Optimal Model Selection in Contextual Bandits with Many Classes via Offline Oracles

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Abstract

We study the problem of model selection for contextual bandits, in which the algorithm must balance the bias-variance trade-off for model estimation while also balancing the exploration-exploitation trade-off. In this paper, we propose the first reduction of model selection in contextual bandits to offline model selection oracles, allowing for flexible general purpose algorithms with computational requirements no worse than those for model selection for regression. Our main result is a new model selection guarantee for stochastic contextual bandits. When one of the classes in our set is realizable, up to a logarithmic dependency on the number of classes, our algorithm attains optimal realizability-based regret bounds for that class under one of two conditions: if the time-horizon is large enough, or if an assumption that helps with detecting misspecification holds. Hence our algorithm adapts to the complexity of this unknown class. Even when this realizable class is known, we prove improved regret guarantees in early rounds by relying on simpler model classes for those rounds and hence further establish the importance of model selection in contextual bandits.

1 Introduction

Contextual bandit algorithms are a fundamental tool for sequential decision making and have been the focus of an increasing amount of research over the past couple of decades (Lattimore and Szepesvári, 2020). These algorithms have been used in a wide range of applications from recommendation systems (Agarwal et al., 2016) to mobile health (Tewari and Murphy, 2017).

In this paper, we study the finite-armed (stochastic) contextual bandit setting. At every round, the learner observes a feature vector (context) drawn from a fixed distribution. The learner then selects an action (or a probability distribution over actions) and receives a reward whose distribution may depend on the context and action. The learner then incorporates its observation of the context, action and reward into its decisions in the next round. The objective of the learner is to maximize the rewards received during the experiment (that is, minimize regret).

A common approach to the contextual bandit problem is to use data collected over prior rounds to estimate the true conditional expected mean reward for any context and action. In this work, we call this the model-based approach to contextual bandits. When the algorithm receives the next context, it uses this estimate to construct a possibly randomized action selection rule that balances two objectives – reduce uncertainty in the estimate for future rounds (exploration) and maximize the reward received in the current round (exploitation).

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To decide at what rate exploration should be decreased, we rely on misspecification test oracles to set of $M$ model classes $\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_M$, such that at least one of these classes is realizable (that is, well-specified). Can we design a contextual bandit algorithm with regret guarantees that match the best guarantees ensured by model-based algorithms corresponding to these classes? 

The central challenge to model selection in contextual bandits is that estimating models from more complex classes requires more exploration. Hence, optimizing the exploration-exploitation trade-off for one class may lead to under or over exploration for learning models from other classes, which can lead to additional costs in terms of regret. Broadly speaking, prior work has taken two strategies to solve this problem, which we here refer to as sequential search strategies (e.g. Foster et al., 2019) and parallel search strategies (e.g. Agrawal et al., 2017). Both strategies consider bandit algorithms corresponding to model each class $\mathcal{F}_i$, and they propose solutions that try to identify the single best model class $\mathcal{F}_i^*$ such that the corresponding algorithm minimizes regret.

Sequential search strategies have largely focused on model selection over a nested sequence of linear classes (e.g. Foster et al., 2019). That is, $\mathcal{F}_1 \subset \mathcal{F}_2 \subset \cdots \subset \mathcal{F}_M$ and these classes are linear over a nested sequence of feature maps. For notational convenience, let $i^*$ denote the index of the smallest realizable class. The key idea is to sequentially run contextual bandits with increasing class complexities with the goal of eventually using an algorithm corresponding to model class $\mathcal{F}_{i^*}$. While running a contextual bandit with model class $\mathcal{F}_i$, some share of rounds are dedicated to sampling arms uniformly at random, and this uniformly sampled data is used to test if the current class $\mathcal{F}_i$ is misspecified. If $\mathcal{F}_i$ is determined to be misspecified, the strategy moves on to using an algorithm corresponding to the class $\mathcal{F}_{i+1}$. As identifying the class $\mathcal{F}_{i^*}$ is critical to this strategy, these strategies also rely on stringent distributional assumptions for model identification known as diversity conditions – i.e., they assume that the minimum eigenvalue of the covariance matrix for these feature maps is greater than some positive constant.\footnote{This may not be easily satisfied for feature maps with many correlated features.}

Parallel search strategies use master algorithms (e.g. Agrawal et al., 2017) to run in parallel $M$ contextual bandit algorithms, one corresponding to each of the $M$ classes. The key idea is to design a master algorithm that allocates rounds to these $M$ base algorithms, learns which of these algorithms will maximize expected cumulative reward, and eventually allocates most rounds to this algorithm. Regret guarantees for both sequential and parallel search strategies tend to have a fractional polynomial dependency on either $i^*$ or $M$ – which contrasts the logarithmic dependency obtained in excess risk bounds for model selection in the classical statistical learning.

This paper starts with the observation that a fundamental issue with both these strategies is that there isn’t one model based algorithm that is optimal for all time horizons. Instead, there is a bias-variance trade-off for model-based contextual bandits (Foster et al., 2020a, Krishnamurthy et al., 2021a,b). That is, algorithms corresponding to simpler model classes have better guarantees for smaller time horizons, whereas algorithms corresponding to more expressive classes have better guarantees for larger horizons. Hence, attempting to find the single best performing model-based algorithm may not be the most effective approach.

Instead, this paper proposes a single contextual bandit algorithm that uses estimators that balance the classical bias-variance trade-off for regression. That is, these estimators are constructed by any offline model selection oracle for regression. From classical statistical learning theory, the risk of this estimator will decrease at a faster rate in early rounds. This follows because the oracle tends to select estimators from simpler (low variance) classes in early rounds characterized by small data, while it selects more complex and expressive classes (high variance) in later rounds where more data is available. To optimize the exploration-exploitation trade-off, our algorithm accordingly reduces exploration more rapidly in earlier rounds and reduces exploration at a slower rate in later rounds. To decide at what rate exploration should be decreased, we rely on misspecification test oracles to estimate at what rate risk for the model selection oracle is decreasing. By reducing exploration at
different rates for different rounds, we sidestep the key challenge for model selection in contextual bandits, which was that learning from different model classes requires different exploration rates. Hence our approach optimizes both the bias-variance and exploration-exploitation trade-offs.

Our algorithm provides the first reduction from model selection for contextual bandits to offline model selection oracles, and our regret guarantees only have a logarithmic dependency on the number of classes. When one of the classes in our set is realizable, up to logarithmic dependencies, our algorithm guarantees optimal minimax regret bounds if one of the following two conditions hold: (i) the time-horizon is large enough, or (ii) there is no policy that makes a misspecified class seem well-specified. Hence our algorithm adapts to the complexity of this unknown realizable class. Even when this realizable class is known, as discussed earlier, we prove improved regret guarantees in early rounds by relying on the faster model estimation rates of simpler model classes for small data regimes. We describe the differences between our results and other related work in the next section, Section 1.1.

1.1 Related Work

Model selection for the classical statistical learning setting has been well-studied and is by now well understood (see [Arlot et al., 2010; Koltchinskii, 2011; Massart, 2007] for a comprehensive review). As discussed in Section 1, prior work on model selection in contextual bandits can be largely categorized into sequential and parallel search. Here, we provide more details about key contributions for each strategy.

Sequential search strategies. [Chatterji et al., 2020] propose an algorithm that selects between two classes. They guarantee optimal problem-dependent rates for the (non-contextual) multi-arm bandit setting, and guarantee minimax optimal rates in the linear contextual bandit setting when the context distribution is sufficiently diverse. In concurrent work, [Foster et al., 2019] propose an algorithm that selects between a nested sequence of linear classes. In particular, they consider a nested sequence of model classes \( F_1 \subset F_2 \subset \cdots \subset F_M \) such that the model class \( F_i \) is a \( d_i \)-dimensional linear class and the corresponding features are sufficiently diverse. They design an algorithm that achieves a regret guarantee of \( \hat{O}(T \sqrt{K d_i}) \). Where \( F_{\hat{i}} \) is the smallest class that contains the true model (realizability), \( T \) denotes the number of arms, and \( K \) denotes the number of rounds. For this setup, if we use the misspecification test described in [Foster et al., 2019], our algorithm achieves the optimal minimax guarantee of \( \hat{O}(\sqrt{K d_{\hat{i}}} T) \). [Ghosh et al., 2021] primarily study model selection for stochastic linear bandits, but also provide an algorithm that achieves the optimal minimax guarantee for this setup up to an additive error of \( \hat{O}(d_{\hat{i}}^2) \).

Under linear realizability and sufficiently strong assumptions on diversity of features for the optimal region of every arm, prior work argues that advanced exploration is not needed ([Bastani and Bavai, 2015; Bastani et al., 2021] [Kamran et al., 2018; Raghavan et al., 2018], which considerably simplifies the problem. Recent work also show that under certain symmetry assumptions on the distribution of features, regularized greedy algorithms induce sufficient exploration ([Arora et al., 2020] [Oh et al., 2020], and the guarantees of these algorithms degrade when these distributions are less symmetric. The assumptions required to make greedy algorithms work are fairly strong and as such, these results should be seen complementary to our own.

Parallel search strategies. Another popular approach is to combine multiple contextual bandit algorithms with the goal of creating a master algorithm that performs almost as well as the best base algorithm ([Agarwal et al., 2017]). That is, the master algorithm allocates rounds to these base algorithms, and learns to allocate more rounds to the best base learner. This problem is fairly more challenging compared to the standard multi-arm bandit problem as the performance of base algorithms improve the more times they are used. Since the introduction of this general setup ([Agarwal et al., 2017]), several master algorithms have been proposed (e.g. [Arora et al., 2021; Pacchiano et al., 2020]). We compare our results in a setting where we wish to select among a set of classes with finite VC sub-graph dimension. In particular, consider a sequence of model classes \( F_1, F_2, \ldots, F_M \) such that the model class \( F_i \) has VC-sub-graph dimension \( d_i \). Again for notational convenience, let \( d_1 \leq d_2 \leq \cdots \leq d_M \) and let \( F_{\hat{i}} \) be the smallest class that contains the true model (realizability). For simplicity, we only compare against regret guarantees that achieve a square-root dependency on the number of rounds for this setup. Among such guarantees, the algorithms proposed in ([Agarwal et al., 2017; Arora et al., 2021; Pacchiano et al., 2020]) achieve a regret bound that...
is at least as large as $\tilde{O}(\sqrt{MK}d_i T + d_i \sqrt{i^2 K T})$. In comparison, our algorithm guarantees a regret bound of $O(d_i \sqrt{KT})$. Moreover, for $T \geq \tilde{\Omega}(d_i^2)$, our algorithm achieves the optimal minimax guarantee of $O(\sqrt{K d_i T})$. That is, we get a better dependency on the number of classes, and achieve equally good or better dependency on the other parameters.

Our analysis builds on recent work that quantify the bias-variance trade-off in contextual bandits (Foster et al., 2020a; Krishnamurthy et al., 2021b). In particular, to quantify and optimize the bias-variance trade-off for contextual bandits, we use several technical observations made in Krishnamurthy et al. (2021a).

Our work also builds on the literature of reducing contextual bandit problems to supervised learning tasks (Langford and Zhang, 2007; Dudik et al., 2011; Agarwal et al., 2012, 2014; Foster et al., 2018; Foster and Rakhlin, 2020; Simchi-Levi and Xu, 2020; Xu and Zeevi, 2020). In particular, we leverage several lemmas and observations from Simchi-Levi and Xu (2020), which in turn leverages insights from Agarwal et al. (2014) and Foster and Rakhlin (2020). Our algorithm is a modification of the inverse-gap weighting algorithm, which was originally proposed by Abe and Long (1999), and has recently become a popular tool for contextual bandits (e.g., Foster and Rakhlin, 2020; Simchi-Levi and Xu, 2020).

2 Preliminaries

In this section, we setup some basic notation and preliminaries to formalize our problem and to discuss our algorithm. We work in the stochastic contextual bandit setting, which is defined by a set of contexts $\mathcal{X}$, a finite set of arms $\mathcal{A}$, and a distribution $D$ over contexts and arm rewards. We let $K$ denote the number of arms (i.e., $K := |\mathcal{A}|$), $T$ denote the number of rounds, and use the notation $[n]$ to denote the set $\{1, \ldots, n\}$. At every time-step $t \in [T]$, the environment draws a context $x_t \in \mathcal{X}$ and reward vector $r_t \in [0, 1]^K$ from the fixed but unknown distribution $D$. The learner observes context $x_t$, chooses an arm $a_t$, and observes a reward $r_t(a_t)$. Where $r_t(a)$ denotes the reward for choosing arm $a$ at time $t$. Unless stated otherwise, all expectation are taken with respect to the distribution $D$.

We let $f^* : \mathcal{X} \times \mathcal{A} \rightarrow [0, 1]$ denote the true conditional expectation reward function given contexts and actions; i.e. $f^*(x, a) := \mathbb{E}[r_t(a)|x_t = x]$. A model $f$ is any map from $\mathcal{X} \times \mathcal{A}$ to $[0, 1]$, and a model class $\mathcal{F}$ is simply a set whose elements are models. We also let $D_X$ denote the marginal distribution of $D$ on the set of contexts $\mathcal{X}$.

A policy $\pi$ is any function from $\mathcal{X}$ to $\mathcal{A}$, and we let $\pi^*$ denote the policy that maximizes the conditional mean reward; i.e., $\pi^*(x) = \arg\max_a f^*(x, a)$. In this paper, we study contextual bandit algorithms that minimize (expected) cumulative regret $R_T$. Where for any round $t$, $R_t$ denotes the (expected) cumulative regret up to round $t$:

$$R_t := \sum_{t'=1}^{t} \left[ f^*(x_{t'}, \pi^*(x_{t'})) - f^*(x_{t'}, a_{t'}) \right].$$

We let $\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_M$ be a sequence of $M$ model classes. At a high-level, our algorithm (Mod-IGW) uses regression oracles over these classes in order to estimate the conditional expected reward ($f^*$), and then uses these estimates for arm selection. Similar to prior work on model selection for contextual bandits, we aim for refined guarantees that scale with the complexity of the class that best approximates $f^*$.

