Valid Post-Selection Inference in Robust Q-Learning

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Abstract

Constructing an optimal adaptive treatment strategy becomes complex when there are a large number of potential tailoring variables. In such scenarios, many of these extraneous variables may contribute little or no benefit to an adaptive strategy while increasing implementation costs and putting an undue burden on patients. Although existing methods allow selection of the informative prognostic factors, statistical inference is complicated by the data-driven selection process. To remedy this deficiency, we adapt the Universal Post-Selection Inference procedure to the semiparametric Robust Q-learning method and the unique challenges encountered in such multistage decision methods. In the process, we also identify a uniform improvement to confidence intervals constructed in this post-selection inference framework. Under certain rate assumptions, we provide theoretical results that demonstrate the validity of confidence regions and tests constructed from our proposed procedure. The performance of our method is compared to the Selective Inference framework through simulation studies, demonstrating the strengths of our procedure and its applicability to multiple selection mechanisms.
1 Introduction

It can be difficult to construct desirable adaptive strategies in the presence of a large number of potential tailoring variables. Often, it is important to encourage sparsity in the estimated rule through some form of variable selection. The statistical community has long recognized that the advantages of sparsity are introduced at the cost of complicating classical statistical inference. Classical inference frameworks fail to accommodate selection because of bias that is introduced by only performing inference on those variable coefficients which are estimated to be further away from zero than others (Leeb and Pötscher 2005, 2008; Berk et al. 2013). Several authors have proposed techniques that address this issue. For a recent review of this body of work, see Kuchibhotla et al. (2020), who motivate the study of post-selection inference as a response to the replicability crisis in the sciences. Additional motivation for this perspective is provided in Benjamini (2020).

Typical formulations cast the problem of estimating an optimal strategy as one in which a “best” strategy is targeted among some class. An optimum is estimated either directly, as in direct-policy methods, or through outcome modeling algorithms such as Q-learning (Zhao et al. 2015; Schulte et al. 2014; Zhao et al. 2012; Murphy 2003). One strength of such methods is that the concepts of reward or utility can be used to balance patient outcomes with other considerations, such as side effects. Although tradeoffs may be evaluated with respect to individual patients, other factors may be relevant when comparing decision rules. For example, some rules may differ in the cost or difficulty to implement in practice.

Sparsity may be one factor to weigh when comparing multiple strategies. For example, when comparing two decision rules with very similar performance in terms of patient utility, the rule which uses fewer tailoring variables might be preferred. This is because the comparatively sparse rule may reduce the cost of individualized treatment by eliminating variables that are costly to measure and only slightly improve expected patient utility (Flores et al. 2013). This can also reduce the burden on future patients when collecting such information is invasive. Additionally, the future performance of the sparse rule may be improved relative to the non-sparse rule by increased precision and elimination of spurious or weak predictors (Lu et al. 2013). When the in-sample estimates of patient utility are relatively similar between these two rules, these other considerations might lead an analyst to prefer the sparse rule.

A complication for outcome-modeling methods such as Q-learning is the role of confounding in the outcome model. The form of the decision rules in Q-learning do not depend on the full outcome model, but on the so-called “blip” (Robins 2004; Robins et al. 2008) or “contrast” function (Zhang et al. 2012; Schulte et al. 2014). Motivated in part by this fact, Ertefaie et al. (2021) proposed the Robust Q-learning algorithm as a method to focus inference on projections of the blip function by leveraging the Robinson-Speckman transformation (Robinson 1988; Speckman 1988) in a two-stage treatment decision setting.

Our contributions in this paper take place in this framework for targeting finite-dimensional treatment strategies. Although alternative algorithms have been proposed for learning the unrestricted optimal strategy (Zhao et al. 2012; Zhang et al. 2012; van der Laan and Luedtke 2015), we have four reasons for focusing on such strategies: (1) these finite-dimensional models lead to more interpretable and understandable decision rules; (2) effect modifier selection may be performed via existing methods; (3) the targeted parameters have a valid causal interpretation in terms of the conditional average treatment effect; and (4) the class of
parametric rules, while not necessarily containing an optimal rule, may nonetheless result in rules with competitive value while providing parametric rates of convergence and better finite-sample efficiency.

Data-driven selection of tailoring variables has received some recent attention. Wallace et al. (2019) developed an information criterion for the G-estimation framework, although such methods do not scale well with dimension. Lu et al. (2013) proposed an adaptive lasso technique in the A-learning setting (Schulte et al., 2014), while Bian et al. (2021) introduced a Lasso-type penalty in the framework of Wallace and Moodie (2015). One benefit of the Robust Q-learning framework is that adapting regression-based selection methods is relatively straightforward, as only the blip model is estimated parametrically. As will be discussed in Section 4.2, this framework allows many common selection techniques to be applied. Additionally, and in contrast to the method of Wallace and Moodie (2015), this framework does not require a correctly-specified blip function in order to target a meaningful projection of the blip function. This result will be further explored in Section 3.2.

Although selection may be easily applied, several complications prevent a straightforward application of existing post-selection inference techniques. The backwards-recursive nature of the problem means that the first-stage estimation problem depends on the model used in the second stage. This implies that existing methods based on selective likelihood ratios and related methods in regression contexts (e.g., Lee et al., 2016; Tian and Taylor, 2017; Tibshirani et al., 2018) do not account for the second-stage model selection event. Additionally, these methods in practice make restrictive assumptions regarding the homogeneity of the underlying error distribution, which in general will not hold in the first stage due to the estimation of the pseudo-outcome. A third complication is that the design of many approaches is generally considered fixed, (the previously-listed methods, plus Berk et al., 2013; Fithian et al., 2014). This has consequences for the implied target parameter and inferential framework, as we will see in Section 6. The final complication is that the asymptotic behavior of the Robust Q-learning estimators has only been characterized when the models are non-random.

In Section 2, we establish some general notation and frame the general adaptive strategy estimation problem. In Section 3 we review the Robust Q-learning algorithm as it occurs for fixed, non-random models and establish some more specialized notation around these concepts. The method for cross-fitting and the perturbation bootstrap are also discussed. We also formally define the model selection problem in the context of adaptive strategies in Section 4 along with the complications this creates in terms of the pseudo-outcome, target rules, subspaces, and parameters due to the backward-inductive nature of the problem. The strengths of the Robust Q-learning algorithm in terms of the general model selection problem are also presented. We provide a discussion of our novel result that cross-fitting behaves uniformly over all models of bounded sparsity, so that model selection may occur alongside nuisance parameter estimation with some asymptotic guarantees.

