pi')$$
Proof. The goal of this section is to construct an error bound for which we can optimize \( \pi \) without needing to compute any uncertainties. To do this, we must replace this quantity with a looser upper bound. Note that since Bellman uncertainty \( u_{D,\delta} \leq \frac{1}{1-\gamma} \) and \( (I - \gamma P_D A^\pi)^{-1} \leq \frac{1}{1-\gamma} \), we have

\[
\mu_{D,\delta}^* \leq \frac{1}{(1-\gamma)^2} \mathbf{1}.
\]

If we substitute it into the second term (after ensuring that all coefficients are positive), we see:

\[
\begin{align*}
\mu_{D,\delta}^* & \leq \mu_{D,\delta}^* + (I - \gamma A^\pi P_D)^{-1}(\gamma)|A^\pi - A^\pi'| P_D \mu_{D,\delta}^* \\
& \leq \mu_{D,\delta}^* + (I - \gamma A^\pi P_D)^{-1}(\gamma)|A^\pi - A^\pi'| P_D \frac{1}{(1-\gamma)^2} \mathbf{1} \\
& = \mu_{D,\delta}^* + (I - \gamma A^\pi P_D)^{-1}\left(\frac{\gamma}{(1-\gamma)^2}\right)|A^\pi - A^\pi'| P_D \mathbf{1} \\
& = \mu_{D,\delta}^* + (I - \gamma A^\pi P_D)^{-1}\left(\frac{\gamma}{(1-\gamma)^2}\right)|A^\pi - A^\pi'| \mathbf{1}
\end{align*}
\]

The last line follows from noting that \( P_D \) is stochastic. Finally, note that since the positive and negative components of the state-wise difference between policies must be symmetric, \( |A^\pi - A^\pi'| \mathbf{1} \) is precisely equivalent to the state-wise total variation distance, \( \text{TV}_S(\pi, \pi') \). Thus, we have

\[
\mu_{D,\delta}^* \leq \mu_{D,\delta}^* + (I - \gamma A^\pi P_D)^{-1}\left(\frac{\gamma}{(1-\gamma)^2}\right)\text{TV}_S(\pi, \pi').
\]

Finally, invoking Lemma 2, we arrive at the desired result. \( \square \)

A.6 Suboptimality of Uncertainty-Aware Pessimistic FDPO Algorithms

Let \( v_D^\pi := \mathcal{E}_{\text{naive}}(D, \pi) \). From the definition of the UA family, we have the fixed-point property \( v_D^\pi = A^\pi (r_D + \gamma P_D v_D^\pi) - \alpha u_{D,\delta}^\pi \), and the standard geometric series rearrangement yields \( v_D^\pi = (I - \gamma A^\pi P_D)^{-1}(A^\pi r_D - \alpha u_{D,\delta}^\pi) \). From here, we see:

\[
\begin{align*}
v_D^\pi &= (I - \gamma A^\pi P_D)^{-1}(A^\pi r_D - \alpha u_{D,\delta}^\pi) \\
&= (I - \gamma A^\pi P_D)^{-1} A^\pi r_D - (I - \gamma A^\pi P_D)^{-1} \alpha u_{D,\delta}^\pi \\
&= \mathcal{E}_{\text{naive}}(D, \pi) - \alpha \mu_{D,\delta}^*
\end{align*}
\]

We now use this to bound overestimation and underestimation error of \( \mathcal{E}_{\text{naive}}(D, \pi) \) by invoking Lemma 2, which holds with probability at least \( 1 - \delta \). First, for underestimation, we see:

\[
\begin{align*}
v_M^\pi - v_D^\pi &= v_M^\pi - (\mathcal{E}_{\text{naive}}(D, \pi) - \alpha \mu_{D,\delta}^*) \\
&= (v_M^\pi - \mathcal{E}_{\text{naive}}(D, \pi)) + \alpha \mu_{D,\delta}^*
\end{align*}
\]

and thus, \( v_M^\pi - v_D^\pi \leq (1 + \alpha) \mu_{D,\delta}^* \). Next, for overestimation, we see:

\[
\begin{align*}
v_D^\pi - v_M^\pi &= (\mathcal{E}_{\text{naive}}(D, \pi) - \alpha \mu_{D,\delta}^*) - v_M^\pi \\
&= (\mathcal{E}_{\text{naive}}(D, \pi) - v_M^\pi) - \alpha \mu_{D,\delta}^* \\
&\leq \mu_{D,\delta}^* - \alpha \mu_{D,\delta}^* \\
&= (1 - \alpha) \mu_{D,\delta}^*
\end{align*}
\]

and thus, \( v_D^\pi - v_M^\pi \leq (1 - \alpha) \mu_{D,\delta}^* \). Substituting these bounds into Lemma 1 gives the desired result.
A.7 Suboptimality of Proximal Pessimistic FDPO Algorithms