In this paper, probability kernels always refer to probability kernels from $\mathcal{A} \times \mathcal{X}$ to $[0, 1]$. That is, a probability kernel $p$ is a (possibly randomized) arm selection rule given by the distribution $p(\cdot|x)$ at context $x$. For any probability kernel $p$, we let $D(p)$ be the induced distribution over $\mathcal{X} \times \mathcal{A} \times [0, 1]$, where sampling $(x, a, r(a)) \sim D(p)$ is equivalent to sampling $(x, r) \sim D$ and then sampling $a \sim p(\cdot|x)$.

To quantify how well a class $\mathcal{F}_i$ can approximate $f^*$, we use the definition of average squared misspecification error studied in Krishnamurthy et al. (2021a). Similar definitions of misspecification were studied in Foster et al. (2020a; Krishnamurthy et al., 2021b). We denote by $B_i$ the “average squared misspecification error relative to $\mathcal{F}_i$,’’ that is:

$$B_i := \max_p b_i(p).$$
Where \( b_i(p) \) denotes the average squared misspecification error relative to \( \mathcal{F}_i \) under the distribution \( D(p) \).

\[
b_i(p) := \min_{f \in \mathcal{F}_i} \mathbb{E}_{x \sim D, a \sim p(x)} [(f(x, a) - f^*(x, a))^2].
\]  

We say the the model class \( \mathcal{F}_i \) is misspecified if \( B_i \) is greater than zero, and we say it is well-specified or realizable if \( B_i \) is zero. In this paper, we assume that one of these \( M \) model classes is realizable (Assumption 1), and let \( i^* \) denote the smallest class index with zero squared misspecification error.

**Assumption 1 (Realizability).** We assume that there exists a class index \( i \in [M] \) such that \( B_i \) is zero.

Assumption 1 allows our algorithm to use more complex classes reliably upon detecting misspecification for simpler classes. We argue that Assumption 1 isn’t too stringent as our analysis immediately extends to the case where the number of classes \( M \) is infinite (see Section 4).

For simplicity, in the main paper, we use the VC subgraph dimension as our measure for class complexity and require our classes to have finite VC subgraph dimension. We discuss extensions to the general case in the appendix. We let \( d_i \) denote the VC subgraph dimension for model class \( \mathcal{F}_i \). For notational convenience we order the classes so that they increase in complexity; i.e. \( d_1 \leq d_2 \leq \cdots \leq d_M \). In Section 2.1 we discuss a model selection oracle for estimation.

### 2.1 Estimation Oracle

We use a model selection oracle for estimation over the set of classes \( \{\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_M\} \) as a subroutine for our algorithm Mod-IGW. In Assumption 2 we state our requirements of this estimation oracle and outline one of many approaches to construct such an oracle.

**Assumption 2 (Estimation Oracle).** For every index \( i \in [M] \), we assume access to an offline model selection oracle for estimation (EstOracle\(_i\)) over the sequence of classes \( \mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_i \) that satisfies the following property. There exists a constant \( C_0 \geq 1 \) such that for any probability kernel \( p \), any natural number \( n \), and any \( \zeta \in (0, 1) \), the following holds with probability at least \( 1 - \zeta \):

\[
\mathbb{E}_{x \sim D, a \sim p(x)} [(\hat{f}(x, a) - f^*(x, a))^2] \leq \min_{j \in [i]} \left( C_0 \cdot b_j(p) + \xi_j(n, \zeta/i) \right).
\]  

Where \( \hat{f} \) is the output of EstOracle\(_i\) fitted on \( n \) independently and identically drawn samples from the distribution \( D(p) \). Here \( b_j(p) \) is defined by (3), and \( \xi_j \) is a known function given by:

\[
\xi_j(n, \zeta) := \frac{C_1 d_j \ln(n) \ln(1/\zeta)}{n}
\]  

For some known constant \( C_1 > 0 \).

We refer to the function \( \xi_i(\cdot, \cdot) \) as the estimation rate for model class \( \mathcal{F}_i \) as it can be used to bound the excess risk of a regression oracle on model class \( \mathcal{F}_i \). In the appendix, we outline one of many approaches to construct an oracle that achieves the “fast rates” of Assumption 2. The approach we describe there is based on using empirical risk minimization over training and validation sets. Other approaches one could use include aggregation algorithms (see Lecué et al., 2014, and references therein), penalized regression (see relevant chapters in Koltchinskii, 2011; Wainwright, 2019), cross validation, etc.

### 3 Algorithm

In this section, we describe our algorithm Mod-IGW, which is an algorithm based on inverse gap weighting (Abe and Long, 1999; Foster and Rakhlin, 2020; Foster et al., 2020b; Simchi-Levi and Xu, 2020). We use an inverse gap weighting approach because it can be used to develop optimal algorithms, and gives us a simple analytical handle on important quantities like the expected inverse probability weight for any policy at any round. Our algorithm is implemented in epochs indexed by \( m \), with epoch \( m \) beginning at round \( \tau_{m-1} + 1 \) and ending at \( \tau_m \). For all \( m \geq 1 \), \( \tau_{m+1} = 2\tau_m \). Where \( \tau_1 \geq 2 \) is an input parameter and \( \tau_0 = 0 \). For any time-step \( t \) in epoch
At the end of any epoch, the algorithm observes context \( x_t \) and sample action \( a_t \) from the distribution \( p_m(\cdot|x_t) \). Where \( p_m \) is called the action selection kernel for epoch \( m \) and is given by:

\[
p_m(a|x) := \begin{cases} 
\frac{1}{K+\gamma_m(f_m(x,a) - f_m(x,\hat{a}))} & \text{for } a \neq \hat{a}, \\
1 - \sum_{a' \neq \hat{a}} p(a'|x) & \text{for } a = \hat{a}.
\end{cases}
\] (6)

Here \( \hat{f}_m \) is an estimate of the reward model obtained using data from previous epochs, \( \hat{a} = \max_a f_m(x,a) \) is the predicted best action, \( \gamma_m > 0 \) is a parameter that controls how much the algorithm explores. The algorithm also maintains a set of possibly well-specified model-class indices denoted by \( \mathcal{I}_m \), sometimes referred to as the "index set" for convenience.

**Algorithm 1** Mod-IGW (Model Selection with Inverse Gap Weighting)

**input:** Initial epoch length \( \tau_1 \geq 2 \), and confidence parameter \( \delta \).

1: Set \( \tau_0 = 0 \), and \( \tau_{m+1} = 2\tau_m \) for all \( m \geq 1 \).
2: Let \( \hat{f}_1 \equiv 0 \), \( \mathcal{I}_1 = [M] \), and \( \gamma_1 = 1 \).
3: for epoch \( m = 1, 2, \ldots \) do
4: Let \( p_m \) be given by (6).
5: for round \( t = \tau_m + 1, \ldots, \tau_m \) do
6: Observe context \( x_t \), sample \( a_t \sim p_m(\cdot|x_t) \), and observe \( r_t(a_t) \).
7: end for
8: Let \( S_m \) denote the data collected in epoch \( m \).
9: \( \hat{f}_{m+1} \leftarrow \text{EstOracle}_M(S_m) \).
10: \( \mathcal{I}_{m+1} := \{ i | i \in \mathcal{I}_m, \text{MTOracle}(i, S_m, \delta/(4Mm^2)) = \text{False} \} \).
11: \( i_{m+1} \) is the smallest index in the set \( \mathcal{I}_{m+1} \).
12: \( \gamma_{m+1} = \gamma_{m+1,i_{m+1}} \).
13: end for

At the end of any epoch \( m \), Mod-IGW uses the data collected in epoch \( m \) (denoted by \( S_m \)) to construct the reward model \( \hat{f}_{m+1} \) and exploration parameter \( \gamma_{m+1} \). The reward model \( \hat{f}_{m+1} \) is the output of a model selection oracle (EstOracle\(_M\)) with input \( S_m \). For every model class \( \mathcal{F}_i \), there is a corresponding exploration parameter denoted by \( \gamma_{m+1,i} \) and given by (7).

\[
\gamma_{m+1,i} := \sqrt{\frac{K}{8\xi((\tau_m - \tau_{m-1}, \delta/(4Mm^2))}}.
\] (7)

The algorithm chooses the exploration parameter \( \gamma_{m+1} \) by first constructing the index set \( \mathcal{I}_{m+1} \), choosing \( i_{m+1} \) to denote the smallest index in this set, and setting the the exploration parameter \( \gamma_{m+1} \) to be the exploration parameter corresponding to the model class \( \mathcal{F}_{i_{m+1}} \). The index set \( \mathcal{I}_{m+1} \) is constructed by using a misspecification test oracle (MTOracle) on every class index in \( \mathcal{I}_m \) and removing those class indices that are determined to be misspecified with high probability. We describe our requirements of the misspecification test oracle (MTOracle) in Section 3.1 and describe constructions of such oracles in Section 3.2.

### 3.1 Understanding Mod-IGW

Contextual bandit algorithms are designed to balance the exploration-exploitation trade-off. In particular, under-exploration in any epoch can lead to construction of less accurate reward models for future epochs. For every class index \( i \in [M] \), we define a "safe" epoch denoted by \( m^*_i \) and show that the exploration parameter \( \gamma_{m,i} \) induces sufficient exploration up to the end of this epoch. A similar quantity was originally defined in [Krishnamurthy et al. (2021a)](https://www.venue.com), and we explain its importance in the following paragraph.

\[
m^*_i := \max \left\{ m \mid \xi_i((\tau_m - \tau_{m-1}, \delta/(4Mm^2)) \geq C_0 \min_{i'} B_{i'} \right\}.
\] (8)

Note that the epoch \( m^*_i \) represents the epoch after which the average misspecification error for every class in the set \( \{ \mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_i \} \) dominates the estimation rate for model class \( \mathcal{F}_i \). Hence from
Assumption 2 up to epoch \( m_i^* \), the risk of the estimation oracle (EstOracle\(_M\)) can be bounded by \( \tilde{O}(d_i/\tau_m) \). We use this observation to show that the exploration parameter \( \gamma_{m,i} \) induces sufficient exploration up to the end of this epoch. Further note that larger values of \( \gamma \) correspond to less exploration. As less exploration is needed for later rounds, \( \gamma_{m,i} \) increases in the epoch index \( m \). The class index \( i \) only controls how rapidly \( \gamma_{m,i} \) increases in \( m \), with larger class indices corresponding to slower rates of increase. At a high-level, to optimize the exploration-exploitation trade-off, we want to use an exploration parameter that performs as little exploration as possible, subject to the constraint of performing sufficient exploration for accurate reward model construction. Therefore, if we knew the parameter \( m_i^* \) for every class index \( i \), we could optimize the exploration-exploitation trade-off by using the exploration parameter \( \gamma_{m,i} \) for every epoch \( m \in (m_{i-1}, m_i^*] \). For convenience, we define \( m_i^* \) to be equal to one. Note that under Assumption 1 \( B_{i'} \) is zero and hence \( m_i^* \) is infinity.

Unfortunately, we do not know the average misspecification errors \( (B_i) \) and hence cannot calculate the value of safe epochs \( (m_i^*) \). Therefore Mod-IGW relies on MTOracle to implicitly construct estimates \( (\hat{m}_i) \) of the safe epoch \( (m_i^*) \).

\[
\hat{m}_i := \max \left\{ m \mid i_m \leq i \right\}, \tag{9}
\]

Hence Mod-IGW uses the exploration parameter \( \gamma_{m,i} \) for every epoch \( m \in (\hat{m}_{i-1}, \hat{m}_i] \). In Assumption 3 we state fairly minimalistic requirements for the misspecification test oracle (MTOracle).

**Assumption 3 (Misspecification Test).** We assume that the misspecification test MTOracle satisfies the following property. For any class index \( i \in [M] \), epoch \( m \), and any \( \zeta \in (0, 1) \). If \( \tau_m \leq \beta_i' \tau_{m_i^*} \),

\[
\Pr[\text{MTOracle}(i, S_m, \zeta) = \text{False}] \geq 1 - \zeta,
\]

If \( \tau_m > \beta_i \),

\[
\Pr[\text{MTOracle}(i, S_m, \zeta) = \text{True}] \geq 1 - \zeta,
\]

Where \( \beta_i' \) and \( \beta_i \) are (possibly unknown) parameters for every class index \( i \in [M] \). Such that \( \beta_i \) is non-decreasing in class index \( i \). For every class index \( i \in [M] \), \( \beta_i' \in (0, 1) \) and \( \beta_i \geq \beta_i' \tau_{m_i^*} \). For convenience we define \( \beta_0 \) to be equal to zero.

The parameters \( \beta_i, \beta_i' \) in Assumption 3 will depend on both the problem instance and the misspecification test, and allow us to quantify how close the estimate \( \hat{m}_i \) is to \( m_i^* \). In particular, under Assumption 3 with high-probability we have that \( \tau_{m_i^*}, \tau_m \in [\beta_i' \tau_{m_i^*}, \beta_i] \). Also note that \( m_i^* \) is infinity, hence a test satisfying Assumption 3 will never claim that \( F_{m_i^*} \) is misspecified. In Section 3.2 we construct a misspecification test that satisfies Assumption 3.