In Sections 5 and 6 Universal Post-Selection Inference (Kuchibhotla et al., 2020) hereafter referred to as “UPoSI”) is generalized to Robust Q-learning. Section 5 derives the most general case, in which the randomness of the design is acknowledged. In addition to generalizing the UPoSi methods, an amendment to the confidence intervals proposed by Kuchibhotla et al. (2020) is introduced which uniformly shortens their length without impacting their post-selection inference guarantees. The perturbation bootstrap is also discussed in relation to this multi-stage problem. The theoretical properties of the proposed methods are established
under some relatively mild assumptions. We close the section with a brief discussion that motivates the study of the fixed-design framework.

This alternative framework is derived in Section 6 with a characterization of the fixed-design targets, along with a UPoSI-based method for providing inference for such parameters. We contrast the population-level parameters derived throughout the earlier sections and the “fixed-design” targets considered throughout many other post-selection inference methods. We also adapt our theoretical results to such an inferential framework and prove the fixed-design versions of the previous results.

We illustrate these ideas through simulation studies and examine the ability of different methods to provide statistically valid inference for the targeted rule parameters in Section 7. Comparisons are drawn between the coverage properties guaranteed by each method. The performance of each method in terms of confidence interval length is also explored.

## 2 Notation and Problem Statement

Suppose that we observe $n$ i.i.d. trajectories of $O := (X_1, A_1, X_2, A_2, Y)$ from an unknown distribution $P_0$. For each stage $\ell = 1, 2$, the candidate tailoring variables $X_\ell \in X_\ell \subseteq \mathbb{R}^{a_\ell}$ are assumed to precede the Stage $\ell$ binary treatment, $A_\ell \in \mathcal{A}_\ell := \{0, 1\}$, and $Y$ represents the continuous outcome observed after both stages. It is convenient to collect all of the history preceding $A_\ell$ into the variable $\bar{X}_\ell$, so that $\bar{X}_2 := (X_1^\top, A_1, X_2^\top)^\top$ and $\bar{X}_1 := X_1$. These take values in $\bar{X}_2 := X_1 \times A_1 \times X_2$ and $\bar{X}_1 := X_1$, respectively.

Let $Y^*(a_1, a_2)$ denote the potential outcome of $Y$ if the treatments are set to $\{A_1 = a_1, A_2 = a_2\}$. We make the commonly used assumptions for studying causal effects: stable unit treatment value assumption and positivity assumption (Rubin, 1978; Robins, 1986, 1989). To accommodate the longitudinal nature of the data, we additionally assume sequential ignorability at each stage given $\bar{X}_\ell$ (Robins et al., 2000; Murphy, 2003), with treatment propensity $\mu_{A_0}(\bar{x}_\ell) := \mathbb{E}(A_\ell | \bar{X}_\ell = \bar{x}_\ell)$. Let $d_\ell(\cdot) \in \mathcal{D}_\ell$ be a decision rule that maps observed history to treatment at Stage $\ell$, formalized as a map $\bar{X}_\ell \mapsto \mathcal{A}_\ell$, with $\mathcal{D}_\ell$ the set of all such rules. An adaptive strategy is a collection $\tilde{d} = (d_1, d_2) \in \mathcal{D} := \mathcal{D}_1 \times \mathcal{D}_2$ of these maps which consequently maps any trajectory to a sequence of treatments.

Assuming that higher outcomes are more desirable, we are interested in strategies that maximize expected future outcomes. We call the function $V : \mathcal{D} \mapsto \mathbb{R}$ defined as $V(\tilde{d}) := \mathbb{E}\{Y^*(\tilde{d})\}$ the value function. A value-optimal strategy optimizes this objective—i.e., $d_{opt} \in \arg\max_{d \in \mathcal{D}} V(d)$. Using a backwards induction argument, Q-learning proceeds by writing the optimal Stage 2 decision rule as

$$d_{opt}^2(\bar{x}_2) \in \arg\max_{a \in \{0, 1\}} \mathbb{E}\{Y^*(A_1, a) | \bar{X}_2 = \bar{x}_2\}$$

$$= \arg\max_{a \in \{0, 1\}} \mathbb{E}\{Y^*(A_1, 0) + a\{Y^*(A_1, 1) - Y^*(A_1, 0)\} | \bar{X}_2 = \bar{x}_2\}$$

$$= \arg\max_{a \in \{0, 1\}} \{\eta_2^*(\bar{x}_2) + a\Delta_2^*(\bar{x}_2)\}.$$
We will also restrict the set of submodels being studied in each stage to only those submodels with a certain level of sparsity; we will use the notation...

\[ \Delta_{2}^{*}({\bar{x}}_{2}) = \mathbb{E}\left\{ Y^{*}(A_{1}, 1) - Y^{*}(A_{1}, 0) \big| {\bar{X}}_{2} = {\bar{x}}_{2} \right\}, \]

and, consequently, \( d^{*}_{2}({\bar{x}}_{2}) := 1\{\Delta_{2}^{*}({\bar{x}}_{2}) > 0\} \) maximizes \( V(\mu_{1,0}, d_{2}) \) in \( d_{2} \in D_{2} \), where we view the data-generating propensity \( \mu_{1,0} \) also as a stochastic decision rule.

This argument may be followed again in the first stage in order to find the optimal strategy. If \( Y^{*}(A_{1}, d^{*}_{2}) \) were known, then we might again decompose

\[
d^{*}_{1}(\bar{x}_{1}) \in \arg\max_{a \in \{0,1\}} \mathbb{E}\left\{ Y^{*}(a, d^{*}_{2}) \big| {\bar{X}}_{1} = \bar{x}_{1} \right\}
\]

\[
\equiv \arg\max_{a \in \{0,1\}} \left\{ \eta_{1}^{*}(\bar{x}_{1}) + a\Delta_{1}^{*}(\bar{x}_{1}) \right\},
\]

for \( \Delta_{1}^{*}(\bar{x}_{1}) \equiv \mathbb{E}\{ Y^{*}(1, d^{*}_{2}) - Y^{*}(0, d^{*}_{2}) \big| {\bar{X}}_{1} = \bar{x}_{1} \} \).

This algorithm results in a \( d^{*} = (d_{1}^{*}, d_{2}^{*}) \) with maximal value (Watkins and Dayan, 1992; Chakraborty and Moodie, 2013; Butler et al., 2018; Nahum-Shani et al., 2012).