Let $v^*_D := \mathcal{E}_{\text{proximal}}(D, \pi)$. From the definition of the proximal family, we have the fixed-point property

$$v^*_D = A^\pi(r_D + \gamma P_D v^*_D) - \alpha \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')$$

and the standard geometric series rearrangement yields

$$v^*_D = (I - \gamma A^\pi P_D)^{-1} \left(A^\pi r_D - \alpha \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)$$

From here, we see:

$$v^*_D = (I - \gamma A^\pi P_D)^{-1} \left(A^\pi r_D - \alpha \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)$$

$$= (I - \gamma A^\pi P_D)^{-1} A^\pi r_D - (I - \gamma A^\pi P_D)^{-1} \alpha \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')$$

$$= \mathcal{E}_{\text{naive}}(D, \pi) - (I - \gamma A^\pi P_D)^{-1} \alpha \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')$$

Next, we define a new family of FDPO algorithms,

$$\mathcal{E}_{\text{proximal-full}}(D, \pi) := \mathcal{E}_{\text{naive}}(D, \pi) - \alpha \left(\mu^*_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)$$

We use Lemma 5, which holds with probability at least $1 - \delta$, to bound the overestimation and underestimation.

$$v^*_M - \mathcal{E}_{\text{proximal-full}}(D, \pi) = v^*_M - \left(\mathcal{E}_{\text{naive}}(D, \pi) - \alpha \left(\mu^*_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)\right)$$

$$= (v^*_M - \mathcal{E}_{\text{naive}}(D, \pi)) + \alpha \left(\mu^*_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)$$

$$\leq (1 + \alpha) \left(\mu^*_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)$$

Next, we analogously bound the overestimation:

$$\mathcal{E}_{\text{proximal-full}}(D, \pi) - v^*_M = \left(\mathcal{E}_{\text{naive}}(D, \pi) - \alpha \left(\mu^*_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)\right) - v^*_M$$

$$= (v^*_M - \mathcal{E}_{\text{naive}}(D, \pi)) - \alpha \left(\mu^*_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)$$

$$\leq (1 - \alpha) \left(\mu^*_{D,\delta} + (I - \gamma A^\pi P_D)^{-1} \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right)$$

We can now invoke Lemma 1 to bound the suboptimality of any value-based FDPO algorithm which uses $\mathcal{E}_{\text{proximal-full}}$, which we denote with $\mathcal{O}^{\text{VB}}_{\text{proximal-full}}$. Substituting and rearranging, we see that with probability at least $1 - \delta$,

$$\text{SUBOPT}(\mathcal{O}^{\text{VB}}_{\text{proximal-full}}(D)) \leq (1 - \alpha) \cdot \mathbb{E}_\rho[\mu^*_{D,\delta}] + \inf_{\pi} \mathbb{E}_\rho[v^*_M - v^*_M] + (1 + \alpha) \cdot \mathbb{E}_\rho \left[(I - \gamma A^\pi P_D)^{-1} \frac{\gamma TV_S(\pi, \hat{\pi}_D)}{(1-\gamma)^2}\right]$$

$$+ \sup_{\pi} (1 - \alpha) \cdot \mathbb{E}_\rho \left[(I - \gamma A^\pi P_D)^{-1} \frac{\gamma TV_S(\pi, \hat{\pi}_D)}{(1-\gamma)^2}\right]$$