### 3.2 Misspecification Test

In this section, we describe a straight-forward "goodness of fit" approach to construct a misspecification test (MTOracle) using the estimation oracle (EstOracle\(_M\)) described in Assumption 2. Consider any class index \( i \in [M] \), epoch \( m \), and any \( \zeta \in (0, 1) \). Our test starts by splitting the data collected in epoch \( m \) (\( S_m \)) into "training" and "hold-out" sets denoted by \( S_{m,\text{tr}} \) and \( S_{m,\text{ho}} \), such that \( S_{m,\text{tr}} \) contains \( \lfloor \alpha_0 |S_m| \rfloor \) samples. Where \( \alpha_0 \in (0, 1) \) is an algorithmic parameter. With \( S_{m,\text{tr}} \) as input, let \( \hat{g}_i \) and \( \hat{g}_M \) be the output of EstOracle\(_i\) and EstOracle\(_M\) respectively. Our test says the class \( \cup_{j \in [i]} F_j \) is possibly well-specified when (10) holds and is misspecified otherwise. We state a guarantee for this test in Theorem 1 and provide a more detailed guarantee in the appendix.

\[
\hat{L}(S_{m,\text{ho}}, \hat{g}_i) \leq \hat{L}(S_{m,\text{ho}}, \hat{g}_M) + 4 \xi_i (|S_{m,\text{tr}}|, \zeta/(6i)) + \frac{26 \log(6/\zeta)}{3 |S_{m,\text{ho}}|} \tag{10}
\]

Where \( \hat{L}(S, f) \) denote the empirical square loss of model \( f \) on a dataset \( S \), that is:

\[
\hat{L}(S, f) := \frac{1}{|S|} \sum_{(x,a,r(a)) \in S} (f(x,a) - r(a))^2. \tag{11}
\]
Algorithm 2 Misspecification test

**input:** Data from epoch \(m\) \((S_{m})\), class index \(i \in [M]\), \(\alpha_{ho} \in (0, 1)\), and confidence parameter \(\zeta\).

1. Split \(S_{m}\) into training \((S_{m, \text{tr}})\) and holdout \((S_{m, \text{ho}})\) data such that \(|S_{m, \text{ho}}| = |\alpha_{ho}|S_{m}|\).
2. \(\hat{g}_{i} \leftarrow \text{EstOracle}_{i}(S_{m, \text{tr}})\).
3. \(\hat{g}_{M} \leftarrow \text{EstOracle}_{M}(S_{m, \text{tr}})\).
4. if \(\hat{L}(S_{m, \text{ho}}, \hat{g}_{i}) \leq \hat{L}(S_{m, \text{ho}}, \hat{g}_{M}) + 4\xi(|S_{m, \text{ho}}|, \zeta/(6\xi)) + \frac{26 \log(6\xi)}{|S_{m, \text{ho}}|}\) then
5.   Return \textbf{False}. (\(\cup_{j \in [t]} \mathcal{F}_{j}\) may be well-specified)
6. else
7.   Return \textbf{True}. (\(\cup_{j \in [t]} \mathcal{F}_{j}\) is misspecified with probability at least \(1 - \zeta\)).
8. end if

**Theorem 1.** Suppose Assumption 1 and Assumption 2 hold. Consider any class index \(i \in [M]\), epoch \(m\), and confidence parameter \(\zeta \in (0, 1)\), the following hold with probability \(1 - \zeta\): (i) Algorithm 2 outputs \textbf{"False"} if \(\tau_{m} \leq \tau_{m}^{*}\); (ii) Algorithm 2 outputs \textbf{"True"} if \(\tau_{m} \geq \Omega(\max_{i \in [t]} d_{i}/b_{i}(p_{m}))\).

We now want to use Theorem 1 to show that Algorithm 2 satisfies Assumption 3. To do this, we need to lower bound \(\min_{i \in [t]} \max_{r \neq i} b_{i}(p_{m})\). While we can bound this quantity without any assumptions, we can clearly get a tighter bound under Assumption 4. Together these bounds give us Corollary 1 from Theorem 1.

**Assumption 4** (Clear Misspecification). For every model class \(\mathcal{F}_{i}\) that is misspecified \((B_{i} > 0)\), there exists a constant \(\kappa_{i} > 0\) such that \(b_{i}(p_{m}) \geq \kappa_{i}\) for every probability kernel \(p\).

**Corollary 1.** Suppose Assumption 1 and Assumption 2 hold. Then Algorithm 2 satisfies Assumption 3 with \(\beta_{r-1} \leq \tilde{O}(d_{i}^{2})\) and \(\beta_{i} = 1\) for all \(i \in [M]\). Further when Assumption 4 also holds, we have \(\beta_{i} \leq \tilde{O}(d_{i})\).

Assumption 4 simply ensures that there is no policy that can make a misspecified class look well-specified. That is, if \(\mathcal{F}_{i}\) is misspecified, there is no probability kernel \(p\) such that the average squared misspecification error relative to \(\mathcal{F}_{i}\) under the distribution \(D(p)\) is arbitrarily small. It may be reasonable to make this assumption for several real world instances where we may never use an action selection kernel that makes misspecified classes look well-specified. When this assumption is satisfied, we get optimal minimax regret bounds.

## 4 Main Result

Our guarantees for Mod-IGW rely on Assumption 1 Assumption 2, and Assumption 3. In Corollary 5, we also show improved regret guarantees under Assumption 4. We start by stating our main guarantee in Theorem 2.

**Theorem 2.** Suppose Assumption 2 and Assumption 3 hold. Then with probability at least \(1 - \delta\), for all \(i, j \in [M]\), and \(t \in [\beta_{i}^{*} \tau_{m}^{*}]\), Mod-IGW attains the following regret guarantee:

\[
R_{i} \leq \mathcal{O}\left(\beta_{j-1} \ln(d_{i}/d_{j}) + \sqrt{\frac{d_{i}}{d_{j}}} \sqrt{Kd_{i}t \ln(t) \ln\left(\frac{M \ln(t)}{\delta}\right)}\right) \tag{12}
\]

To better understand Theorem 2, we discuss several corollaries. Corollary 2 shows that when \(t \in [\beta_{i}^{*} \tau_{m}^{*}]\), up to an additive cost of \(\tilde{O}(\beta_{i-1})\), Mod-IGW gets optimal realizability based bounds for model class \(\mathcal{F}_{i}\). It is easy to see that Corollary 2 follows from setting \(j\) equal to \(i\) in Theorem 2.

**Corollary 2.** Suppose Assumption 2 and Assumption 3 hold. Then with probability at least \(1 - \delta\), for all \(i \in [M]\), and \(t \in [\beta_{i}^{*} \tau_{m}^{*}]\), Mod-IGW attains the following regret guarantee:

\[
R_{i} \leq \mathcal{O}\left(\beta_{i-1} \ln(d_{i}/d_{j}) + \sqrt{Kd_{i}t \ln(t) \ln\left(\frac{M \ln(t)}{\delta}\right)}\right). \tag{13}
\]

Corollary 3 shows that Mod-IGW balances the bias-variance trade-off for contextual bandits over several rounds. One interesting special case to consider is regret guarantees in terms of the complexity of the simplest realizable class \(\mathcal{F}_{i}^{*}\). Since \(\tau_{m}^{*}\) is unbounded, we get Corollary 3 by setting \(i\) equal to \(i^{*}\) in Corollary 2.
Further when Assumption 4 also holds, with probability at least 1 - δ, for all rounds t, Mod-IGW attains the following regret guarantee:

\[
R_t \leq O\left(\beta_{i^* - 1} \ln(d_{i^*} / d_1) + \sqrt{Kd_{i^*}t \ln\left(\frac{M \ln(t)}{\delta}\right)}\right).
\] (14)

Alternatively, by setting \( j \) equal to one and \( i \) equal to \( i^* \) in Theorem 2, we get Corollary 4.

**Corollary 4.** Suppose Assumption 1, Assumption 2, and Assumption 3 hold. Then with probability at least 1 - δ, for all rounds \( t \), Mod-IGW attains the following regret guarantee:

\[
R_t \leq O\left(d_{i^*} \sqrt{Kt \ln(t) \ln\left(\frac{M \ln(t)}{\delta}\right)}\right).
\] (15)

At a high-level, Corollary 4 quantifies the cost of under-exploration that may have happened. Under Assumption 3 with high-probability, within the first \( \beta_{i^* - 1} \) rounds, MOracle determines that the model classes in the set \( \{F_1, F_2, \ldots, F_{i^* - 1}\} \) are misspecified and Mod-IGW returns to using an exploration parameter that optimizes the exploration-exploitation trade-off. Corollary 3 shows that within \( \tilde{O}(\beta_{i^* - 1}) \) rounds, the algorithm self-corrects for any under-exploration that may have happened and gets back to ensuring optimal realizability based bounds for model class \( F_{i^*} \). Now, by combining Corollary 1 and Corollary 3, we provide a regret guarantee for Mod-IGW with the misspecification test described in Algorithm 2, and state the result in Corollary 5.

**Corollary 5.** Suppose Assumption 1 and Assumption 2 hold. Suppose we run Mod-IGW with the misspecification test described in Algorithm 2. Then with probability at least 1 - δ, this algorithm attains the following regret guarantee:

\[
R_T \leq \tilde{O}\left(d_{i^*}^2 + \sqrt{Kd_{i^*}T}\right).
\] (16)

Further when Assumption 2 also holds, with probability at least 1 - δ, this algorithm attains the following regret guarantee:

\[
R_T \leq \tilde{O}\left(\sqrt{Kd_{i^*}T}\right).
\] (17)

**Implications for open problems:** Corollary 5 affirmatively answers open problem 2 in Foster et al. (2019) under one of two conditions: (i) \( T \) is large enough, or (ii) Assumption 4 holds. We also affirmatively answer question 1 in Foster et al. (2019) that was asked in their discussion section. Under the setup and assumptions in Foster et al. (2019), they describe a sub-linear misspecification test that would satisfy Assumption 3 with \( \beta_{i^* - 1} \leq \tilde{O}(d_{i^*}) \). Hence from Corollary 5 under the same setup and assumptions, Mod-IGW with this misspecification test gets the optimal minimax bound of \( \tilde{O}(\sqrt{Kd_{i^*}T}) \). Hence showing that the price for model selection is negligible under this setup.

**Infinite classes:** It is straightforward to see that our results also hold for the case with infinite classes. Consider an infinite sequence of classes \( (M = \infty) \) such that \( d_i \) is strictly increasing in class index \( i \). Note that at the end of any epoch \( m \), at most \( \tau_m / C_1 \) classes have a non-trivial estimation rate on the dataset \( S_m \). Hence if we implement a version of Mod-IGW that only considers the first \( \tau_m / C_1 \) classes for the construction of the action selection kernel \( p_{m+1} \), all bounds on \( R_t \) that we discussed in this section continue to hold with the \( \log(M) \) factor being replaced by \( \log(t) \). From the same argument, at the end of every epoch \( m \), we can add a fixed number of classes with VC subgraph dimension greater than \( \tau_m / C_1 \) to our sequence of classes. These classes could be constructed using data collected in prior epochs, and similar bounds on \( R_t \) would continue to hold.

5 Conclusion

This paper concerns model selection for contextual bandits. We provide the first reduction of this problem to offline model selection oracles, propose an algorithm that can select from many classes, and also achieve minimax optimal guarantees under favorable/non-pathological instances (Assumption 3) or when the time-horizon is large enough.
**Limitations:** Practical implementations should tweak Mod-IGW to allow for more flexible epoch schedules and allow for more efficient data usage. A more careful analysis would allow for such modifications. Algorithmic ideas from [Krishnamurthy et al. (2021)](https://www.arXiv.org) should also be incorporated to weaken the dependency on Assumption 1. One interesting direction for future work would be to expand the scope of our solution to account for possible distribution shifts that may occur over the course of the bandit.

**Broader Impact:** Applications in health care, social science, and public policy offer an opportunity for positive impact. However, ethical considerations must be taken into account when designing exploration mechanisms for sensitive situations. As algorithms get better at learning personalized policies, some organizations may be incentivized to collect as much personal data as possible. Making it important to develop some framework that steers the usage of such algorithms in a direction that respects rights of users.

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A Additional Preliminaries

In this section we describe additional preliminaries to help with analyzing Mod-IGW. We setup additional notation in Appendix A.1 describe a more general estimation oracle in Appendix A.2 state helpful properties of the action selection kernel in Appendix A.3 describe important high-probability events in Appendix A.4 and state implicit policy evaluation guarantees for direct method via model selection in Appendix A.5. In Appendix B we use these concepts to analyze Mod-IGW. Finally, we analyze Algorithm 2 in Appendix C. We also provide additional details in Appendix D.

A.1 Additional Notation

In this paper, we follow notation used in Simchi-Levi and Xu (2020), similar notation has been used in other papers as well (e.g. Agarwal et al., 2014; Foster and Rakhlin, 2020). Let \( \Gamma_t \) denote the set of observed data points up to and including time \( t \). That is

\[
\Gamma_t := \{(x_i, a_i, r_i)\}_{i=1}^t
\]

(18)

Given a model \( f \) and policy \( \pi \), we let \( R_f(\pi) \) denote the expected instantaneous reward of the policy \( \pi \) with respect to the model \( f \).

\[
R_f(\pi) := \mathbb{E}_{x \sim D_x} [f(x, \pi(x))].
\]

(19)

Similarly, we let \( \text{Reg}_f(\pi) \) denote the expected instantaneous regret for policy \( \pi \) with respect to model \( f \).

\[
\text{Reg}_f(\pi) := \mathbb{E}_{x \sim X} [f(x, \pi_f(x)) - f(x, \pi(x))].
\]

(20)

Here \( \pi_f \) denote the policy induced by the model \( f \), that is \( \pi_f(x) := \max_a f(x, a) \) for every \( x \). Note that this policy has the highest instantaneous reward with respect to the model \( f \), that is \( \pi_f = \arg \max_{\pi \in \Psi} R_f(\pi) \). When there is no possibility of confusion, we will write \( R(\pi) \) and \( \text{Reg}(\pi) \) to mean \( R_f(\pi) \) and \( \text{Reg}_f(\pi) \) respectively.