The observed data in \( \bar{X}_{\ell} \) defines a maximal amount of information which can be used for treatment decisions at Stage \( \ell \). In this work, we will consider sparse linear models as working models for the contrast functions. We may consider the \( p_{\ell} \)-dimensional vector \( \bar{X}_{\ell}^{0} \) to be a fixed-dimensional transformation of the vector \( \bar{X}_{\ell} \), such that \( \bar{X}_{\ell}^{0} \) is fixed when conditioning upon \( \bar{X}_{\ell} \). If an analyst decides \textit{a priori} on a dictionary of possible terms to include in a working model (e.g. all main effects and one-way interactions), we may view such a dictionary as a “full model” represented through the entire vector \( \bar{X}_{\ell}^{0} \) in each stage. Submodels are created by subsetting this full vector. We may identify this subsetting operation with the indices of \( \bar{X}_{\ell}^{0} \) used to create the sub-vector. That is, the “full model” at Stage \( \ell \) may be identified with the object \( S_{\ell}^{F} := \{1, \ldots, p_{\ell}\} \) and submodels of \( S_{\ell}^{F} \) are those sets \( S_{\ell} \subseteq S_{\ell}^{F} \). The maximal set of all possible submodels is given by the power set \( M_{\ell} := \{S_{\ell} : S_{\ell} \subseteq S_{\ell}^{F}\} \). We will also restrict the set of submodels being studied in each stage to only those submodels with a certain level of sparsity; we will use the notation \( M_{\ell}(C_{\ell}) := \{S_{\ell} \in M_{\ell} : |S_{\ell}| \leq C_{\ell}\} \) to represent the set of all \( C_{\ell} \)-sparse models based on the data in \( \bar{X}_{\ell}^{0} \).

We will often use the notation of \( S_{\ell} \in M_{\ell} \) to refer to an arbitrary (fixed) submodel. That is, \( S_{\ell} \) represents a particular specification of the elements of \( \bar{X}_{\ell}^{0} \) that will be used to assess effect modification and thereby tailor future treatment. A data-dependent model will be denoted as \( \hat{S}_{\ell} \). Let \( A(S_{\ell}) \) represent a sub-matrix or sub-vector of \( A \) corresponding to the model indices \( S_{\ell} \). For example, when \( \bar{X}_{1}^{0} \) is a column vector of dimension 5 and \( S_{1} = \{1, 2\} \), then \( \bar{X}_{1}^{0}(S_{1}) \) represents the 2-dimensional sub-vector of \( \bar{X}_{1}^{0} \) constructed from the first two elements of \( \bar{X}_{1}^{0} \). Similarly, if \( A \) is a \( 5 \times 5 \) real matrix, \( A(S_{1}) \) represents the \( 2 \times 2 \) sub-matrix of \( A \) with entries corresponding to first two rows and columns. Based on the description of \( M_{\ell} \), we may think of any \textit{a priori}-specified model \( S_{\ell} \in M_{\ell} \) as representing the set of indices \( j \) corresponding to the covariates \( \bar{X}_{\ell}^{0}(\{j\}) \) to be included in said model; that is, the component \( \bar{X}_{\ell}^{0}(\{j\}) \) is included in the linear predictor under model \( S_{\ell} \) if and only if \( j \in S_{\ell} \).

Several norms will be of use. For vectors or column matrices, we use \( \| \cdot \|_{q} \) to represent the \( \ell_{q} \) norm. For real square matrices, we will use \( \| \cdot \|_{\infty} \) to represent the maximal element of the matrix. We will also make use of the \( L_{2}(P_{0}) \) norm for random functions: \( \| h \|_{P_{0},2} = \{ \mathbb{E}_{P_{0}} h^{2} \}^{1/2} \).
Additionally, we will denote the minimal and maximal eigenvalues of a matrix $A$ by $\lambda_{\min}(A)$ and $\lambda_{\max}(A)$, respectively. We will also use the shorthand $a \vee b$ and $a \wedge b$ to represent the minimum and maximum, respectively, of the scalar variables $a$ and $b$.

### 3 Robust Q-learning with Fixed Submodels

This section will serve as an overview and exposition for the Robust Q-learning technique in the situation where the specification of the linear models for the contrast functions are \textit{a priori} fixed—i.e., the case where $S_1$ and $S_2$ are nonrandom. The notation introduced in this section will define several quantities related to the Robust Q-learning technique for different levels of knowledge: full knowledge of the conditional expectations (which we will refer to as “oracle”), complete knowledge of the data-generating distribution (which we call “population”), and complete ignorance, which will be ameliorated by the use of cross-fitting. Additionally, we will propose a perturbation bootstrap technique which will prove useful for handling the post-selection inference problem we discuss in a later section. We can envision the perturbation bootstrap at any of these levels of knowledge. As such, our notation will reflect this fact. In general, quantities overset by a $\sim$ will represent the oracle level of knowledge, quantities subscripted by zero will relate to the population, and “hatted” quantities will relate to cross-fitting. The application of the perturbation bootstrap to either the oracle or cross-fitting situations will involve a superscript $b$ along with either a superscript $\sim$ or $\wedge$.

#### 3.1 The Centering Approach in Two Stages

The binary treatments considered here result in a saturated nonparametric model:

$$Y = \eta_2(\bar{X}_2) + A_2\Delta_2(\bar{X}_2) + \varepsilon_2, \quad (1)$$

where $\mathbb{E}(\varepsilon_2 | \bar{X}_2, A_2) = 0$. The function $Q_2(\bar{x}_2, a_2) = \mathbb{E}(Y | \bar{X}_2 = \bar{x}_2, A_2 = a_2)$ is decomposed by the functions $\eta_2(\bar{x}_2) = Q(\bar{x}_2, 0)$ and $\Delta_2(\bar{x}_2) = Q(\bar{x}_2, 1) - Q(\bar{x}_2, 0)$. The previous causal assumptions imply for any $\bar{x}_2 \in \bar{X}_2$ that $\Delta_2(\bar{x}_2) \equiv \Delta_2^{*}(\bar{x}_2)$ and $\eta_2(\bar{x}_2) \equiv \eta_2^{*}(\bar{x}_2)$, so that optimization of expected potential outcomes is accomplished through study of $\Delta_2(\bar{x}_2)$.

This contrast function is a value-optimal basis for making optimal treatment decisions for future patients. The usual approach to Q-learning imposes models on both the $\eta_2$ and $\Delta_2$ functions. For example, linear parametric models are commonly used as a class of functions for the treatment-free outcome model. However, the validity of this approach relies heavily on the accuracy of the $\eta_2$ model. It would be preferable if the latter did not affect interpretations of the targeted decision rules, since it is irrelevant to the fundamental problem.