Finally, we see that FDPO algorithms which use $\mathcal{E}_{\text{proximal-full}}$ as their subroutine will return the same policy as FDPO algorithms which use $\mathcal{E}_{\text{proximal}}$:

$$\arg \max_{\pi} \mathbb{E}_\rho[\mathcal{E}_{\text{proximal-full}}(D, \pi)] = \arg \max_{\pi} \mathbb{E}_\rho \left[\mathcal{E}_{\text{naive}}(D, \pi) - \mu^*_{D,\delta} - (I - \gamma A^\pi P_D)^{-1} \alpha \left(\frac{\gamma}{(1-\gamma)^2}\right) TV_S(\pi, \pi')\right]$$
\[
= \arg \max_{\pi} \mathbb{E}_\rho \left[ \mathcal{E}_\text{na"ive}(D, \pi) - (I - \gamma A^\pi P_D)^{-1} \alpha \left( \frac{\gamma}{(1 - \gamma)^2} \right) \text{TV}(\pi, \pi') \right]
\]

\[
= \arg \max_{\pi} \mathbb{E}_\rho [\mathcal{E}_\text{proximal}(D, \pi)]
\]

Thus, the suboptimality of \( \arg \max_{\pi} \mathbb{E}_\rho [\mathcal{E}_\text{proximal}(D, \pi)] \) must be equivalent to that of \( \arg \max_{\pi} \mathbb{E}_\rho [\mathcal{E}_\text{proximal-full}(D, \pi)] \), leading to the desired result.

### B Algorithms

In the main body of the text, we primarily focus on families of algorithms, rather than specific members. In this section, we provide pseudocode from example algorithms in each family. The majority of these algorithms are simple empirical extensions of well-studied algorithms, so we do not study their properties (e.g. convergence) in detail. The sets of algorithms described here are not intended to be comprehensive, but rather, a few straightforward examples to illustrate key concepts and inspire further research. To simplify presentation, we avoid hyperparameters, e.g. learning rate, wherever possible.

#### B.1 Na"ive

The na"ive algorithms presented here are simply standard dynamic programming approaches applied to the empirical MDP constructed from the dataset, using \( r_D, P_D \) in place of \( r, P \). See [29] for analysis of convergence, complexity, optimality, etc. of the general dynamic programming approaches, and note that the empirical MDP is simply a
particular example of an MDP, so all results apply directly.

**Algorithm 1: Tabular Fixed-Dataset Policy Evaluation**

**Input:** Dataset $D$, policy $\pi$, discount $\gamma$.
Construct $r_D, P_D$ as described in Section 2;
$v \leftarrow (I - \gamma A^\pi P_D)^{-1} A^\pi r_D$;
return $v$;

**Algorithm 2: Tabular Fixed-Dataset Policy Iteration**

**Input:** Dataset $D$, discount $\gamma$.
Initialize $\pi, v$ Construct $r_D, P_D$ as described in Section 2;
while $\pi$ not converged do
  $\pi \leftarrow \arg \max_{\pi\in\Pi} A^\pi (r_D + \gamma P_D v)$; // argmax policy is state-wise max action
  $v \leftarrow (I - \gamma A^\pi P_D)^{-1} A^\pi r_D$;
end
return $\pi$;

**Algorithm 3: Tabular Fixed-Dataset Value Iteration**

**Input:** Dataset $D$, discount $\gamma$.
Initialize $\pi, v$ Construct $r_D, P_D$ as described in Section 2;
while $v$ not converged do
  $\pi \leftarrow \arg \max_{\pi\in\Pi} A^\pi v$; // argmax policy is state-wise max action
  $v \leftarrow r_D + \gamma P_D A^\pi v$;
end
return $\pi$;

**Algorithm 4: Neural Fixed-Dataset Value Iteration**

**Input:** Dataset $D$, discount $\gamma$.
Initialize $\theta, \theta'$ while $\theta$ not converged do
  for each $s$ in $D$ do
    $\pi(s) \leftarrow \arg \max_{a\in\mathcal{A}} q_\theta(s, a)$;
  end
while $\theta'$ not converged do
  Sample $(s, a, r, s')$ from $D$;
  $L \leftarrow (r + \gamma q_\theta(s', \pi(s')) - q_\theta(s, a))^2$;
  $\theta' \leftarrow \theta' - \nabla_{\theta'} L$;
end
$\theta \leftarrow \theta'$
end
return $\pi$;

**B.2 Pessimistic**

In this section, we provide pseudocode for concrete implementations of algorithms in the pessimistic families we have discussed. Since the algorithms are not the focus of this work, we do not provide an in-depth analysis of these algorithms. We briefly note that, at a high level, the standard proof technique used to show convergence of policy iteration [36] can be applied to all of these approaches. These algorithms utilize a penalized Bellman update, and the penalty is state-wise and independent between states. Thus, performing a local greedy policy improvement in any one state will strictly increase the value of all states. Thus, policy iteration guarantees strict monotonic improvement of the values of all states, and thus eventual convergence to an optimal policy (as measured by the penalized values).
B.2.1 Uncertainty-Aware

In this section, we provide pseudocode for a member of the UA pessimistic family of algorithms.