Let \( \Psi = \mathcal{A}^X \) denote the universal policy space containing all possible policies. Given any probability kernel \( p \) we can construct a unique product probability measure on \( \Psi \), given by: (see lemma 3 in Simchi-Levi and Xu, 2020)

\[
Q_p(\pi) := \prod_{x \in X} p(\pi(x)|x),
\]

(21)

and it satisfies the following property

\[
p(a|x) = \sum_{\pi \in \Psi} I\{\pi(x) = a\}Q_p(\pi).
\]

(22)

For short-hand, we let \( Q_m \equiv Q_{p_m} \) denote the product probability measure on \( \Psi \) induced by the action selection kernel \( p_m \) defined in (6). Now, for any action selection kernel \( p \) and any policy \( \pi \), we let \( V(p, \pi) \) denote the expected inverse probability weight.

\[
V(p, \pi) := \mathbb{E}_{x \sim D_x} \left[ \frac{1}{p(\pi(x)|x)} \right]
\]

(23)

The variance term for several policy evaluation estimators like IPW depend on this expected inverse probability weight (see e.g. Agarwal et al., 2014). We also let \( m(t) \) denote the epoch containing round \( t \) – that is, \( m(t) := \min\{m|t \leq \tau_m\} \).

A.2 General Estimation Oracle

Recall that Mod-IGW uses a model selection oracle for estimation over the set of classes \( \{\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_M\} \). In this section, we state a generalized version of Assumption 2 that allows for more flexible estimation rates (\( \xi_i \)). We start by stating two fairly benign conditions that we expect our estimation rates to satisfy, and say that our rates are “valid” if they satisfy these conditions. First, we require \( \xi_i \) to be a non-increasing function of \( n \). In particular, we require:

For all \( i \in [M] \) and \( \zeta \in (0, 1), \xi_i(n, \zeta/\ln(n)) \) is non-increasing in \( n \).

\[\text{(24)}\]

\[\text{We require the first condition to ensure that } \gamma_{m,i} \text{ is non-decreasing in } m.\]
The second condition helps us simplify notation. At a high-level, it requires larger classes indices to correspond to more complex classes and have slower estimation rates.

For all $i \in [M]$ and $\zeta \in (0, 1)$, \(\frac{\xi_i(n, \zeta/n \ln(n))}{\xi_{i-1}(n, \zeta/n \ln(n))}\) is non-increasing in $n$ and is $\geq 1$. (25)

Where we define $\xi_0(n, \zeta) := \ln(1/\zeta)/n$, which is the estimation rate for estimating the mean of a one-dimensional bounded random variable.

We finally state Assumption 5, which weakens the requirements in Assumption 2 by allowing for general estimation rates.

**Assumption 5 (Estimation Oracle).** For every index $i \in [M]$, we assume access to an offline model selection oracle for estimation ($\text{EstOracle}_i$) over the sequence of classes $F_1, F_2, \ldots, F_i$ that satisfies the following property. There exists a constant $C_0 \geq 1$ such that for any probability kernel $p$, any natural number $n$, and any $\zeta \in (0, 1)$, the following holds with probability at least $1 - \zeta$:

\[
\mathbb{E}_{x \sim D_p} \mathbb{E}_{a \sim p(x)} [(\hat{f}(x, a) - f^*(x, a))^2] \leq \min_{j \in [i]} \left( C_0 \cdot b_j(p) + \xi_j(n, \zeta/i) \right). \tag{26}
\]

Where $\hat{f}$ is the output of $\text{EstOracle}_i$, fitted on $n$ independently and identically drawn samples from the distribution $D_p$. Here $b_j(p)$ is defined by (3). The functions $\xi_1, \xi_2, \ldots, \xi_M : \mathbb{N} \times [0, 1] \rightarrow [0, \infty)$ are known “valid” estimation rates; i.e., they satisfy (24) and (25).

For clarity, we note that saying Assumption 2 holds is equivalent to saying Assumption 5 holds with the estimation rates given by (5). As Assumption 5 allows for more general rates, we will prove our main results while assuming that our estimation oracle satisfies Assumption 5. This will directly imply the results discussed earlier where we required our estimation oracle to satisfy Assumption 2.

### A.3 Properties of the Action Selection Kernel

We now state helpful properties of the action selection kernel, and only include the proofs for completeness. These properties are explicitly stated and proved in Simchi-Levi and Xu (2020), but also show up in the analysis for Foster and Rakhlin (2020) (see section B.1 of their paper). Arguably, these properties characterize the key features of inverse gap weighting algorithms. Lemma 1 establishes an helpful notational equivalence between the expected instantaneous regret at any round $t$ in epoch $m$ and the expected regret of the randomized policy $Q_m$ that is induced by the action selection kernel used in epoch $m$.

**Lemma 1.** For any epoch $m \geq 1$ and time-step $t \geq 1$ in epoch $m$, we have:

\[
\mathbb{E}_{x, r, a_t} [r_t(\pi^*(x)) - r_t(a_t)|\Gamma_{t-1}] = \sum_{\pi \in \Psi} Q_m(\pi) \text{Reg}(\pi).
\]
Proof. Consider any epoch $m \geq 1$ and time-step $t \geq 1$ in the active phase of epoch $m$, then from Equation (22) we have:

$$E_{x_t, r_t, a_t} [r_t(\pi^*(x)) - r_t(a_t) | \Gamma_{t-1}]$$

$$= E_{x \sim D_x, a \sim p_m(:|x)} [f^*(x, \pi^*) - f^*(x, a)]$$

$$= E_{x \sim D_x} \left[ \sum_{a \in A} p_m(a|x) (f^*(x, \pi^*) - f^*(x, a)) \right]$$

$$= E_{x \sim D_x} \left[ \sum_{a \in A} \sum_{\pi \in \Psi} \mathbb{I}(\pi(x) = a) Q_m(\pi) (f^*(x, \pi^*) - f^*(x, a)) \right]$$

$$= \sum_{\pi \in \Psi} Q_m(\pi) E_{x \sim D_x} \left[ (f^*(x, \pi^*) - f^*(x, \pi(x))) \right]$$

$$= \sum_{\pi \in \Psi} Q_m(\pi) \text{Reg}(\pi).$$

$$\square$$

Lemma 2 and Lemma 3 bound the estimated instantaneous regret and the expected inverse probability weight for the action selection kernel constructed by inverse gap weighting.

**Lemma 2.** For any epoch $m \geq 1$, we have:

$$\sum_{\pi \in \Psi} Q_m(\pi) \text{Reg}_{f_m}(\pi) \leq \frac{K}{\gamma_m}.$$

**Proof.** Note that:

$$\sum_{\pi \in \Psi} Q_m(\pi) \text{Reg}_{f_m}(\pi) = \sum_{\pi \in \Psi} Q_m(\pi) E_{x \sim D_x} \left[ \hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, \pi(x)) \right]$$

$$= E_{x \sim D_x} \left[ \sum_{\pi \in \Psi} Q_m(\pi) (\hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, \pi(x))) \right]$$

$$= E_{x \sim D_x} \left[ \sum_{a \in A} \sum_{\pi \in \Psi} \mathbb{I}(\pi(x) = a) Q_m(\pi) (\hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, a)) \right]$$

$$= E_{x \sim D_x} \left[ \sum_{a \in A} p_m(a|x) (\hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, a)) \right]$$

$$= E_{x \sim D_x} \left[ \sum_{a \in A} \frac{(\hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, a))}{K + \gamma_m (\hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, a))} \right] \leq \frac{K}{\gamma_m}. $$

$$\square$$

**Lemma 3.** For all policies $\pi \in \Psi$ and epochs $m \geq 1$, we have:

$$V(p_m, \pi) \leq K + \gamma_m E_{x \sim D_x} \left[ (\hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, \pi(x))) \right]$$

**Proof.** Consider any policy $\pi \in \Psi$ and epoch $m \geq 1$. For any context $x \in X$ and action $a \in A \setminus \{\pi_{f_m}(x)\}$, from our choice for $p_m$, we get:

$$\frac{1}{p_m(a|x)} = K + \gamma_m (\hat{f}_m(x, \pi_{f_m}(x)) - \hat{f}_m(x, a)).$$

For the action $a = \pi_{f_m}(x)$, we have:

$$\frac{1}{p_m(a|x)} = \frac{1}{1 - \sum_{a' \neq a} \frac{1}{K + \gamma_m (f_m(x, \pi_{f_m}(x)) - f_m(x, a'))} \leq K$$
In particular, putting the above inequality together, we get:

\[
\frac{1}{p_m(\pi(x)|x)} \leq K + \gamma_m \left( \hat{f}_m(x, \pi f_m(x)) - \hat{f}_m(x, \pi(x)) \right).
\]

The lemma now follows by taking expectation over \( x \sim D_X \).

A.4 High probability events

In this section, we define two events \( \mathcal{W}_1 \) and \( \mathcal{W}_2 \) that hold with high-probability under Assumption 5 and Assumption 3 respectively. At a high-level, \( \mathcal{W}_1 \) defines the event where the prediction guarantees of EstOracle hold. That is, this event bounds the expected squared error difference between the true model (\( f^* \)) and the estimated model (\( \hat{f}_{m+1} \)).

\[
\mathcal{W}_1 := \left\{ \forall m \in [m^*_\ell], \mathbb{E}_{x \sim D_X} \mathbb{E}_{a \sim p_m(\cdot|x)} [(\hat{f}_{m+1}(x, a) - f^*(x, a))^2] \leq 2\xi_1(\tau_m - \tau_{m-1}, \frac{\delta}{4Mm^2}) \right\}.
\]

Similarly, \( \mathcal{W}_2 \) defines the event where the guarantees of MTOracle hold. That is, this event requires that, \( \tau_{\hat{m}_i} \in [\beta_i^c \tau_{m^*_i}, \beta_i] \) for any class index \( i \in [M] \). Recall \( \hat{m}_i \) is the implicit estimate of \( m^*_i \) constructed by MTOracle, it is the last epoch where model class \( \mathcal{F}_i \) was thought to be well-specified.

\[
\mathcal{W}_2 := \left\{ \forall i \in [M], \tau_{\hat{m}_i} \in [\beta_i^c \tau_{m^*_i}, \beta_i] \right\}.
\]

In Lemma 4 and Lemma 5 we use standard union bound arguments to show that the events \( \mathcal{W}_1 \) and \( \mathcal{W}_2 \) hold with high-probability.

**Lemma 4.** Suppose Assumption 5 holds. Then the event \( \mathcal{W}_1 \) holds with probability at least \( 1 - \delta/2 \).

**Proof.** Consider any epoch \( m \). Note that, conditional on \( \Gamma_{\tau_{m-1}} \) the samples in epoch \( m \) are i.i.d. samples from the distribution \( D(p_m) \). Hence with probability \( 1 - \delta/(4m^2) \), from Assumption 5, for all \( i \in [M] \) such that \( m \in [m^*_i] \) we have:

\[
\mathbb{E}_{x \sim D_X} \mathbb{E}_{a \sim p_m(\cdot|x)} [(\hat{f}_{m+1}(x, a) - f^*(x, a))^2] \leq \min_{i^* \in [M]} \left( C_0 B_{\epsilon} + \xi_{\epsilon} (\tau_m - \tau_{m-1}, \delta/(4Mm^2)) \right)
\]

\[
\leq 2\xi_1(\tau_m - \tau_{m-1}, \delta/(4Mm^2)).
\]

Where the last inequality follows from the definition of \( m^*_i \) and the fact that \( m \leq m^*_i \). Therefore, the probability that \( \mathcal{W}_1 \) does not hold can be bounded by:

\[
\sum_{m=1}^{\infty} \frac{\delta}{4Mm^2} \leq \delta/2.
\]

**Lemma 5.** Suppose Assumption 3 holds. The event \( \mathcal{W}_2 \) holds with probability at least \( 1 - \delta/2 \).

**Proof.** Consider any epoch \( m \) and any model index \( i \). From Assumption 3 with probability at least \( 1 - \delta/(4Mm^2) \), we have that MTOracle(\( i, S_m, \delta/(4Mm^2) \)) outputs \text{False} if \( \tau_m \leq \beta_i^c \tau_{m^*_i} \) and outputs \text{True} if \( \tau_m > \beta_i \). Therefore, we have \( \tau_{\hat{m}_i} \in [\beta_i^c \tau_{m^*_i}, \beta_i] \) for all \( i \in [M] \) with probability at least:

\[
1 - \sum_{i=1}^{M} \sum_{m=1}^{\infty} \frac{\delta}{4Mm^2} \geq 1 - \delta/2.
\]

\( D(p_m) \) depends on \( \Gamma_{\tau_{m-1}} \) because \( p_m \) is constructed using the data in \( \Gamma_{\tau_{m-1}} \).
A.5 Direct Method

Given any estimated model $\hat{f}$, $R_f(\pi)$ gives us an implicit estimate for any policy $\pi$. Moreover, as discussed earlier, $\pi_f$ is the policy that maximizes these implicitly estimated rewards. This approach to policy optimization is known as the direct method for policy optimization. Several papers have analyzed the direct method for policy evaluation/optimization. In Lemma 6 we state a guarantee on the direct method via a model selection oracle for estimation. The proof is essentially the same as the proof of prior guarantees on the direct method (e.g. Qian and Murphy, 2011; Simchi-Levi and Xu, 2020; Krishnamurthy et al., 2021).