The Robust Q-learning algorithm [Ertefaie et al., 2021] applies the Robinson-Speckman transformation (Robinson, 1988; Speckman, 1988) to Q-learning. In particular, these authors re-express the model (1) in its equivalent centered form to find:

$$Y - \mu_{2Y0}(\bar{X}_2) = \{ A_2 - \mu_{2A0}(\bar{X}_2) \} \Delta_2(\bar{X}_2) + \varepsilon_2, \quad (2)$$

where $\mu_{2Y0}(\bar{x}_2) := \mathbb{E}(Y | \bar{X}_2 = \bar{x}_2)$ and $\mu_{2A0}(\bar{X}_2)$ is the propensity defined in Section 2. This model exhibits a number of features. First, the explicit dependence upon the treatment-free
outcome model $\eta_{2}(\bar{X}_{2})$ is eliminated by introducing the conditional expectations $\mu_{2A0}$ and $\mu_{2Y0}$. Second, the residual $\varepsilon_2$ is the same as that of the saturated model (1) since no assumptions have yet been placed on the data-generating distribution. Further, the mean functions $\mu_{2A0}$, $\mu_{2Y0}$ are relatively easy to estimate and are disentangled from the contrast model. If $\mu_{2Y0}$ and $\mu_{2A0}$ were known exactly, an analyst could impose a blip model, say $X_2^\top \theta_2$. If we additionally require that the model only makes use of the data in $S_2 \in M_2(C_2)$, then we could express the equation as

$$ Y - \mu_{2Y0}(X_2) = \{A_2 - \mu_{2A0}(X_2)\} \bar{X}_2^0(S_2)^\top \theta_{20,S_2} + \varepsilon_{2,S_2}, $$

(3)

$$ \varepsilon_{2,S_2} = \varepsilon_2 + \{A_2 - \mu_{2A0}(\bar{X}_2)\} \{\Delta_2(\bar{X}_2) - \bar{X}_2^0(S_2)^\top \theta_{20,S_2}\}, $$

(4)

where $\theta_{20,S_2}$ is a non-random population-level parameter which is defined in (13) in Section 3.2. In this case, the imposition of a model for $\Delta_2$ as well as the selection of a particular $S_2$ induces a change in the residuals. Nonetheless, these residuals are uncorrelated with any function of $\bar{X}_2$, which can be seen by applying expectations that condition on $\bar{X}_2$ to both sides of (4). This verifies the property $\mathbb{E}(\varepsilon_{2,S_2} \mid \bar{X}_2) = 0$ for any $S_2 \in M_2(C_2)$.

Mimicking the backwards induction argument of the previous section, we may define:

$$ Y_{1|S_2} := Y + \xi \{A_2, \bar{X}_2^0(S_2); \theta_{20,S_2}\} $$

(5)

$$ \xi(a_2, x; \theta) := x^\top \theta \{1(x^\top > 0) - a_2\}, $$

(6)

and then apply similar arguments to arrive at the first-stage models:

$$ Y_{1|S_2} - \mu_{Y1S_20}(\bar{X}_1) = \{A_1 - \mu_{1A0}(\bar{X}_1)\} \Delta_{1,S_2}(\bar{X}_1) + \varepsilon_{1,S_2} $$

(7)

$$ Y_{1|S_2} - \mu_{Y1S_20}(\bar{X}_1) = \{A_1 - \mu_{1A0}(\bar{X}_1)\} \bar{X}_1^0(S_1)^\top \theta_{10,S_1,S_2} + \varepsilon_{1,S_1,S_2}, $$

(8)

where the error $\varepsilon_{1,S_2}$ obeys $\mathbb{E}(\varepsilon_{1,S_2} \mid \bar{X}_1, A_1) = 0$ and $\varepsilon_{1,S_1,S_2}$ has a representation similar to (4). Similar logic as in the second stage case may be employed to verify that the model-based residuals satisfy $\mathbb{E}(\varepsilon_{1,S_2} \mid \bar{X}_1) = 0$ for all $S_1 \in M_1(C_1)$, $S_2 \in M_2(C_2)$. The blip function $\Delta_{1,S_2}(\bar{X}_1):= \mathbb{E}(Y_{1S_2} \mid \bar{X}_1, A_1 = 1) - \mathbb{E}(Y_{1S_2} \mid \bar{X}_1, A_1 = 0)$ in (7) represents the contrast in outcomes from different first stage treatments. Finally, note that the second-stage model $S_2$ impacts the pseudo-outcome $Y_{1|S_2}$ and its corresponding conditional expectation $\mu_{Y1S_20}(\bar{X}_1)$, which will go on to influence our derivation of the first-stage quantities.

### 3.2 The Submodel Parameters and their Oracle Estimators

In this section, we explore how estimation could proceed if the conditional expectation functions were known. Such estimation might start from the least-squares objective function, which for any $S_2 \in M_2$ may be viewed as a random function of an $\mathbb{R}^{|S_2|}$—valued argument:

$$ R_{2n,S_2}(\theta_{2,S_2}) := \frac{1}{n} \sum_{i=1}^{n} \left[ Y_i - \mu_{2Y0}(\bar{X}_{2i}) - \{A_2 - \mu_{2A0}(\bar{X}_{2i})\} \bar{X}_{2i}^0(S_2)^\top \theta_{2,S_2}\right]^2. $$

(9)

In this expression, $\theta_{2,S_2}$ is a free parameter to the function $R_{2n,S_2}$ with dimension depending on the size of $S_2$. This function is convex and has a minimizer depending on its quadratic behavior. This objective function is equivalent, up to a constant, to

$$ R_{2n,S_2}(\theta_{2,S_2}) - R_{2n,S_2}(0) = -2 \bar{G}_{2n}(S_2)^\top \theta_{2,S_2} + \theta_{2,S_2}^\top \bar{H}_{2n}(S_2) \theta_{2,S_2}, $$

(10)
which makes use of the following quantities related to the gradient and Hessian:

\[
\begin{align*}
\tilde{G}_{2n} & := \frac{1}{n} \sum_{i=1}^{n} \left\{ A_{2i} - \mu_{2A0}(\bar{X}_{2i}) \right\} \left\{ Y_i - \mu_{2Y0}(X_{2i}) \right\} X_{2i}^0 \\
\tilde{H}_{2n} & := \frac{1}{n} \sum_{i=1}^{n} \left\{ A_{2i} - \mu_{2A0}(\bar{X}_{2i}) \right\}^2 (X_{2i}^0)^\otimes 2.
\end{align*}
\]  

(11)

Notice that the choice of model \(S_2\) only serves to subset the full vector \(\tilde{G}_{2n}\) and matrix \(\tilde{H}_{2n}\)—i.e., the choice of model impacts the minimand through subsetting operations. The representation \([10]\) recovers the normal equations for least-squares estimators by equating the gradient of the LHS to the \(|S_2|\)-dimensional zero vector. For example, the oracle estimator \(\tilde{\theta}_{2n,S_2}\), which leverages knowledge of the true \(\mu_{2Y0}\) and \(\mu_{2A0}\) functions, satisfies

\[
0 = \tilde{G}_{2n}(S_2) - \tilde{H}_{2n}(S_2)\tilde{\theta}_{2n,S_2}.
\]

(12)

Taking the expectation of the \(R_{2n,S_2}\) translates the empirical squared-error criterion into its population analogue. The best-fitting population parameter, \(\theta_{20,S_2}\), minimizes this expected error. As such, we apply similar arguments: taking expectations on both sides of \([10]\) and using the gradient argument, the parameter \(\theta_{20,S_2}\) satisfies

\[
0 = G_{20}(S_2) - H_{20}(S_2)\theta_{20,S_2},
\]

(13)

where the components \(G_{20}\) and \(H_{20}\) of the quadratic function are defined as

\[
\begin{align*}
G_{20} & := \mathbb{E} \left[ \left\{ A_2 - \mu_{2A0}(\bar{X}_2) \right\}^2 \Delta_2(X_2)X_2^0 \right] \\
H_{20} & := \mathbb{E} \left[ \left\{ A_2 - \mu_{2A0}(\bar{X}_2) \right\}^2 (X_2^0)^\otimes 2 \right].
\end{align*}
\]

(14)

The subsetting due to \(S_2\) has an analogous impact on \([13]\) as in \([12]\).