Algorithm 5: Tabular Uncertainty-Aware Pessimistic Fixed-Dataset Policy Iteration

**Input:** Dataset $D$, discount $\gamma$, error rate $\delta$.

1. Initialize $v, \pi$ Construct $r_D, P_D, \tilde{u}_D$ as described in Section 2;
2. Compute $u_{D,\delta}^{\pi}$ as described in Appendix C;
3. **while** $\pi$ not converged **do**
   1. $\pi \leftarrow \arg \max_{\pi \in \Pi} A^{\pi}(v - u_{D,\delta}^{\pi})$;
   2. $v \leftarrow (I - \gamma A^{\pi} P_D)^{-1} (A^{\pi} r_D - u_{D,\delta}^{\pi})$;
4. **end**
5. **return** $\pi$;

Algorithm 6: Neural Uncertainty-Aware Pessimistic Fixed-Dataset Value Iteration

**Input:** Dataset $D$, discount $\gamma$.

1. Initialize $\theta, \theta', \Psi$
2. **while** $\theta$ not converged **do**
   1. // update policy
      1. **while** $\Psi$ not converged **do**
         1. Sample $\langle s, \cdot, \cdot, \cdot \rangle$ from $D$;
         2. $R \leftarrow \mathbb{E}_{a \sim \pi_{\phi}(\cdot|s)}[q_{\theta}(s, a)] - u_{D,\delta}^{\pi}(s)$;
         3. $\Psi' \leftarrow \Psi' + \nabla_{\theta} R$;
      2. **end**
   2. // update value function
      1. **while** $\theta'$ not converged **do**
         1. Sample $\langle s, a, r, s' \rangle$ from $D$;
         2. $L \leftarrow (r + \gamma (\mathbb{E}_{a' \sim \pi_{\phi}(\cdot|s')}[q_{\theta'}(s', a')] - q_{\theta'}(s, a'))^2$;
         3. $\theta' \leftarrow \theta' - \nabla_{\theta'} L$;
      2. **end**
   3. $\theta \leftarrow \theta'$
3. **end**
4. **return** $\pi$;

As discussed in the main text, count-based Bellman uncertainty functions, such as those derived from concentration inequalities in Appendix C.1, do not apply to non-tabular environments. The correct way to compute epistemic uncertainty with neural networks is still an open question. Therefore, our pseudocode for a neural implementation of the UA pessimistic approach is in some sense incomplete: a full implementation would need to specify a technique for computing $u_{D,\delta}^{\pi}$. We hope that future work will identify such a technique.
B.2.2 Proximal

In this section, we provide pseudocode for a member of the proximal pessimistic family of algorithms.

**Algorithm 7:** Tabular Proximal Pessimistic Fixed-Dataset Policy Iteration

**Input:** Dataset $D$, discount $\gamma$, error rate $\delta$.

- Initialize $v, \pi$ Construct $r_D, P_D, u_D$ as described in Section 2;
- Compute $u^\pi_{\delta,\delta}$ as described in Appendix C;

  **while** $\pi$ not converged **do**
  
  $\pi \leftarrow \arg \max_{a \in A} A^\pi (v - \frac{\alpha}{(1-\gamma)^2} |\hat{\pi} - \hat{\pi}_D|)$;
  
  $v \leftarrow (I - \gamma A^\pi P_D)^{-1} (A^\pi r_D - \frac{\alpha}{2(1-\gamma)^2} |\hat{\pi} - \hat{\pi}_D|)$;

  **end**

  return $\pi$;

**Algorithm 8:** Neural Proximal Pessimistic Fixed-Dataset Value Iteration

**Input:** Dataset $D$, discount $\gamma$.

- Initialize $\theta, \theta', \Psi$ **while** $\theta$ not converged **do**
  
  // update policy
  
  While $\Psi$ not converged **do**
  
  Sample $(s, \cdot, \cdot, \cdot)$ from $D$;
  
  $R \leftarrow (E_{a \sim \pi}(s) | q_\theta(s, a)) - \frac{\alpha}{(1-\gamma)^2} |\hat{\pi} - \hat{\pi}_D(s)|$;
  