Lemma 6. Suppose the event $\mathcal{W}_1$ defined in (27) holds. Then, for all policies $\pi$, class indices $i \in [M]$, and epochs $m \in [m_t^+]$, we have:

$$|R_{f_{m+1}}(\pi) - R(\pi)| \leq \frac{\sqrt{V(p_m, \pi)\sqrt{K}}}{2\gamma_{m+1,i}}$$

Proof. For any policy $\pi$, class index $i$, and epoch $m \in [m_t^+]$, note that:

$$|R_{f_{m+1}}(\pi) - R(\pi)|$$

$$\leq \mathbb{E}_{x \sim D_x} \left[ \left| \hat{f}_{m+1}(x, \pi(x)) - f^*(x, \pi(x)) \right| \right]$$

$$= \mathbb{E}_{x \sim D_x} \left[ \frac{1}{p_m(\pi(x)|x)} p_m(\pi(x)|x) \left( \hat{f}_{m+1}(x, \pi(x)) - f^*(x, \pi(x)) \right)^2 \right]$$

$$\leq \mathbb{E}_{x \sim D_x} \left[ \frac{1}{p_m(\pi(x)|x)} \mathbb{E}_{a \sim p_m(x|a)} \left( \hat{f}_{m+1}(x, a) - f^*(x, a) \right)^2 \right]$$

$$\leq \mathbb{E}_{x \sim D_x} \left[ \frac{1}{p_m(\pi(x)|x)} \right] \mathbb{E}_{x \sim D_x} \mathbb{E}_{a \sim p_m(x|a)} \left( \hat{f}_{m+1}(x, a) - f^*(x, a) \right)^2$$

$$\leq \sqrt{V(p_m, \pi)} \sqrt{2K \xi_t (\tau_m - \tau_{m-1}) \frac{\delta}{4Mm^2}} = \frac{\sqrt{V(p_m, \pi)\sqrt{K}}}{2\gamma_{m+1,i}}.$$ 

The first inequality follows from Jensen’s inequality, the second inequality is straightforward, the third inequality follows from Cauchy-Schwarz inequality, and the last inequality follows from assuming that $\mathcal{W}_1$ from (27) holds.

Since the accuracy of the direct method for policy evaluation only depends on the prediction error of the underlying estimator. A simple observation we make is that when the underlying estimator is constructed by a model selection oracle for estimation, the prediction error will decrease more rapidly in terms of sample size for small datasets, and will allow us to accordingly reduce the corresponding exploration more rapidly for earlier rounds.

B Analyzing Mod-IGW

In this section, we state and prove our main guarantee (Theorem 3), and show that Theorem 2 is a direct corollary of Theorem 3. At a high-level, the proof of Theorem 3 is simply a series of inductive arguments.

Theorem 3. Suppose Assumption 5 and Assumption 2 hold. Then with probability at least $1 - \delta$, for all $i, j \in [M]$, and $t \in [\beta_t^\tau m_t^+]$, Mod-IGW attains the following regret guarantee:

$$R_t \leq O\left( \beta_{j-1} \ln \left( \frac{\gamma_m(b_{j-1}, 1)}{\gamma_m(b_{j-1}, i)} \right) + \sum_{t' = \tau_{t+1}}^t \gamma_{m(t')-1, 1} \sqrt{K \xi_t (\tau_m(t') - \tau_{m(t')-2}) \frac{\delta}{4M(m(t')^2)}} \right)$$

(30)
B.1 Inductive argument

In Lemma 7, we establish a key inductive guarantee for implicit estimates of instantaneous regret for Mod-IGW. The proof of Lemma 7 is a modification of similar inductive guarantees proved in Agarwal et al. (2014) and Simchi-Levi and Xu (2020).

Lemma 7. Suppose the event \( \mathcal{W}_1 \) defined in (27) holds. Consider any class index \( i \in [M] \) and consider any epoch \( m \in [m^*] \). Suppose there exists a constant (\( \eta > 0 \)) such that for all policies \( \pi \), we have:

\[
\begin{align*}
\text{Reg}(\pi) &\leq 2\text{Reg}_{f_m}(\pi) + \frac{\eta K}{\gamma_{m,i}} \\
\text{Reg}_{f_m}(\pi) &\leq 2\text{Reg}(\pi) + \frac{\eta K}{\gamma_{m,i}}.
\end{align*}
\]

We then have that:

\[
\begin{align*}
\text{Reg}(\pi) &\leq 2\text{Reg}_{f_{m+1}}(\pi) + \frac{\eta' K}{\gamma_{m+1,i}} \\
\text{Reg}_{f_{m+1}}(\pi) &\leq 2\text{Reg}(\pi) + \frac{\eta' K}{\gamma_{m+1,i}}.
\end{align*}
\]

Where \( \eta' = 2 \max \left( \frac{\gamma_m}{\gamma_{m,i}}, \sqrt{1 + \frac{\gamma_{m,i}}{\gamma_m}} \right) \).

Proof. Let \( \alpha \) be a positive constant, and let \( \alpha' = \gamma_m/\gamma_{m,i} \). Note that:

\[
\begin{align*}
\text{Reg}(\pi) - \text{Reg}_{f_{m+1}}(\pi) &= \left( R(\pi^*) - R(\pi) \right) - \left( R_{f_{m+1}}(\pi_{f_{m+1}}) - R_{f_{m+1}}(\pi) \right) \\
&\leq \left( R(\pi^*) - R(\pi) \right) - \left( R_{f_{m+1}}(\pi^*) - R_{f_{m+1}}(\pi) \right) \\
&\leq |R(\pi^*) - R_{f_{m+1}}(\pi^*)| + |R(\pi) - R_{f_{m+1}}(\pi)| \\
&\leq \sqrt{V(p_m, \pi^*) \sqrt{K}} + \sqrt{V(p_m, \pi) \sqrt{K}} \\
&\leq \frac{V(p_m, \pi^*)}{\alpha \gamma_{m+1,i}} + \frac{V(p_m, \pi)}{\alpha \gamma_{m+1,i}} + \alpha K \leq \alpha K + \frac{\eta K}{\gamma_{m,i}} - (1 + \alpha' \eta)K.
\end{align*}
\]

Where the first inequality follows from the definition of \( \pi_{f_{m+1}} \), the third inequality follows from Lemma 6 and the last inequality follows from the AM-GM inequality. Now note that:

\[
\begin{align*}
\text{Reg}(\pi) &= \text{Reg}_{f_m}(\pi) + \text{Reg}(\pi) - \text{Reg}_{f_{m+1}}(\pi) \\
&\leq \frac{K + \gamma_m \text{Reg}_{f_m}(\pi^*)}{\alpha \gamma_{m+1,i}} - 1 + \alpha' \eta K + \frac{\eta K}{\gamma_{m,i}} \\
&\leq \frac{K + \gamma_m \left( 2\text{Reg}(\pi^*) + \frac{\eta K}{\gamma_{m,i}} \right)}{\alpha \gamma_{m+1,i}} = (1 + \alpha' \eta)K.
\end{align*}
\]

Where the first inequality follows from Lemma 6 and the last inequality follows from the fact that \( \text{Reg}(\pi^*) \) is equal to zero. Similarly note that:

\[
\begin{align*}
\text{Reg}(\pi) &= \text{Reg}_{f_{m+1}}(\pi) + \text{Reg}(\pi) - \text{Reg}_{f_{m+1}}(\pi) \\
&\leq \frac{K + \gamma_m \text{Reg}_{f_{m+1}}(\pi^*)}{\alpha \gamma_{m+1,i}} - 1 + \alpha' \eta K + \frac{\eta K}{\gamma_{m,i}} \\
&\leq \frac{K + \gamma_m \left( 2\text{Reg}(\pi) + \frac{\eta K}{\gamma_{m,i}} \right)}{\alpha \gamma_{m+1,i}} \leq 2\alpha' \text{Reg}(\pi) + \frac{K(1 + \alpha' \eta)}{\alpha \gamma_{m+1,i}}.
\end{align*}
\]

Where the first inequality follows from Lemma 6. Now from combining (31), (32), and (33), we get:

\[
\begin{align*}
\text{Reg}(\pi) - \text{Reg}_{f_{m+1}}(\pi) &\leq \frac{\alpha K}{\gamma_{m+1,i}} + \frac{2(1 + \alpha' \eta)K}{\alpha \gamma_{m+1,i}} + \frac{2\alpha' \text{Reg}(\pi)}{\alpha} \\
\Rightarrow \frac{\alpha - 2\alpha'}{\alpha} \text{Reg}(\pi) &\leq \text{Reg}_{f_{m+1}}(\pi) + \frac{\alpha K}{\gamma_{m+1,i}} + \frac{2(1 + \alpha' \eta)K}{\alpha \gamma_{m+1,i}} \\
\Rightarrow \text{Reg}(\pi) &\leq \frac{\alpha}{\alpha - 2\alpha'} \text{Reg}_{f_{m+1}}(\pi) + \frac{\alpha^2 K}{\gamma_{m+1,i}} + \frac{2(1 + \alpha' \eta)K}{\alpha - 2\alpha' \gamma_{m+1,i}}.
\end{align*}
\]
Where we finally get the required result by combining (34), (37), (38), and (39).

Further, we get:

\[ \lVert R \pi \rVert_{\text{Reg}} \leq \left( R_{f_{m+1}}(\pi_{f_{m+1}}) - R_{f_{m+1}}(\pi) \right) - \left( R(\pi^*) - R(\pi) \right) \]

with the first inequality follows from the definition of Lemma 8. Suppose the event \( W_1 \) holds. Consider any class index \( i \in [M] \). For all policies \( \pi \) and epochs \( m \leq m_1 + 1 \), we have:

\[ \text{Reg}(\pi) \leq 2 \text{Reg}(\pi) \leq 2 \text{Reg}(\pi) \]

Now by choosing \( \alpha = 4 \max(\alpha', \sqrt{1 + \alpha' \eta}) \), we have that:

\[ \alpha + 2\alpha' \leq 2, \text{ and } \frac{\alpha}{\alpha - 2\alpha'} \leq 2 \]

Further, we get:

\[ \frac{\alpha^2}{8(\alpha - 2\alpha')} + \frac{2(1 + \alpha' \eta)}{(\alpha - 2\alpha')^{\gamma_{m+1,i}}} \leq \frac{\alpha}{4} + \frac{4(1 + \alpha' \eta)}{\alpha} \leq \frac{\alpha}{2} \]

We finally get the required result by combining (34), (37), (38), and (39).

\[ \Box \]

**B.2 Under Exploration and Self Correction**

Under exploration can lead to less accurate (implicit) estimates of instantaneous regret. Lemma 8 bounds the prediction error of these implicit estimates, and quantifies the cost of under-exploration that may happen. For notational convenience, we let \( \gamma_{0,i} = \gamma_{1,i} = 1 \) for all class indices \( i \in [M] \).

**Lemma 8.** Suppose the event \( W_1 \) holds. Consider any class index \( i \in [M] \). For all policies \( \pi \) and epochs \( m \leq m_1 + 1 \), we have:

\[ \text{Reg}(\pi) \leq 2 \text{Reg}(\pi) \]

\[ \text{Reg}(\pi) \leq 2 \text{Reg}(\pi) \]

Where \( \eta_{k,m} = 2 + 4\gamma_{m-1,i}/\gamma_{m-1,i} \).
**Proof.** We will prove this by induction. The base case then follows from the fact that for all policies \( \pi \), we have:

\[
\text{Reg}(\pi) \leq 1 \leq \eta_1 K / \gamma_{1,i},
\]

\[
\text{Reg}_{f_i}(\pi) \leq 1 \leq \eta_1 K / \gamma_{1,i}.
\]

For the inductive step, fix some \( m \leq m^*_i \). Assume for all policies \( \pi \), we have:

\[
\text{Reg}(\pi) \leq 2 \text{Reg}_{f_m}(\pi) + \frac{\eta_{i,m} K}{\gamma_{m,i}},
\]

\[
\text{Reg}_{f_m}(\pi) \leq 2 \text{Reg}(\pi) + \frac{\eta_{i,m} K}{\gamma_{m,i}}.
\]

Therefore, from Lemma 7 we have:

\[
\text{Reg}(\pi) \leq 2 \text{Reg}_{f_{m+1}}(\pi) + \frac{\eta'_{m+1} K}{\gamma_{m+1,i}},
\]

\[
\text{Reg}_{f_{m+1}}(\pi) \leq 2 \text{Reg}(\pi) + \frac{\eta'_{m+1} K}{\gamma_{m+1,i}}.
\]

Where,

\[
\eta'_{i,m+1} = 2 \max \left( \frac{\gamma_{m,i}}{\gamma_{m,i}} \sqrt{1 + \frac{\gamma_{m,i}}{\gamma_{m,i}} \eta_{i,m}} \right) \leq 2 \max \left( \frac{\gamma_{m,i}}{\gamma_{m,i}} \sqrt{1 + \frac{\gamma_{m,i}}{\gamma_{m,i}} \eta_{i,m}} \right)
\]

\[
\leq 2 \max \left( \frac{\gamma_{m,i}^2}{\gamma_{m,i}^2} \sqrt{1 + 4 \frac{\gamma_{m,i}^2}{\gamma_{m,i}^2} + 2 \frac{\gamma_{m,i}^2}{\gamma_{m,i}^2}} \right) = \max \left( 2 \frac{\gamma_{m,i}^2}{\gamma_{m,i}^2} \eta_{i,m+1} \right) = \eta_{i,m+1}.
\]

This completes the inductive argument.  