There is some additional complication arising due to the pseudo-outcome in the first stage. Specifically, \([5]\) depends upon an unknown target parameter \(\theta_{20,S_2}\). In the oracle setting where all the conditional expectations are known, we could use \(\tilde{\theta}_{2n,S_2}\) as the parameter for the blip function \([6]\) to define the pseudo outcome \(\tilde{Y}_{1,S_2}\). The objective function in Stage 1 for a pair of models \(S_1\) and \(S_2\) is a function of an \(\mathbb{R}^{|S_1|}\)-valued argument, taking the form

\[
R_{1n,S_1S_2}(\theta_{1,S_1}) := \frac{1}{n} \sum_{i=1}^{n} \left( \tilde{Y}_{1S_2i} - \mu_{1YS_20}(\bar{X}_{1i}) - \{ A_{1i} - \mu_{1A0}(\bar{X}_{1i}) \} X_{1i}^0(S_1)^\top \theta_{1,S_1} \right)^2
\]

(15)

Identical arguments as in the second-stage case lead to the following representation:

\[
R_{1n,S_1S_2}(\theta_{1,S_1}) - R_{1n,S_1S_2}(0) = -2G_{1n,S_2}(S_1)^\top \theta_{1,S_1} + \theta_{1,S_1}^\top H_{1n}(S_1)\theta_{1,S_1}.
\]

(16)

Consequently, the oracle estimator \(\tilde{\theta}_{1n,S_1S_2}\) and population minimizer \(\theta_{10,S_1S_2}\) each satisfy

\[
0 = \tilde{G}_{1n,S_2}(S_1) - \tilde{H}_{1n}(S_1)\tilde{\theta}_{1n,S_1S_2},
\]

(17)

\[
0 = G_{10,S_2}(S_1) - H_{10}(S_1)\theta_{10,S_1S_2}.
\]

(18)
The vectors and matrices in these expressions take the forms presented below:

\[
\tilde{G}_{1n,S_2} := \frac{1}{n} \sum_{i=1}^{n} \left\{ A_{1i} - \mu_{1A0}(\tilde{X}_{1i}) \right\} \left\{ \hat{Y}_{1i} - \mu_{1Y_{S_0}}(\tilde{X}_{1i}) \right\} \tilde{X}_{1i}^0
\]

\[
\tilde{H}_{1n} := \frac{1}{n} \sum_{i=1}^{n} \left\{ A_{1i} - \mu_{1A0}(\tilde{X}_{1i}) \right\}^2 \left( \tilde{X}_{1i}^0 \right)^{\otimes 2}
\]

\[
G_{1n,S_2} := \mathbb{E} \left[ \left\{ A_{1} - \mu_{1A}(\tilde{X}_{1}) \right\} \Delta_{1,S_2}(\tilde{X}_{1}) \tilde{X}_{1}^0 \right]
\]

\[
H_{10} := \mathbb{E} \left[ \left\{ A_{1} - \mu_{1A0}(\tilde{X}_{1}) \right\}^2 \left( \tilde{X}_{1}^0 \right)^{\otimes 2} \right].
\]

Because of the dependence of the pseudo-outcomes on \( S_2 \), the \( p_1 \)-dimensional vectors \( \tilde{G}_{1n,S_2} \) and \( G_{1n,S_2} \) also depend on this model. This is a departure from the second-stage problem, in which the impact of the model \( S_2 \) only serves to subset the vectors \( \tilde{G}_{2n} \) and \( G_{20} \). In other words, the second-stage vector \( \tilde{G}_{2n} \) only serves to subset the vectors \( \tilde{G}_{1n,S_2} \), but the full first-stage vector \( \tilde{G}_{1n,S_2} \) changes based on \( S_2 \), even if the full model \( S_{1}^F \) is used. The latter imposes some additional complexities for inference outside of the fixed-model scenario.

### 3.3 Estimation via Cross-fitting

In practice, the conditional expectations in each stage are nuisance functions that must be estimated. In this section, we describe the \( K \)-fold cross-fitting technique for estimation by general statistical learners. Let \( K \) represent some fixed number of folds and \( \mathcal{P}_K \) represent a partition of \( \{1, \ldots, n\} \) into \( K \) indexing sets of roughly-equal size; i.e. \( \mathcal{P}_K = \{I_k : k = 1, \ldots, K\} \) with \( \bigcup_{k=1}^{K} I_k = \{1, \ldots, n\} \) and \( I_k \cap I_{k'} = \emptyset \) for \( k \neq k' \). Let \( D_I := \{O_i : i \in I\} \) for any indices \( I \). Then using \( I^c \) for the set complement, we write \( D_{I^c} \) to represent the observed data outside of \( I_k \). We demonstrate cross-fitting by applying it to the \( \mu_{2Y_{S_0}}(\cdot) \) function. To estimate the value of this function at \( \tilde{X}_{2i} \), for \( i \in I_k \), use \( \tilde{D}_{I^c_k} \) to train an estimator \( \hat{\mu}_{2Y}(\cdot; \tilde{D}_{I^c_k}) \) for the whole function and obtain a prediction at \( \tilde{X}_{2i} \) for every \( i \in I_k \). Continue changing the held-out fold \( I_k \) until all of the necessary predictions have been made. Because \( \mathcal{P}_K \) is a partition, the sum over \( i = 1, \ldots, n \) may equivalently be written as a double-sum over \( k = 1, \ldots, K \) and \( i \in I_k \).

Employing this cross-fitting strategy, we obtain predictions for each \( k = 1, \ldots, K, \ i \in I_k \) using the trained functions \( \hat{\mu}_{2Y}(\tilde{X}_{2i}; \tilde{D}_{I^c_k}) \) and \( \hat{\mu}_{2A}(\tilde{X}_{2i}; \tilde{D}_{I^c_k}) \). This gives rise to \( \hat{R}_{2n,S_2}(\theta_{2,S_2}) \), which differs from (9) by replacing the unknown functions with their cross-fitted estimates.