  $\Psi' \leftarrow \Psi' + \nabla_\theta R$;

  **end**

  // update value function
  
  While $\theta'$ not converged **do**
  
  Sample $(s, \cdot, \cdot, \cdot)$ from $D$;
  
  $L \leftarrow (r + \gamma (E_{a \sim \pi}(s') | q_\theta(s', a')) - \frac{\alpha}{(1-\gamma)^2} |\hat{\pi}(s') - \hat{\pi}_D(s')| - q_\theta'(s, a))$;
  
  $\theta' \leftarrow \theta' - \nabla_\theta L$;

  **end**

  $\theta \leftarrow \theta'$

  return $\pi$;

One important nuance of proximal algorithms is that the optimal policy may not be deterministic, since the penalty term is minimized when the policy matches the empirical policy, which may itself be stochastic. It is not enough to select $\pi_{t+1}(s) = \arg \max_{a \in A} v(s, a)$; we must instead select $\pi_{t+1}(\cdot | s) = \sup_{\pi} v^\pi (s) = \sup_{\pi} \sum_{a \in A} \pi(a | s) v(s, a) - \frac{\alpha}{(1-\gamma)^2} |\pi(a | s) - \hat{\pi}_D(a | s)|$, which is a more difficult optimization problem. Fortunately, it has a closed-form solution.

**Proposition 1.** Consider any state-action values $q$ and empirical policy $\hat{\pi}_D$. Let

\[
\begin{align*}
    z &:= \max_{a \in A} q(s, a) - \frac{\alpha \gamma}{(1-\gamma)^2} \\
    \pi_{\text{localopt}}(a | s) &\begin{cases}
        \hat{\pi}_D(a | s) + (1 - \sum_{a' \text{ st. } q(s, a') > z} \hat{\pi}_D(a' | s)) & \text{if } a = \arg \max_{a' \in A} q(s, a') \\
        0 & \text{if } q(s, a) > z,
    \end{cases}
\end{align*}
\]

has the property

\[
\begin{align*}
    \sum_{a \in A} \pi_{\text{localopt}}(a | s) q(s, a) - \alpha \gamma (2(1-\gamma)^2 |\pi_{\text{localopt}}(a | s) - \hat{\pi}_D(a | s)| \geq \sum_{a \in A} \pi(a | s) q(s, a) - \frac{\alpha \gamma}{2(1-\gamma)^2} |\pi(a | s) - \hat{\pi}_D(a | s)|,
\end{align*}
\]

for all $s \in S, \pi \in \Pi$. 

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Proof. We provide a brief outline of the proof. Consider any policy \( \pi \neq \pi_{\text{localopt}} \) in some state \( s \). First, assume that exactly two cells of \( \pi(s) - \pi_{\text{localopt}}(s) \) are non-zero, meaning that one term is \( x \) and the other is \( -x \) (since both distributions sum to 1). If \( |x| > 0 \), the change in penalized return is non-positive, so \( \pi \) is worse that \( \pi_{\text{localopt}} \). To see this, we simply consider all possible mappings between \( x, -x \) and actions. Actions fall into three categories, corresponding to the three cases of the construction: argmax-actions, empirical-actions, and zero-actions, respectively. It’s easy to check each case, moving probability mass from any category of action to any other, and see that penalized return is always non-positive. Finally, if more than two cells of \( \pi(s) - \pi_{\text{localopt}}(s) \) are non-zero, we can always rewrite it as a sum of positive/negative pairs, and thus the overall change in penalized return is a sum of non-positive terms, and is itself non-positive. \( \square \)

C Computing Uncertainties

C.1 State-action-wise Bound

We seek to construct an \( u_{D,\delta} \) such that \( |A^\pi(r_M + \gamma P_M v) - A^\pi(r_D + \gamma P_D v)| \leq u_{D,\delta} \) with probability at least \( 1 - \delta \).