To help with understanding Lemma 8 it may be helpful to consider selection among classes with finite VC sub-graph dimension. Under this setup, according to Lemma 8 the worst case cost of under exploration up to epoch \( m^*_i \) is \( \eta_{i,m} = O(\sqrt{d_i/d_i}) \). This agrees with the discussion in Section 4. Lemma 10 shows that Mod-IGW can self-correct when the amount of under-exploration is reduced, and Lemma 9 is a key step towards showing the self-correction property of Mod-IGW.

**Lemma 9.** Suppose the event \( \mathcal{W}_i \) holds. Consider any class indices \( i, j \in [M] \) such that \( j \leq i \). For all policies \( \pi \) and epochs \( m \in [m_{j-1} + 1, m^*_i + 1] \), we have:

\[
\text{Reg}(\pi) \leq 2 \text{Reg}_{f_{m}}(\pi) + \eta_{m,j} (\gamma_{m,j-1,i}) \frac{\gamma_{m,j-1,i}}{\gamma_{m,j-1,i}} \frac{K}{\gamma_{m,i}} \leq 2 \text{Reg}(\pi) + \frac{\eta'_{m} K}{\gamma_{m,i}}.
\]

\[
\text{Reg}_{f_{m}}(\pi) \leq 2 \text{Reg}(\pi) + \frac{\eta'_{m} K}{\gamma_{m,i}}.
\]

**Proof.** Consider any class indices \( i, j \in [M] \) such that \( j \leq i \). We will prove the required bound by induction. The bound for the base case \( m = m_{j-1} + 1 \) follows from Lemma 8. Suppose the bound in Lemma 9 holds for class indices \( i, j \) and for some epoch \( m \in [m_{j-1} + 1, m^*_i] \). From Lemma 7 we have:

\[
\text{Reg}(\pi) \leq 2 \text{Reg}_{f_{m+1}}(\pi) + \frac{\eta'_{m+1} K}{\gamma_{m+1,i}}
\]

\[
\text{Reg}_{f_{m+1}}(\pi) \leq 2 \text{Reg}(\pi) + \frac{\eta'_{m+1} K}{\gamma_{m+1,i}}.
\]
Where:

\[ \eta' = 2 \max \left( \frac{\gamma_m}{\gamma_{m,i}} \left( 1 + \frac{\gamma_{m,j}}{\gamma_{m,i}} \left( \frac{\gamma_{m,j,1}}{\gamma_{m,j,i}} \right)^{1/2^{m-m_i-1}} \right) \right) \]

\[ \leq 2 \max \left( \frac{\gamma_{m,j}}{\gamma_{m,i}} \left( 1 + \frac{\gamma_{m,j}}{\gamma_{m,i}} \left( \frac{\gamma_{m,j,1}}{\gamma_{m,j,i}} \right)^{1/2^{m-m_i-1}} \right) \right) \]

\[ \leq \gamma \left( \frac{\gamma_{m,j,1}}{\gamma_{m,j,i}} \right)^{1/2^{m-m_i-1}} \]

Where the first inequality follows from the fact that \( \gamma_m \leq \gamma_{m,j} \). The second inequality follows from Lemma 10, and the second inequality follows from Lemma 9.

This completes the proof of Lemma 10.

To help with understanding Lemma 10, it may be helpful to consider selection among classes with finite VC sub-graph dimension. Note that for any class index \( i \in [M] \), Mod-IGW isn’t under-exploring for epochs in \([\hat{m}_i - 1 + [\log_2(\gamma_{m_i,1}/\gamma_{m_i,i})]], m_i, 1)\]. Hence from Lemma 10 we get that Mod-IGW self corrects and gets accurate implicit estimates for expected instantaneous regret (that is \( \eta_{m_i-1,m} = O(1) \)) for all \( m \in [\hat{m}_i - 1 + [\log_2(\gamma_{m_i,1}/\gamma_{m_i,i})]], m_i, 1)\).

### B.3 Bounding Instantaneous Regret of Action Selection Kernel

Recall that the action selection kernel \( q_m \) induces a distribution over deterministic policies, denoted by \( Q_m \). In this section, we bound the expected instantaneous regret of the randomized policy \( Q_m \).

**Lemma 11.** Suppose the event \( \mathcal{W}_1 \) defined in (27) holds. Consider any class indices \( i, j \in [M] \) such that \( j \leq i \). Then for all epochs \( m \in [\hat{m}_j - 1 + [\log_2(\gamma_{m_j,1}/\gamma_{m_j,i})]], m_i^*, 1) \) we have:

\[ \sum_{\pi \in \Psi} Q_m(\pi) \text{Reg}(\pi) \leq 2K \frac{2K}{\gamma_m} \frac{\eta_{i,j,m} K}{\gamma_m} \]

Where \( \eta_{i,j,m} = 32\gamma_{m-1,j}/\gamma_{m-1,i} \).

**Proof.** Consider any class indices \( i, j \in [M] \) such that \( j \leq i \). For any \( m \in [\hat{m}_j - 1 + [\log_2(\gamma_{m_j,1}/\gamma_{m_j,i})]], m_i^*, 1) \):

\[ \sum_{\pi \in \Psi} Q_m(\pi) \text{Reg}(\pi) \leq \sum_{\pi \in \Psi} Q_m(\pi) \left( 2\text{Reg}_{m}(\pi) + \frac{\eta_{i,j,m} K}{\gamma_m} \right) \leq 2K \frac{2K}{\gamma_m} \frac{\eta_{i,j,m} K}{\gamma_m} \]

Where the first inequality follows from Lemma 10 and the second inequality follows from Lemma 9. 

\[ \Box \]
B.4 Proof of Theorem 3

In this section we prove Theorem 3 and restate it for convenience.

**Theorem 3.** Suppose Assumption 5 and Assumption 3 hold. Then with probability at least $1 - \delta$, for all $i, j \in [M]$, and $t \in \left[\beta_i' \tau_{m_i^*}\right]$, Mod-IGW attains the following regret guarantee:

$$R_t \leq \mathcal{O}\left(\beta_{j-1} \ln\left(\frac{\gamma_m(\beta_{j-1})}{\gamma_{m(\beta_{j-1})}}\right) + \sum_{t' = \tau_{t+1}}^t \frac{\gamma_{m(t')-1,j}}{\gamma_{m(t')-1,i}} \sqrt{K\xi_i \left(\tau_{m(t')-1} - \tau_{m(t')-2}, \frac{\delta}{4M(m(t'))^2}\right)}\right)$$

(30)

**Proof.** From Lemma 4 and Lemma 5 we have that both $W_1$ and $W_2$ hold with probability at least $1 - \delta$. We now bound the expected cumulative regret up to round $t$ while assuming that this high-probability event holds. Consider any class indices $i, j \in [M]$ and round $t \in \left[\beta_i' \tau_{m_i^*}\right]$. Note that under $W_2$, if $j > i$, then $\beta_{j-1} \geq \beta_i \geq \beta_i' \tau_{m_i^*} \geq t$. Hence the bound in Theorem 3 trivially holds. So, we only focus on the case when $j \leq i$.

For notational convenience, let $m' = \max(1, m_{j-1} + \lceil \log_2(\log_2(\gamma_{m_{j-1},1}/\gamma_{m_{j-1},i}))\rceil)$. Therefore, as $W_2$ holds, we have $\tau_{m'} \geq \max(\tau_1, 2\beta_{j-1} \log_2(\gamma_{m(\beta_{j-1},1)/\gamma_{m(\beta_{j-1},i)}})$. If $m(t) \leq m'$, then we have that $\tau_{m(t)} \leq \mathcal{O}(\beta_{j-1} \ln(\gamma_{m(\beta_{j-1},1)/\gamma_{m(\beta_{j-1},i)}})$. Hence the bound in Theorem 3 again trivially holds. So, we only focus on the case when $m(t) > m'$.

Consider any round $t' \in [t]$. Since under $W_2$ we have $t' \leq t \leq \beta_i' \tau_{m_i^*} \leq \tau_{m_i}$, we get that $1/\gamma_{m(t')} \leq 1/\gamma_{m(t),i}$. Hence, from Lemma 11 we have that:

$$R_t = \sum_{t'=1}^t \sum_{\pi \in \Psi} Q_{t'}(\pi)R(\pi)$$

$$\leq \tau_{m'} + \sum_{t' = \tau_{m'}+1}^t \left(2 + \eta_{i,j,m(t')}\right) K \frac{\gamma_{m(t')},i}{\gamma_{m(t')},i}$$

$$\leq \tau_{m'} + 68\sqrt{2} \sum_{t' = \tau_{m'}+1}^t \frac{\gamma_{m(t')-1,j}}{\gamma_{m(t')-1,i}} \sqrt{K\xi_i \left(\tau_{m(t')-1} - \tau_{m(t')-2}, \frac{\delta}{4M(m(t'))^2}\right)}$$

(40)

Now the bound in Theorem 3 follows from noting that:

$$\tau_0 \leq \tau_{m'} \leq \max(\tau_1, 2\beta_{j-1} \log_2(\gamma_{m(\beta_{j-1},1)/\gamma_{m(\beta_{j-1},i)}})$$

\hfill \square

B.5 Proof of Theorem 2

In this section, we show that Theorem 2 is a simple corollary of Theorem 3.

**Theorem 2.** Suppose Assumption 2 and Assumption hold. Then with probability at least $1 - \delta$, for all $i, j \in [M]$, and $t \in \left[\beta_i' \tau_{m_i^*}\right]$, Mod-IGW attains the following regret guarantee:

$$R_t \leq \mathcal{O}\left(\beta_{j-1} \ln(d_i/d_1) + \sqrt{\frac{d_i}{d_j}} \sqrt{Kd_i t \ln(t) \ln\left(\frac{M \ln(t)}{\delta}\right)}\right)$$

(12)

**Proof.** Consider any class indices $i, j \in [M]$ and consider any round $t \in \left[\beta_i' \tau_{m_i^*}\right]$. Under Assumption 2 we have that:

$$\sum_{t' = \tau_{t+1}}^t \sqrt{\xi_i \left(\tau_{m(t')-1} - \tau_{m(t')-2}, \frac{\delta}{4M(m(t'))^2}\right)} \leq \sqrt{C_i d_i \ln(t) \ln\left(\frac{4M \ln(t)}{\delta}\right)} \sum_{m=2}^{m(t)} \frac{\tau_m - \tau_{m-1}}{\sqrt{\tau_{m-1} - \tau_{m-2}}}$$

(41)
Since for all $m \geq 1$, $\tau_{m+1} = 2\tau_m$, we have that:
\begin{equation}
\sum_{m=2}^{m(t)} \frac{\tau_m - \tau_{m-1}}{\sqrt{\tau_{m-1} - \tau_{m-2}}} \leq \sqrt{2} \sum_{m=2}^{m(t)} \frac{\tau_m - \tau_{m-1}}{\sqrt{\tau_{m-1}}} \leq \sqrt{2} \sum_{m=2}^{m(t)} \int_{\tau_{m-1}}^{\tau_m} dy \sqrt{y} \tag{42}
\end{equation}
\begin{equation*}
= \sqrt{2} \int_{\tau_1}^{\tau_{m(t)}} \frac{dy}{\sqrt{y}} \leq \sqrt{8\tau_{m(t)}} \leq 4\sqrt{7}.
\end{equation*}
Further under the estimation rates in Assumption $\ref{assumption:estimation}$, we have that $\gamma_{m,j} / \gamma_{m,i} = \sqrt{d_i / d_j}$ for all epoch $m$. Therefore the bound in Theorem $\ref{theorem:main_theorem}$ follows from Theorem $\ref{theorem:classification_error}$ (41), (42), and the fact that $\gamma_{m,j} / \gamma_{m,i} = \sqrt{d_i / d_j}$ for all $m$.

\section{Analyzing Algorithm $\ref{algorithm:misspecification_test}$}

In this section, we state and prove our main guarantee (Theorem $\ref{theorem:misspecification_test}$) for the misspecification test described in Algorithm $\ref{algorithm:misspecification_test}$.

\begin{theorem}
Suppose Assumption $\ref{assumption:misspecification}$ holds. Consider any class index $i \in [M]$, epoch $m$, and confidence parameter $\zeta \in (0,1)$, the following hold with probability $1 - \zeta$: (i) Algorithm $\ref{algorithm:misspecification_test}$ outputs “False” if $\tau_m \leq \tau^*_m$. (ii) Algorithm $\ref{algorithm:misspecification_test}$ outputs “True” if (43) holds.
\end{theorem}

Recall that Algorithm $\ref{algorithm:misspecification_test}$ takes as input a class index $i$, epoch $m$, algorithm parameter $\alpha_{ho} \in (0,1)$, and confidence parameter $\zeta \in (0,1)$. For convenience, unless stated otherwise, we keep these parameters fixed throughout this section. We start with a brief recap of Algorithm $\ref{algorithm:misspecification_test}$ with these input parameters.

\begin{algorithm}
Our test starts by splitting the data collected in epoch $m$ ($S_m$) into "training" and "hold-out" sets denoted by $S_m$ and $S_m$ ho. Such that $S_m$ contains $[\alpha_{ho} |S_m|]$ samples. With $S_m$ ho as input, let $\hat{g}_i$ and $\hat{g}_M$ be the output of EstOracle and EstOracleM respectively (see Assumption $\ref{assumption:estimation}$). Our test says the class $U_{j \in [i]} F_j$ is possibly well-specified when (43) holds and is misspecified otherwise.
\begin{equation}
\hat{L}(S_m, ho, \hat{g}_i) \leq \hat{L}(S_m, ho, \hat{g}_M) + 4\xi_i(|S_{m, ho}|, \zeta / (6M)) + 8\xi_i(|S_{m, ho}|, \zeta / (6i)) + \frac{36 \log(6/\zeta)}{|S_{m, ho}|}.
\end{equation}
\end{algorithm}

We want to show that if $\tau_m \leq \tau^*_m$ then with high-probability (43) holds. If the $U_{j \in [i]} F_j$ is well-specified then $\tau^*_m$ is unbounded and hence we will always have that $\tau_m \leq \tau^*_m$. If $U_{j \in [i]} F_j$ is misspecified, then $\tau^*_m$ is bounded, and we want to detect misspecification. In this case, we show that (43) is not satisfied with high-probability if $\tau_m$ is large enough (if (43) holds).