For completeness, we can write the expression as

\[
\hat{R}_{2n,S_2}(\theta_{2,S_2}) := \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in I_k} \left[ Y_i - \hat{\mu}_{2Y}(\tilde{X}_{2i}; \tilde{D}_{I^c_k}) - \left\{ A_{2i} - \hat{\mu}_{2A}(\tilde{X}_{2i}; \tilde{D}_{I^c_k}) \right\} \tilde{X}_{2i}^0(S_2)^\top \theta_{2,S_2} \right]^2.
\]

Notice that this function is also a convex, quadratic function in its argument. Consequently, similar arguments as those leading to (10) and (12) establish

\[
\hat{R}_{2n,S_2}(\theta_{2,S_2}) - \hat{R}_{2n,S_2}(0) = -2 \hat{G}_{2n}(S_2)^\top \theta_{2,S_2} + \theta_{2,S_2}^\top \hat{H}_{2n}(S_2) \theta_{2,S_2}
\]

\[
0 = \hat{G}_{2n}(S_2) - \hat{H}_{2n}(S_2) \hat{\theta}_{2n,S_2}.
\]
where the vector $\hat{G}_{2n}$ and matrix $\hat{H}_{2n}$ are defined as

$$
\hat{G}_{2n} := \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in I_k} \bar{X}_{2i}^0 \{ A_{2i} - \hat{\mu}_{2A}(\bar{X}_{2i}; D_{I_k}) \} \{ Y_i - \hat{\mu}_{2Y}(\bar{X}_{2i}; D_{I_k}) \}
$$

$$
\hat{H}_{2n} := \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in I_k} \{ A_{2i} - \hat{\mu}_{2A}(\bar{X}_{2i}; D_{I_k}) \}^2 (\bar{X}_{2i}^0)^\otimes 2.
$$

(23)

With the second-stage estimator $\hat{\theta}_{2n,S_2}$ defined, we move to the first stage. Using $\hat{\theta}_{2n,S_2}$ as the parameter in the blip function [6], we define the pseudo outcome $\hat{Y}_{1S_2}$. Together with the cross-fitted predictions $\hat{\mu}_{1Y,S_2}(\bar{X}_{1i}; D_{I_k})$ and $\hat{\mu}_{1A,S_2}(\bar{X}_{1i}; D_{I_k})$, we obtain a quadratic objective function $\hat{R}_{1n,S_1,S_2}$ with a minimizer $\hat{\theta}_{1n,S_1,S_2}$, both satisfying

$$
\hat{R}_{1n,S_1,S_2}(\theta_{1,S_1}) - \hat{R}_{1n,S_1,S_2}(0) = -2\hat{G}_{1n,S_2}(S_1)^\top \theta_{1,S_1} + \theta_{1,S_1}^\top \hat{H}_{1n}(S_1)\theta_{1,S_1}
$$

$$
0 = \hat{G}_{1n,S_2}(S_1) - \hat{H}_{1n}(S_1)\hat{\theta}_{1n,S_1,S_2},
$$

(24) (25)

where these relationships make use of the following definitions:

$$
\hat{G}_{1n,S_2} := \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in I_k} \bar{X}_{2i}^0 \{ A_{1i} - \hat{\mu}_{1A}(\bar{X}_{1i}; D_{I_k}) \} \{ \hat{Y}_{1S_2i} - \hat{\mu}_{1Y,S_2}(\bar{X}_{1i}; D_{I_k}) \}
$$

$$
\hat{H}_{1n} := \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in I_k} \{ A_{1i} - \hat{\mu}_{1A}(\bar{X}_{1i}; D_{I_k}) \}^2 (\bar{X}_{2i}^0)^\otimes 2
$$

$$
\hat{Y}_{1S_2} := Y + \zeta \{ A_2, \bar{X}_{2}^0(S_2); \hat{\theta}_{2n,S_2} \}.
$$

(26)

3.4 The Perturbation Bootstrap with Cross-fitting

The development of the cross-fitted empirical functions lends itself to a perturbation bootstrap approach. While the perturbation bootstrap has been used as an inference method when tied to specific, nearly unbiased variable selection techniques like the adaptive lasso [Das et al. 2019; Minnier et al. 2011; Zou 2006], we will develop a more general method for post-selection inference that leverages the bootstrap to strongly control false coverages.

To fix ideas, let $\omega \sim P_\omega$ be an analyst-specified random variable satisfying $\mathbb{E}(\omega) = 1$, $\mathbb{E}(\omega - 1)^2 = 1$ with $\omega_1, \ldots, \omega_n$ i.i.d. from $P_\omega$. We create the perturbed oracle and cross-fitted minimands in Stage 2 by multiplying the $i^{th}$ contribution by $\omega_i$ in each of (9) and (20) respectively. Analogous definitions also let us create the perturbed cross-fitted objective function. Representing the components related to the perturbation bootstrap by the superscript $b$, a decomposition similar to (10) yields

$$
\hat{R}_{2n,S_2}^b(\theta_{2,S_2}) - \hat{R}_{2n,S_2}^b(0) = -2\hat{G}_{2n}^b(S_2)^\top \theta_{2,S_2} + \theta_{2,S_2}^\top \hat{H}_{2n}^b(S_2)\theta_{2,S_2},
$$

(27)

where $\hat{G}_{2n}^b$ and $\hat{H}_{2n}^b$ are defined as in (11) but with the multiplier $\omega_i$ included in the sum. The perturbation concept naturally accommodates cross-fitting: let $\hat{R}_{2n,S_2}^b$ represent a similar perturbation of the cross-fitted objective (20), and allow the components $\hat{G}_{2n}^b$ and $\hat{H}_{2n}^b$ be
defined analogously to those in (23) except for the inclusion of the factor \( \omega_i \). These describe the quadratic behavior of \( \bar{R}^b_{2n,S_2} \), which follows from arguments similar to those leading to (21). Consequently, first-order conditions can be derived for \( \bar{\theta}^b_{2n,S_2} \) and \( \hat{\theta}^b_{2n,S_2} \) as minimizers of \( \bar{R}^b_{2n,S_2} \) and \( \hat{R}^b_{2n,S_2} \), respectively.