Firstly, let’s consider the simplest possible bound. \( v \) is bounded in \( [0, \frac{1}{1 - \gamma}] \), so both \( A^\pi(r_M + \gamma P_M v) \) and \( A^\pi(r_D + \gamma P_D v) \) must be as well. Thus, their difference is also bounded:

\[
|A^\pi(r_M + \gamma P_M v) - A^\pi(r_D + \gamma P_D v)| \leq \frac{1}{1 - \gamma} \]

Next, consider that for any \( \langle s, a \rangle \), the expression \( r_D(\langle s, a \rangle) + \gamma P_D(\langle s, a \rangle) v^\pi \) can be equivalently expressed as an average of random variables,

\[
r_D(\langle s, a \rangle) + \gamma P_D(\langle s, a \rangle) v = \frac{1}{n_D(\langle s, a \rangle)} \sum_{r, s' \in D(\langle s, a \rangle)} r + \gamma v(s'),
\]

each with expected value

\[
E_{r, s' \in D(\langle s, a \rangle)}[r + \gamma v(s')] = E_{r \sim \mathcal{R}(\langle s, a \rangle)}[r + \gamma v(s')] = [r_M + \gamma P_M v](\langle s, a \rangle).
\]

Note also that each of these random variables is bounded \([0, \frac{1}{1 - \gamma}]\). Thus, Hoeffding’s inequality tells us that this mean of bounded random variables must be close to their expectation with high probability. By invoking Hoeffding’s at each of the \(|S \times A|\) state-actions, and taking a union bound, we see that with probability at least \( 1 - \delta \),

\[
|(r_M + \gamma P_M v) - (r_D + \gamma P_D v)| \leq \frac{1}{1 - \gamma} \sqrt{\frac{1}{2} \ln \frac{2|S \times A|}{\delta}} n_D^{-\frac{1}{2}}
\]

We can left-multiply \( A^\pi \) and rearrange to get:

\[
|A^\pi(r_M + \gamma P_M v) - A^\pi(r_D + \gamma P_D v)| = \left( \frac{1}{1 - \gamma} \sqrt{\frac{1}{2} \ln \frac{2|S \times A|}{\delta}} \right) A^\pi n_D^{-\frac{1}{2}}
\]

Finally, we simply intersect this bound with the \( \frac{1}{1 - \gamma} \) bound from earlier. Thus, we see that with probability at least \( 1 - \delta \),

\[
|A^\pi(r_M + \gamma P_M v) - A^\pi(r_D + \gamma P_D v)| \leq \frac{1}{1 - \gamma} \cdot \min \left( \left( \frac{1}{1 - \gamma} \sqrt{\frac{1}{2} \ln \frac{2|S \times A|}{\delta}} \right) A^\pi n_D^{-\frac{1}{2}}, 1 \right)
\]
C.2 State-wise Bound

This bound is similar to the previous, but uses Hoeffding’s to bound the value at each state all at once, rather than bounding the value at each state-action.

For any $s$, the expression $[A^\pi(r_D + \gamma P_D v)](s)$ can be equivalently expressed as a mean of random variables,

$$[A^\pi(r_D + \gamma P_D v)](s) = \frac{1}{n_D(s)} \sum_{a, r, s' \in D(s)} \frac{\pi(a|s)}{\pi_D(a|s)} (r + \gamma v(s')),$$

each with expected value

$$E_{a, r, s' \in D(s)} \left[ \frac{\pi(a|s)}{\pi_D(a|s)} (r + \gamma v(s')) \right] = E_{a \sim \pi(\cdot|s)} E_{r \sim R(s, a)} E_{s' \sim P(\cdot|s, a)} [r + \gamma v(s')] = [A^\pi(r_M + \gamma P_M v)](s).$$

Note also that each of these random variables is bounded $[0, 1-\gamma \pi_D(a|s)]$. Thus, Hoeffding’s inequality tells us that this sum of bounded random variables must be close to its expectation with high probability. By invoking Hoeffding’s at each of the $|S|$ state-actions, and taking a union bound, we see that with probability at least $1 - \delta$,

$$|A^\pi(r_M + \gamma P_M v) - A^\pi(r_D + \gamma P_D v_M)| \leq \frac{1}{1-\gamma} \sqrt{\frac{1}{2} \ln \frac{2|S|}{\delta} (A^\pi)^{\circ 2} \bar{n}_D^{-1}}$$

where the term $(A^\pi)^{\circ 2}$ refers to the elementwise square. Finally, we once again intersect with $\frac{1}{1-\gamma}$, yielding that with probability at least $1 - \delta$,

$$|A^\pi(r_M + \gamma P_M v) - A^\pi(r_D + \gamma P_D v_M)| \leq \frac{1}{1-\gamma} \cdot \min \left( \sqrt{\frac{1}{2} \ln \frac{2|S|}{\delta} (A^\pi)^{\circ 2} \bar{n}_D^{-1}}, 1 \right)$$

Comparing this to the Bellman uncertainty function in Appendix C.1, we see two differences. Firstly, we have removed a factor of $|A|$, tightening the bound somewhat. Secondly, $A^\pi$ has now moved inside of the square root; since the square root is concave, Jensen’s inequality says that

$$\sqrt{(A^\pi)^{\circ 2} \bar{n}_D^{-1}} \leq (A^\pi)^{\circ 2} \sqrt{\bar{n}_D^{-1}} = A^\pi \bar{n}_D^{-\frac{1}{2}}$$

and so this also represents a tightening of the bound.