\subsection{Bounding Loss Estimates}

In this section we provide high-probability upper and lower bounds on the loss estimates, see Lemma $\ref{lemma:loss_bound}$ and Lemma $\ref{lemma:loss_bound2}$. We also state a high-probability upper bound on the expected loss, see Lemma $\ref{lemma:expected_loss_bound}$. Finally, we define a high-probability event where all these bound hold.

\begin{lemma}
With probability at least $1 - \zeta / 3$, we have that:
\begin{equation}
\hat{L}(S_m, ho, \hat{g}_i) - \hat{L}(S_m, ho, f^*) \leq 2 \cdot \frac{\mathbb{E}}{(x,a,r) \sim D(p_m)} |(\hat{g}_i(x,a) - f^*(x,a))^2| + \frac{10 \log(6/\zeta)}{3 |S_{m, ho}|}.
\end{equation}
\begin{equation}
\hat{L}(S_m, ho, \hat{g}_M) - \hat{L}(S_m, ho, f^*) \leq 2 \cdot \frac{\mathbb{E}}{(x,a,r) \sim D(p_m)} |(\hat{g}_M(x,a) - f^*(x,a))^2| + \frac{10 \log(6/\zeta)}{3 |S_{m, ho}|}.
\end{equation}
\end{lemma}

\begin{proof}
We only show (45) holds with probability at least $1 - \zeta / 6$. A similar proof shows that (46) holds with probability at least $1 - \zeta / 6$. For notational convenience, for any round $t$, let $Z_t$ be defined by:
\begin{equation}
Z_t := (\hat{g}_i(x_t, a_t) - r_t(a_t))^2 - (f^*(x_t, a_t) - r_t(a_t))^2, \quad \mathbb{E}_{(x,a) \sim D(p_m)} |(\hat{g}_i(x,a) - f^*(x,a))^2|.
\end{equation}
\end{proof}
With some abuse of notation, we say $t \in S_{m,ho}$ if the sample from round $t$ is in $S_{m,ho}$. Note that conditional on $\Gamma_{m-1, S_{m, ho}}$, $\{Z_i | t \in S_{m, ho}\}$ is a set of i.i.d. random variables. We want to use Bernstein inequality (Lemma[19]) to get a tight high-probability bound on the sum of these random variables. To do this, we first quantify the mean and variance of $Z_i$. Note that for any $t \in S_{m, ho}$, we have:

$$
\mathbb{E}[Z_i | \Gamma_{m-1, S_{m, ho}}] = \mathbb{E}[(\hat{g}_i(x, a) - r(a))^2 - (f^*(x, a) - r(a))^2] = \mathbb{E}[(\hat{g}_i(x, a) - f^*(x, a)) (\hat{g}_i(x, a) + f^*(x, a) - 2r(a)) - (\hat{g}_i(x, a) - f^*(x, a))^2] = 0.
$$

Hence, $Z_i$ is mean zero. Now note that for any $t \in S_{m, ho}$, we have:

$$
\mathbb{E}[Z_i^2 | \Gamma_{m-1, S_{m, ho}}] = \mathbb{Var}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2] \\
\leq \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2 (\hat{g}_i(x, a) + f^*(x, a) - 2r(a))] \\
\leq 4 \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2].
$$

(49)

Also note that $|Z_i| \leq 2$, therefore with (48) and (49), we have bounded the quantities needed to use Lemma[19]. Hence, from Lemma[19] (Bernstein’s inequality), we have that the following bound holds with probability at least $1 - \zeta/6$:

$$
\sum_{t \in S_{m, ho}} Z_t \leq \frac{4 \ln(6/\zeta)}{3} + \frac{8 \ln(6/\zeta)}{|S_{m, ho}|} \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2].
$$

(50)

Therefore, by dividing (50) by $|S_{m, ho}|$, we get:

$$
\hat{L}(S_{m, ho}, \hat{g}_i) - \hat{L}(S_{m, ho}, f^*) - \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2] \\
\leq \frac{4 \ln(6/\zeta)}{3|S_{m, ho}|} + \frac{4 \ln(6/\zeta)}{|S_{m, ho}|} \mathbb{E}_{(x,a,r) \sim D(p_m)} [2(\hat{g}_i(x, a) - f^*(x, a))^2] \\
\leq \frac{10 \ln(6/\zeta)}{3|S_{m, ho}|} + \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2].
$$

(51)

Where the last inequality follows from AM-GM inequality. This completes the proof of showing that (45) holds with probability at least $1 - \zeta/6$. The same proof with $\hat{g}_M$ instead of $\hat{g}_i$ shows that (46) holds with probability at least $1 - \zeta/6$. Therefore both inequalities hold with probability at least $1 - \zeta/3$ which completes the proof of Lemma[12].

Lemma 13. With probability at least $1 - \zeta/3$, we have that:

$$
\mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2] \leq 2 \left( \hat{L}(S_{m, ho}, \hat{g}_i) - \hat{L}(S_{m, ho}, f^*) \right) + \frac{32 \log(6/\zeta)}{3 |S_{m, ho}|}
$$

(52)

$$
\mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_M(x, a) - f^*(x, a))^2] \leq 2 \left( \hat{L}(S_{m, ho}, \hat{g}_M) - \hat{L}(S_{m, ho}, f^*) \right) + \frac{32 \log(6/\zeta)}{3 |S_{m, ho}|}
$$

(53)

Proof. The proof of Lemma[13] is similar to that of Lemma[12]. We only show (52) holds with probability at least $1 - \zeta/6$. A similar proof shows that (53) holds with probability at least $1 - \zeta/6$. In (50), we used Lemma[19] (Bernstein’s inequality) to bound the sum of $Z_i$’s (see (47) for the definition of $Z_i$). Using the same argument to bound the sum of $-Z_i$’s, we get that the following bound holds with probability at least $1 - \zeta/6$:

$$
\sum_{t \in S_{m, ho}} (-Z_t) \leq \frac{4 \ln(6/\zeta)}{3} + \frac{8 \ln(6/\zeta)}{|S_{m, ho}|} \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x, a) - f^*(x, a))^2].
$$

(54)
Therefore, by dividing (54) by $|S_{m,ho}|$, we get:

$$E_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x,a) - f^*(x,a))^2] - \left( \hat{L}(S_{m,ho}, \hat{g}_i) - \hat{L}(S_{m,ho}, f^*) \right)$$

$$\leq \frac{4 \ln(6/\zeta)}{3|S_{m,ho}|} + \sqrt{\frac{8 \ln(6/\zeta)}{|S_{m,ho}|} \frac{E_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x,a) - f^*(x,a))^2]}{2 (x,a,r) \sim D(p_m)}}$$

$$\leq \frac{16 \ln(6/\zeta)}{3|S_{m,ho}|} + \frac{1}{2} \frac{E_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x,a) - f^*(x,a))^2]}{2 (x,a,r) \sim D(p_m)}$$

(55)

We get (52) by rearranging the terms in (55). This completes the proof of showing that (52) holds with probability at least $1 - \zeta / 6$. The same proof with $\hat{g}_M$ instead of $g_i$ shows that (53) holds with probability at least $1 - \zeta / 6$. Therefore both inequalities hold with probability at least $1 - \zeta / 3$ which completes the proof of Lemma 13.

**Lemma 14.** Suppose Assumption 5 holds. Then with probability at least $1 - \zeta / 3$, we have that:

$$E_{x \sim D_X} E_{a \sim p_m(x)} [(\hat{g}_i(x,a) - f^*(x,a))^2] \leq \min_{j \in [d]} \left( C_0 b_j(p_m) + \xi_j(|S_{m,tr}|, \zeta / (6i)) \right)$$

(56)

$$E_{x \sim D_X} E_{a \sim p_m(x)} [(\hat{g}_M(x,a) - f^*(x,a))^2] \leq \min_{j \in [M]} \left( C_0 b_j(p_m) + \xi_j(|S_{m,tr}|, \zeta / (6M)) \right)$$

(57)

**Proof.** Directly follows from Assumption 5.

To summarize the results of this section, we define the $\mathcal{W}_3$, which is the event where all bounds discussed in this section hold. Following a simple union-bound, we show that $\mathcal{W}_3$ holds with high-probability.

$$\mathcal{W}_3 := \left\{ 45, 46, 52, 53, 56, 57 \right\}.$$

(58)

**Lemma 15.** Suppose Assumption 5 holds. Then with probability at least $1 - \zeta$, we have that the inequalities in $\mathcal{W}_3$ are satisfied.

**Proof.** Follows from Lemma 12 Lemma 13 Lemma 14 and a union bound.

**C.2 Proof of Theorem 4**

In this section, we prove Theorem 4. We start by proving proving parts of this theorem under the high-probability event $\mathcal{W}_3$.

**Lemma 16.** Suppose $\mathcal{W}_3$ holds. Then if $\tau_m \leq \tau_{m,\ast}$, we have that (44) holds.

**Proof.** As $\mathcal{W}_3$ holds, we have:

$$\hat{L}(S_{m,ho}, \hat{g}_i) - \hat{L}(S_{m,ho}, \hat{g}_M) \leq 2 \min_{j \in [d]} \left( C_0 b_j(p_m) + \xi_j(|S_{m,tr}|, \zeta / (6i)) \right)$$

$$\leq 2 \min_{j \in [M]} \left( C_0 b_j(p_m) + \xi_j(|S_{m,tr}|, \zeta / (6M)) \right)$$

Where the first inequality follows from (45). The second inequality follows from (53). And, the third inequality follows from (56), the fact that $m \leq m,\ast$ and $|S_{m,tr}| \leq |S_m|$.

**Lemma 17.** Suppose $\mathcal{W}_3$ holds. Then if (44) holds, we have that (43) does not hold.
Proof. Suppose $\mathcal{W}_3$ holds. Then if (44) holds, we have:
\[
\frac{1}{2} \min_{j \in [i]} b_i(p_m)
\leq \frac{1}{2} \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_i(x,a) - f^*(x,a))^2]
\leq \left( \hat{L}(S_{m, ho}, \hat{g}_i) - \hat{L}(S_{m, ho}, f^*) \right) + \frac{16 \log(6/\zeta)}{3 |S_{m, ho}|}
\leq \left( \hat{L}(S_{m, ho}, \hat{g}_M) - \hat{L}(S_{m, ho}, f^*) \right) + 14 \xi_i(|S_{m, tr}|, \zeta/(6i)) + \frac{14 \log(6/\zeta)}{|S_{m, ho}|}
\leq 2 \mathbb{E}_{(x,a,r) \sim D(p_m)} [(\hat{g}_M(x,a) - f^*(x,a))^2] + 18 \xi_i(|S_{m, tr}|, \zeta/(6i)) + \frac{18 \log(6/\zeta)}{|S_{m, ho}|}
\leq 2 \min_{j \in [M]} \left( C_0 b_j(p_m) + \xi_j(|S_{m, tr}|, \zeta/(6M)) \right) + 18 \xi_i(|S_{m, tr}|, \zeta/(6i)) + \frac{18 \log(6/\zeta)}{|S_{m, ho}|}
\]
Where the first inequality follows from the definition of $b_i(\cdot)$. The second inequality follows from (52). The third inequality follows from (44). The fourth inequality follows from (46), and the last inequality follows from (57).

We now prove Theorem 4. From Lemma 15 we have that $\mathcal{W}_3$ holds with probability at least $1 - \zeta$. Under $\mathcal{W}_3$, when $\tau_m \leq \tau_m^*$, Lemma 16 shows that the condition tested by Algorithm 2 is satisfied – that is, the algorithm does not detect misspecification and outputs False. Under $\mathcal{W}_3$, when (43) holds, then (44) is not satisfied and the algorithm outputs True – that is, the class $\cup_{j \in [i]} \mathcal{F}_j$ was determined to be misspecified. This completes the proof of Theorem 4.

C.3 Understanding Theorem 4

Theorem 4 shows that Algorithm 2 does not detect misspecification for the class $\cup_{j \in [i]} \mathcal{F}_j$ at epoch $m$ when $\tau_m \leq \tau_m^*$. So, this test clearly satisfies Assumption 3 with $\beta_i' = 1$, and can be used along with Mod-IGW. To better understand Theorem 4, we would like to understand when this class is determined to be misspecified.

As we have discussed earlier, if $\cup_{j \in [i]} \mathcal{F}_j$ is well-specified then $\tau_m^*$ is unbounded and Algorithm 2 would not detect misspecification for this class. So it is sufficient to consider the case where $\cup_{j \in [i]} \mathcal{F}_j$ is misspecified. Theorem 4 tells us that, with probability at least $1 - \zeta$, Algorithm 2 will detect misspecification if there is a class index $i' > i$ such that the following holds:
\[
\min_{j \in [i]} b_j(p_m) - 4C_i \min_{j \in [i']} b_j(p_m) > 4\xi_{i'}(|S_{m, tr}|, \zeta/(6i')) + 36 \log(6/\zeta) \frac{36 \log(6/\zeta)}{|S_{m, ho}|}.
\]
Note that the RHS of (59) decreases to zero at the rate given by $O(\xi_{i'}(\tau_m, \delta/(6i'))).$ Hence if $\cup_{j \in [i']} \mathcal{F}_j$ is sufficiently less misspecified compared to $\cup_{j \in [i]} \mathcal{F}_j$ under the distribution induced by any action selection kernels, then the class $\cup_{j \in [i]} \mathcal{F}_j$ will be determined to be misspecified within $O(\xi_{i'}(\tau_m, \delta/(24M^3))^2 i'))$ rounds.