When moving to the first stage, we must take care to incorporate the bootstrap throughout the second-stage estimation procedure. To do so, we perturb the pseudo outcomes as well: create \( \hat{Y}^{b_1}_{1S_2} \) and \( \hat{Y}^{b_2}_{1S_2} \) by using their respective perturbed parameters \( \hat{\theta}^b_{2n,S_2} \) and \( \bar{\theta}^b_{2n,S_2} \) as the parameters inside (6).

\[
R^b_{1n,S_1S_2}(\theta_{1,S_1}) - R^b_{1n,S_1S_2}(0) = -2 \bar{G}^b_{1nS_2}(S_1)^\top \theta_{1,S_1} + \theta_{1,S_1}^\top \bar{H}^b_{1n}(S_1) \theta_{1,S_1},
\]

with \( \bar{G}^b_{1nS_2} \) and \( \bar{H}^b_{1n} \) analogous to their counterparts in (19) except for the inclusion of the multiplier \( \omega_i \) and the replacement of \( \hat{Y}^{b_1}_{1S_2} \) by \( \hat{Y}^{b_2}_{1S_2} \). Arguing along these lines, we obtain the perturbed objective \( \bar{R}^b_{1n,S_1S_2} \) which uses cross-fitting for the conditional expectations and \( \hat{Y}^{b_2}_{1S_2} \) as the pseudo-outcome. Explicit definitions for these pseudo-outcomes are given in Appendix C.2.

4 Submodel Selection in Robust Q-learning

4.1 Random Subspaces of Decision Strategies

In this section, we will formally define the random model selection problem in the general context of adaptive strategy estimation as it appears in Robust Q-learning.

In Section 2, the goal of adaptive strategy estimation was presented as identifying a decision rule maximizing \( V(d) \) over the space of all rules \( \mathcal{D} := \mathcal{D}_1 \times \mathcal{D}_2 \). It was shown that \( d^*_{\ell}(x_\ell) := \mathbbm{1}\{\Delta^*_{\ell}(x_\ell) > 0\} \) may be used to create the strategy \( d^* = (d^*_1, d^*_2) \) maximizing \( V(d) \) over \( \mathcal{D} \). As discussed in the introduction, the expected value to patients may not be the only objective worth pursuing in estimating a rule, as alternative adaptive strategies might achieve a similar value while requiring less invasive or expensive data collection from the patients. In this situation, we might say that there exists \( d' \) making use of only \( S_1 \) and \( S_2 \), with \( V(d') \approx V(d^*) \). In this scenario, the expected regret of \( d' \) might be considered small in relation to the more pragmatic benefits of sparsity. Consequently, we might consider the optimization as being restricted to the space of rules which make use of only \( S_1 \) and \( S_2 \), if it were known ahead of time which models were likely to yield small regrets.

In practice, analyst may not be able to anticipate which submodels are inferior to the full models. As such, making use of the data to adapt to the underlying distribution is an attractive option. Random model selection is formally described as the random variables \( \hat{S}_1, \hat{S}_2 \) that (i) depend at least in part on the observed data and (ii) take their values in the space \( \mathcal{M}_1 \times \mathcal{M}_2 \). In this interpretation, we may view each \( S_\ell \in \mathcal{M}_\ell \) as a potential realization of the random variable \( \hat{S}_\ell \). Thus, model selection acts to select the “relevant” subspace \( \mathcal{D}_{\hat{S}_1\hat{S}_2} \subset \mathcal{D} \) and targeted parameters \( (\theta_{10,S_1S_2}, \theta_{20,S_2}) \) identifying the optimal strategy in that subspace. Here, we use \( \mathcal{D}_{S_1S_2} \) for any pair of models \( (S_1, S_2) \in \mathcal{M}_1 \times \mathcal{M}_2 \) to represent the set of parametric decision rules that use \( \bar{X}^i_1(S_1) \) in the first stage and \( \bar{X}^0_2(S_2) \) in the second.
As a departure from the fixed-model case, the data-dependent choice of subspace $\mathcal{D}_{\hat{S}_1, \hat{S}_2}$ complicates subsequent inference. For example, consider the implicit definitions of the targets (13) and (18) evaluated at $(S_1, S_2) = (\hat{S}_1, \hat{S}_2)$. These targets have random dimension depending on the selected model. One impact is that the number of tests or intervals to be constructed for each element of the target vector depends on the data. Another is that the thresholding behavior of selection creates non-regular estimators which can be difficult to characterize in terms of asymptotic distribution.

Our presentation of the submodel-restricted subspaces also illuminates a fundamental incompatibility with “full model-based” approaches to inference. That is, the value-optimal decision rule over this subspace does not necessarily map to subsets of the parameters corresponding to the optimal rule in the full space (e.g., subsetting $\theta_{20, \hat{S}_2}$ by $S_2$ does not in general yield the second-stage optimal rule over the $S_2$-based subspace of $\mathcal{D}_2$). Consequently, perspectives of estimation or inference that focus on subsets of a “full parameter”—such as de-biased or de-sparsified approaches (Zhang and Zhang, 2014; Van de Geer et al., 2014)—are not focused on our goal. This motivates our adoption of the “post-selection” viewpoint.

4.2 Selection Techniques in Robust Q-learning

There are many possible approaches to variable selection in regression problems. The Lasso (Tibshirani, 1996) is a popular penalized-regression technique that employs the $\ell_1$ penalty. The geometric structure of the $\ell_1$ penalty encourages sparsity, and thereby performs variable selection while allowing one to simultaneously produce a corresponding coefficient estimate. Indeed, the popularity of the Lasso stems in part from the fact that it can be viewed as an estimation procedure, a model selection procedure, or both. Other penalization methods have also been developed, which seek to overcome certain limitations of the Lasso for variable selection (Fan and Li, 2001; Zou, 2006; Zhang, 2010). Other methods for model selection involve information criteria like AIC or BIC, and directly compare the criteria of several different models to perform selection (Takeuchi, 1976). Stepwise regression procedures are one conceptually simple method for performing selection in this manner, although more sophisticated techniques may be leveraged as well.

Variable selection properties have been well-established in these cases when applied to standard linear models, i.e. without the incorporation of nuisance parameters for the mean estimated by cross-fitting. Ertefaie et al. (2021) established an asymptotically linear representation for the decision rule parameters when the model is fixed. As a result, such estimators have a statistical behavior much like the minimizers of the “oracle least-squares criteria” defined in (9) and (15). The reader might wonder if such results are generalizable to the case where the model is selected. Indeed, Lemma E.11 in Appendix E.4 indicates that the error attributable to cross-fitting vanishes uniformly over models of a bounded sparsity. In an asymptotic sense, this rules out the possibility that certain models could have spurious goodness-of-fit that is driven purely by cross-fitting error. In other words, the impact of cross-fitting can be shown, under conditions to be formalized later in Section 5.3, to have a relatively even impact to the estimators across the possible models. This suggests that many selection techniques which compare different subsets in least-squares settings (e.g., using stepwise procedures to select models) may be asymptotically valid in this setting.