When $\pi$ is deterministic, this bound is equivalent to that of Appendix C.1. This can easily be seen by noting that for a deterministic policy, all elements of $(A^\pi)^{\circ 2}$ are either 1 or 0, and so

$$\sqrt{(A^\pi)^{\circ 2} \bar{n}_D^{-1}} = A^\pi \bar{n}_D^{-\frac{1}{2}}$$

Another important property of this bound is that it shows that stochastic policies can be often be evaluated with lower error than deterministic policies. We prove this by example. Consider an MDP with a single state $s$ and two actions $a_0, a_1$, and a dataset with $\bar{n}_D((s, a_0)) = \bar{n}_D((s, a_1)) = 2$. We can parameterize the policy by a single number $\xi \in [0, 1]$ by setting $\pi(a_0|s) = \xi$, $\pi(a_1|s) = 1 - \xi$. The size of this bound will be proportional to $\sqrt{\frac{\xi^2}{2} + \frac{(1-\xi)^2}{2}}$, and setting the derivative equal to zero, we see that the minimum is $\xi = \frac{1}{2}$.

Finding the optimum of this function for larger action spaces is non-trivial, so we leave a full treatment of algorithms which leverage this bound for future work.

C.3 Other Bounds

There are a few other paths by which this bound can be made tighter still. The above bounds take an extra factor of $\frac{1}{1-\gamma}$ because we bound the overall return, rather than simply bounding the reward and transition functions. This
was done because a bound on the transition function would add a cost of $O(\sqrt{S})$. However, this can be mitigated by intersecting the above confidence interval with a Good-Turing interval, as proposed in [38]. Doing so will cause the bound to concentrate much more quickly in MDPs where the transition function is relatively deterministic. We expect this to be the case for most practical MDPs.

Similarly, empirical Bernstein confidence intervals can be used in place of Hoeffding’s, to increase the rate of concentration for low-variance rewards and transitions [24], leading to improved performance in MDPs where these are common.

Finally, we may be able to apply a concentration inequality in a more advanced fashion to compute the value uncertainty directly, rather than computing the Bellman uncertainty and taking the visitation-weighted sum. This would result in an overall tighter bound on value uncertainty by hedging over data across multiple timesteps. However, in doing so, we would sacrifice the monotonic improvement property needed for convergence of algorithms like policy iteration. This idea has a parallel in the robust MDP literature. The bounds in Appendix C.1 can be seen as constructing an $sa$-rectangular robust MDP, whereas Appendix C.2 is similar to constructing an $s$-rectangular robust MDP [45]. More recently, approaches have been proposed which go beyond $s$-rectangular [10], and such approaches likely have natural parallels in implementing value uncertainty functions.

D  Related Work

Bandits. Bandits are equivalent to single-state MDPs, and the fixed-dataset setting has been studied in the bandit literature as the logged bandit feedback setting. Swaminathan & Joachims [37] describe the Counterfactual Risk Minimization principle, and propose algorithms for maximizing the exploitation-only return. The UA pessimistic approach discussed in this work can be viewed as an extension of these ideas to the many-state MDP setting.

Exploration. Since acting pessimistically is the symmetric opposite of acting optimistically, many papers which study exploration leverage math which is nearly identical (though of course used in an entirely different way). For example, the confidence intervals, modified Bellman equation, and dynamic programming approach of [35] closely mirror those used in the UA pessimistic algorithms.

Imitation learning. Imitation learning (IL) [12] algorithms learn a policy which mimics expert demonstrations. The setting in which these algorithms can be applied is closely related to the FDPO setting, in that IL algorithms map from a dataset of trajectories to a single stationary policy, which is evaluated by its suboptimality. (However, note that IL algorithms can be applied to a somewhat more general class of problems; for example, when no rewards are available.) In the FDPO setting, IL algorithms are limited by the fact that they can never improve on the quality of the empirical policy. In contrast, pessimistic FDPO algorithms will imitate the dataset when other actions are uncertain, but are also sometimes able to deviate and improve.