To further simplify the discussion, let us assume that Assumption 1 holds. Further, suppose the estimation rates are given by (5). Recall that this was the setup we considered for Theorem 1. Note that for this setup, Theorem 4 tells us that with probability at least $1 - \zeta$, Algorithm 2 will detect misspecification if the following holds:
\[
\min_{j \in [i]} b_j(p_m) > 12C_i d_{i'} \ln(|S_{m, tr}|) \ln(6i^*/\zeta) + \frac{36 \log(6/\zeta)}{|S_{m, ho}|}.
\]
Therefore, with probability at least $1 - \zeta$, Algorithm 2 determines the class $\cup_{j \in [i]} \mathcal{F}_j$ is misspecified if $\tau_m \geq \Omega(\max_{j \in [i]} d_{i'} / b_j(p_m)).$ Hence, Theorem 1 follows from Theorem 4.

To prove Corollary 1, we must lower bound $\min_{j \in [i]} b_j(p_m)$. Intuitively, one may expect this term to be a problem dependent constant as it is a measure of misspecification for the class $\cup_{j \in [i]} \mathcal{F}_j$. Unfortunately, this may not be the case even when this class is misspecified – that is, even when
$\min_{j \in [n]} B_j > 0$, it may so happen that $\min_{j \in [n]} b_j (p_m)$ goes to zero for large $m$. This is because we may be converging to a policy that makes a misspecified class look well-specified. Such a situation may not occur in practice, and there may be no policy that makes misspecified classes look well-specified on average over the distribution of contexts (Assumption 4). Hence under such conditions, we have that $\min_{j \in [n]} b_j (p_m)$ can be lower bounded by a constant for all epoch $m$. Therefore when Assumption 4 also holds, with probability at least $1 - \zeta$, Algorithm 2 determines the class $\bigcup_{j \in [n]} \mathcal{F}_j$ is misspecified if $\tau_m \geq \tilde{\Omega}(d_{i^*})$.

To complete the proof of Corollary 1 we must also lower bound $\min_{j \in [n]} b_j (p_m)$ when Assumption 4 may not hold. We start by stating and proving Lemma 18 which provides a lower bound on $b_j (p_m)$.

**Lemma 18.** For any model class index $j \in [M]$ and any epoch $m$, we have that:

$$b_j (p_m) \geq \frac{K}{K + \gamma_m} b_j (u)$$

Where $u$ denotes the uniform probability kernel. That is, $u(a|x) = 1/K$ for all $(x, a) \in \mathcal{X} \times \mathcal{A}$.

**Proof.** From the definition of $b_j (p_m)$ (see (3)), we have:

$$b_j (p_m) = \min_{f \in \mathcal{F}_j, x \sim D_X} \mathbb{E} \left[ \sum_{a \in \mathcal{A}} p_m(a|x)(f(x, a) - f^*(x, a))^2 \right]$$

$$\geq \frac{1}{K + \gamma_m} \min_{f \in \mathcal{F}_j, x \sim D_X} \mathbb{E} \left[ \sum_{a \in \mathcal{A}} (f(x, a) - f^*(x, a))^2 \right] = \frac{K}{K + \gamma_m} b_j (u).$$

Where the first inequality follows from the definition of $p_m$ (see (6)).

As the uniform probability kernel $u$ samples all arms at every context with equal probability, we have that $b_j (u) > 0$ if the class $\mathcal{F}_j$ is not well-specified. Therefore we have that:

$$\min_{j \in [n]} b_j (p_m) \geq \frac{K}{K + \gamma_m} \min_{j \in [n]} b_j (u) \geq \tilde{\Omega} \left( \sqrt{\frac{K}{\tau_m}} \right) \geq \tilde{\Omega} \left( \frac{1}{\tau_m} \right)$$

(61)

Note that in (60), the RHS is upper bound by $\tilde{O}(d_{i^*}/\tau_m)$, and now from (61) the LHS of (60) is lower bounded by $\tilde{\Omega}(1/\tau_m)$. Hence, (60) is satisfied if the following holds:

$$\frac{1}{\sqrt{\tau_m}} \geq \tilde{\Omega} \left( \frac{d_{i^*}}{\tau_m} \right)$$

(62)

Recall that we already showed that with probability at least $1 - \zeta$, Algorithm 2 will detect misspecification if (60) holds. Therefore, even when Assumption 4 may not hold, with probability at least $1 - \zeta$, we have that Algorithm 2 will detect misspecification if $\tau_m \geq \tilde{\Omega}(d_{i^*})$. This completes the proof of Corollary 1.

## D Additional Details

### D.1 Bernstein’s Inequality

For completeness, in this section we state a well known form of Bernstein’s inequality, and show that it directly follows from standard Bernstein’s inequality.

**Lemma 19** (Bernstein’s inequality). Let $Z_1, Z_2, \ldots, Z_n$ be i.i.d. random variables with a zero mean. If for all $i$, $\Pr(|Z_i| \leq M) = 1$. Then for any $\delta \in (0, 1)$, with probability at least $1 - \delta$, we have:

$$\sum_{i=1}^{n} Z_i \leq \frac{2M \ln(1/\delta)}{3} + \sqrt{2 \ln(1/\delta) \left( \sum_{i=1}^{n} \mathbb{E}[Z_i^2] \right)}$$

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Proof. From Bernstein’s inequality (see lemma B.9 in Shalev-Shwartz and Ben-David, 2014), for all $t > 0$ we have:

$$\Pr \left[ \sum_{i=1}^{n} Z_i > t \right] \leq \exp \left( - \frac{t^2/2}{Mt/3 + \sum_{i=1}^{n} E[Z_i^2]} \right) \quad (63)$$

We now solve for $t$, by setting the upper bound in (63) to $\delta$.

$$\exp \left( - \frac{t^2/2}{Mt/3 + \sum_{i=1}^{n} E[Z_i^2]} \right) = \delta$$

$$\implies t^2 - \frac{2Mt \ln(1/\delta)}{3} - 2 \ln(1/\delta) \left( \sum_{i=1}^{n} E[Z_i^2] \right) = 0$$

$$\implies t = \frac{M \ln(1/\delta)}{3} + \sqrt{\frac{M^2 \ln^2(1/\delta)}{2} + 2 \ln(1/\delta) \left( \sum_{i=1}^{n} E[Z_i^2] \right)} \quad (64)$$

$$\implies t \leq \frac{2M \ln(1/\delta)}{3} + 2 \ln(1/\delta) \left( \sum_{i=1}^{n} E[Z_i^2] \right)$$

Hence Lemma 19 follows from combining (63) and (64). $\Box$

### D.2 Constructing Estimation Oracle

For completeness, we outline one of many approaches to construct an oracle that achieves the “fast rates” of Assumption 2.

Consider a sequence of classes $\mathcal{F}_1, \mathcal{F}_2, \ldots, \mathcal{F}_i$ with VC subgraph dimensions of $d_1, d_2, \ldots, d_i$ respectively. Consider a probability kernel $p$ and a natural number $n$. Consider $n$ independently and identically drawn samples from the distribution $D(p)$. Let $\hat{f}_j$ be an estimator in $\mathcal{F}_j$ that minimizes empirical squared error loss over the first $\lceil n/2 \rceil$ samples. For any $\zeta \in (0, 1)$, from fairly standard arguments based on local Rademacher complexities (see Theorem 5.2 and example 3 in chapter 5 of Koltchinskii, 2011), with probability $1 - \zeta/(2i)$ we have:

$$\mathbb{E}_{x \sim D_X a \sim p(\cdot|x)} \left[ (\hat{f}_j(x, a) - f^*(x, a))^2 \right] \leq (1 + \epsilon) b_j(p) + O \left( \frac{d_j \ln(n) \ln(i/\zeta)}{n} \right). \quad (65)$$

Where $\epsilon > 0$ is any fixed constant. Now let $\hat{f}$ be an estimator in the set $\{\hat{f}_1, \hat{f}_2, \ldots, \hat{f}_i\}$ that minimizes empirical squared error loss over the remaining $\lfloor n/2 \rfloor$ samples. Again from using the same arguments based on localization (e.g. Mitchell et al., 2009; Koltchinskii, 2011), with probability $1 - \zeta/2$ we have:

$$\mathbb{E}_{x \sim D_X a \sim p(\cdot|x)} \left[ (\hat{f}(x, a) - f^*(x, a))^2 \right]$$

$$\leq (1 + \epsilon') \min_{j \in [i]} \mathbb{E}_{x \sim D_X a \sim p(\cdot|x)} \left[ (\hat{f}_j(x, a) - f^*(x, a))^2 \right] + O \left( \frac{\ln(i/\zeta)}{n} \right). \quad (66)$$

Where $\epsilon' > 0$ is any fixed constant. By combining (65) and (66), with probability $1 - \zeta$, we have:

$$\mathbb{E}_{x \sim D_X a \sim p(\cdot|x)} \left[ (\hat{f}(x, a) - f^*(x, a))^2 \right] \leq (1 + \epsilon)(1 + \epsilon') b_j(p) + O \left( \frac{d_j \ln(n) \ln(i/\zeta)}{n} \right). \quad (67)$$

This completes our outline for the construction of an oracle that satisfies Assumption 2. The approach described here is based on using empirical risk minimization on training and validation sets. Other approaches one could use include aggregation algorithms (see Lecué et al., 2014, and references therein), penalized regression (see relevant chapters in Koltchinskii, 2011; Wainwright, 2019), cross validation, etc.

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6The same approach can be used to construct an oracle that satisfies Assumption 5.

7Note that $\epsilon$ is zero when $\mathcal{F}_j$'s are convex or well-specified.
D.3 Implications for Open Problems

We shed light on two open problems on model selection for contextual bandits.

**Foster et al. (2020b):** Open problem 2 in Foster et al. (2020b) asks for model selection guarantees over a nested sequence of finite classes. In particular, they consider a sequence of finite classes $F_1 \subseteq F_2 \subseteq \cdots \subseteq F_M$ such that some class $F_{i^*}$ is well-specified (Assumption 1). They are looking for contextual bandit algorithms that ensure a regret bound of $O(poly(K,M,\log \log |F_i^*|)T^{\alpha} \log \frac{1}{1-\alpha}|F_{i^*}|)$ for some $\alpha \in [1/2,1)$.

Using techniques outlined in Appendix D.2, one can construct an estimation oracle that satisfies Assumption 5 with estimation rates such that $\xi_i(n,\zeta) = O(ln(\frac{|F_i^*|}{\zeta})/n)$. Hence from Theorem 3, we get a bound of $O(\beta_{i^*-1}\log \log |F_{i^*}| + \sqrt{KT\log(M|F_i^*|\log(T)/\delta)})$ for Mod-IGW with a misspecification test that satisfies Assumption 3.

By additionally assuming Assumption 4, from Theorem 4 we get that Algorithm 2 satisfies Assumption 3 with $\beta_{i^*-1} = O(\log |F_{i^*}|)$. Hence up to a small additive cost, we get near optimal guarantees even when Assumption 3 does not hold.

Even if Assumption 4 does not hold, from Theorem 4 and Lemma 18, we get that Algorithm 2 satisfies Assumption 3 with $\beta_{i^*-1} = O(\log^2 |F_{i^*}|)$. Hence, up to a small additive cost, we get near optimal guarantees even when Assumption 4 does not hold.

**Foster et al. (2019):** Question 1 in the discussion section of Foster et al. (2019) asks if it is possible to achieve a regret bound of $O(\sqrt{d_{i^*}}T)$ (ignoring dependencies on other parameters) for their setup. In particular, they consider a nested sequence of linear classes $F_1 \subseteq F_2 \subseteq \cdots \subseteq F_M$ such that some class $F_{i^*}$ is well-specified (Assumption 1) and the linear feature maps satisfy certain diversity conditions. Here $d_i$ denotes the dimension of the linear class $F_i$.

Under this setup, Foster et al. (2019) provide an algorithm (EstimateResidual) that achieves sub-linear loss estimation. That is, for this setup, they get a rate of $O(\sqrt{d_{i^*}/n})$ instead of the standard $O(d_{i^*}/n)$ rate. Now from Lemma 18 we have that $\min_{j \in [i^*-1]} b_j(p_m) \geq \Omega(\frac{1}{\sqrt{m}})$. Hence, by comparing estimated losses (by EstimateResidual) between successive classes, with high-probability, this procedure will determine $F_{i^*-1}$ to be misspecified when the following holds: (similar to (62))

$$\frac{1}{\sqrt{\tau_m}} \geq \Omega\left(\frac{\sqrt{d_{i^*}}}{\tau_m}\right) \iff \tau_m \geq \Omega(d_{i^*}).$$

Hence $\tau_{i^*-1} \leq \tilde{O}(d_{i^*})$. It is also easy to see that, with high-probability, this test will never wrongly claim that $F_{i^*}$ is misspecified. Therefore from the proof of Theorem 3, we get that Mod-IGW with this misspecification test achieves a regret bound of $\tilde{O}(d_{i^*} + \sqrt{Kd_{i^*}T}) = \tilde{O}(\sqrt{Kd_{i^*}T})$. Hence showing that the price for model selection is negligible under this setup.