Safe reinforcement learning. The sub-field of safe reinforcement learning studies reinforcement learning algorithms with constraints or guarantees that prevent bad behavior from occurring, or reduce it below a certain level [40]. To this end, many algorithms utilize variants of pessimism. Our contribution distinguishes itself from this line of work via its focus on the application of pessimism for worst-case guarantees on the more standard objective of expected suboptimality, rather than for guarantees on safety. However, there is a close relationship between our work and the algorithms and theory used for Safe RL. One popular framework is that of robust MDPs [9, 13, 28, 44], an object which generalizes MDPs to account for specification uncertainty in the transition functions. This framework is closely related to the pessimistic approaches described in this work. In fact, the UA pessimistic approach is precisely equivalent to constructing a robust MDP from data using concentration inequalities, and then solving it for the policy with the optimal performance under an adversarial choice of parameters; this algorithm has been used as a baseline in the literature but not studied in detail [8, 21]. Additionally, the sub-problem of Safe RL known as conservative policy improvement focuses on making small changes to a baseline policy which guarantee that the new policy will have higher value [8, 21, 27, 33, 39, 41], which bears strong resemblance to the proximal pessimistic algorithms discussed in this work.

Proximal algorithms. Several approaches to online deep reinforcement learning, including TRPO and PPO, have been described as “proximal” [31, 32]. In that body of work, this refers to the notion that, after each policy update,
the resulting policy is close to the previous iterate. In contrast, the proximal algorithm described in this work is proximal with respect to a fixed policy (typically, the empirical policy defined by the dataset).

**Deep learning FDPO approaches.** Recently, deep learning FDPO has received significant attention [7, 14, 17, 18, 19, 21, 43, 46, 48]. At a high level, these works are each primarily focused around proposing and analyzing some specific method. In contrast, the objective of this work is theoretical: we focus on providing a clean mathematical framework through which to understand this setting. We now provide specific details for how our contribution relates to each of these works.

The algorithms introduced in [7, 14, 18, 21] can all be viewed as variants of the proximal pessimistic approach described in this paper. The implementations vary in a number of ways, but at its core, the primary difference between these algorithms lies in the choice of regularizer: KL, MMD, or hard constraint. This connection has also been noted in [46], which provides a unifying algorithmic framework for these approaches, BRAC, and also performs various empirical ablations. Interestingly, all of these regularizers can be expressed as upper-bounds to $TV_S(\pi, \hat{\pi}_D)$, and as such, our proof of the suboptimality of proximal pessimistic algorithms can be used to justify all of these approaches. One aspect of our contribution is therefore providing the theoretical framework justifying BRAC. Furthermore, conceptually, these works differ from our contribution due to their focus on error propagation; in contrast, our results show that poor suboptimality of naïve algorithms is an issue even when there is no function approximation error at all.

More recently, [19] propose a technique, CQL, which avoids overestimation by directly penalizing Q-values. The authors provide guarantees on the degree to which they will avoid overestimation. However, CQL does not guarantee reduction of underestimation, and that paper does not provide bounds on its suboptimality. Our work may provide a direction by which such bounds may be derived.

[43] provides an alternative algorithm for pessimistic FDPO, utilizing a policy-gradient based algorithm instead of the value-iteration-style algorithms in other related work. Similarly to [18], this approach utilizes a policy constraint to prevent bootstrapping from actions which are poorly represented in the training data. However, this difference is purely algorithmic: since the fixed-point found by the optimization is the same, this algorithm can also be justified by our proximal pessimistic suboptimality bounds.

Similarly, model-based methods [17, 48] have recently been proposed which implement pessimism via planning in a pessimistic model. This procedure can be viewed as learning a model which defines an implicit value function (derived from applying the planner to the model), and from there defines an implicit policy (which is greedy with respect to the implicit value function). The implicit value functions learned by the algorithms in [17, 48] obey the same fixed-point identity as the solutions to the UA pessimistic approach discussed in our work. Thus, both of these works are implementations of UA pessimistic approaches, and our UA pessimistic suboptimality bound can be viewed as justification for this family of algorithms. However, both of these works rely on ensembles to compute the uncertainty penalty, which is not a theoretically well-motivated technique.