In the UPoSI technique for standard linear regression, almost no restrictions are set on
the model selection technique, other than the requirement that it produce a sufficiently sparse model. Our method inherits a similar agnosticism to the underlying selection method. This allows the selection mechanism employed by the analyst to incorporate constraints in a meaningful way. As an example, the analyst might include in the transformation $X_0^\ell$ at each stage the set of pairwise interactions between predictors along with the corresponding “main effects” terms. After running some selection mechanism, the analyst might wish to enforce that all included interactions are also present alongside their corresponding main effects and manually add the missing main effects to the model. Such an informal technique that encodes these constraints is accommodated by our framework.

In order to extend the theoretical results of UPoSI to Robust Q-learning, we will need to add some slightly stronger restrictions. We will not appeal to an oracle property that requires correctness in the selected model (Fan and Li, 2001; Zou, 2006; Zhao and Yu, 2006). Instead, we merely require that the variability in the model settles in some sense, even if it settles upon an “incorrect” model; see Assumption 5.4. In the previous example involving constraints on interaction terms, if the underlying selection mechanism settles asymptotically, then so does the constraint-enforcing mechanism.

5 UPoSI for Population Parameters

5.1 Adaptation of UPoSI to Robust Q-learning

The UPoSI procedure was presented in Kuchibhotla et al. (2020) as an assumption-lean approach for performing inference on parameters after selection. In this framework, the post-selection inference problem is formulated as providing coverage guarantees for confidence regions that are constructed for parameters, like those defined in (13), after a random model selection event takes place. Unlike selective inference methods (Fithian et al., 2014; Lee et al., 2016), the UPoSI framework is agnostic to the specific random model selection mechanism. This is convenient in light of the myriad options presented in Section 4.2.

The UPoSI regions are derived by examining the post-selection inference problem through the lens of simultaneous inference. To retain focus, more detail on this perspective is given in Appendix B. The regions are constructed on the basis of inequalities that provide a deterministic, simultaneous bound on the stochastic deviations of the post-selection parameters about their respective targets. We complete this section by generalizing the arguments of Kuchibhotla et al. (2020) to the Robust Q-learning setting.

Fix any pair of models $S_1 \in \mathcal{M}_1$ and $S_2 \in \mathcal{M}_2$. Then the following inequalities hold deterministically by simply adding and subtracting components of the empirical and expected versions of the normal equations and using elementary inequalities:

$$\|\hat{H}_{2\text{n}}(S_2)\{\theta_{2n,S_2} - \theta_{20,S_2}\}\|_\infty \leq D_{2\text{n}}^G + D_{2\text{n}}^H\|\theta_{20,S_2}\|_1$$
$$\|\hat{H}_{1\text{n}}(S_1)\{\theta_{1n,S_1S_2} - \theta_{10,S_1S_2}\}\|_\infty \leq D_{1\text{n},S_2}^G + D_{1\text{n}}^H\|\theta_{10,S_1S_2}\|_1.$$  (29, 30)

The quantities on the RHS are related to components defined in Section 3.3:

$$\hat{D}_{2\text{n}}^G := \|\hat{G}_{2\text{n}} - G_{20}\|_\infty, \quad \hat{D}_{2\text{n}}^H := \|\hat{H}_{2\text{n}} - H_{20}\|_\infty, \quad \hat{D}_{1\text{n}}^G := \|\hat{G}_{1\text{n},S_2} - G_{10,S_2}\|_\infty, \quad \hat{D}_{1\text{n}}^H := \|\hat{H}_{1\text{n}} - H_{10}\|_\infty.$$  (31)
The original application of Kuchibhotla et al. (2020) created coordinate-wise confidence intervals by creating the smallest hyperrectangle that enclosed the UPoSI confidence regions. If we were to directly apply this to, say, the second stage parameter vector, we would create confidence intervals of the form $\hat{\theta}_{2n,S_2 \setminus \{j\}} \pm \tilde{L}^\dagger_{2j|S_2}$, where $e_j$ is a column vector of zero with a 1 in the $j^{th}$ index, and

$$\tilde{L}^\dagger_{2j|S_2} := \left\| e_j \left\{ \hat{H}_{2n}(S_2) \right\}^{-1} \right\|_1 \left\{ C^G_{2n}(\alpha) + C^H_{2n}(\alpha) \right\} \|\hat{\theta}_{2n,S_2}\|_1.$$

However, a drawback of this approach is that the first factor multiplying the critical value in braces may grow with $|S_2|$, since it represents the $\ell_1$ norm of the $j^{th}$ row of $\left\{ \hat{H}_{2n}(S_2) \right\}^{-1}$. Each of the $|S_2| - 1$ off-diagonal elements which are nonzero add to the size of the interval.
We propose the confidence intervals with half-length for any $S_2 \in \mathcal{M}_2$ given by

$$
\hat{L}_{2jS_2} := \left| e_j^\top \left\{ \hat{H}_{2n}(S_2) \right\}^{-1} e_j \right| \left\{ C_{2n}^G(\alpha) + C_{2n}^H(\alpha) \| \hat{\theta}_{2n,S_2} \|_1 \right\}. \tag{36}
$$

Compared to (35), the confidence interval length (36) is likely to be much smaller, and is equivalent when the $j^{th}$ row of the inverted matrix $\left\{ \hat{H}_{2n}(S_2) \right\}^{-1}$ is a zero vector with a non-zero element in the $j^{th}$ position. When this condition does not hold, the interval length $\hat{L}_{2jS_2}$ is strictly smaller than $\hat{L}_{2jS_2}$. Similarly, we may construct confidence intervals for the first stage coefficients using half-lengths of

$$
\hat{L}_{1jS_1S_2} := \left| e_j^\top \left\{ \hat{H}_{1n}(S_1) \right\}^{-1} e_j \right| \left\{ C_{1n}^G(\alpha) + C_{1n}^H(\alpha) \| \hat{\theta}_{1n,S_1S_2} \|_1 \right\}. \tag{37}
$$

which have a similar improvement in terms of length as their second-stage counterparts. Using ideas from restricted least-squares, we show in Theorem 5.3 that confidence intervals constructed from $\hat{L}_{2jS_2}$ and $\hat{L}_{1jS_1S_2}$ satisfy similar properties as the original regions. Simulations in Section 7 will demonstrate the improvements seen from these modifications.

### 5.3 Theoretical Results

Before stating our theoretical results, we state the assumptions we use for this setup. For the first assumption, the expression $\Lambda_\ell(C_\ell) := \min_{S_\ell \in \mathcal{M}_\ell(C_\ell)} \lambda_{\min}(H_{0\ell})$ for $\ell = 1, 2$ represents the minimal eigenvalue of $H_{0\ell}$ over all subsets of size bounded by $C_\ell$. The following assumption allows the full matrices $H_{0\ell}$ to be collinear, but requires that any subset of a specified sparsity is uniformly invertible.

**Assumption 5.1.** For each stage $\ell = 1, 2$, there exists $0 < C_\ell < p_\ell$ such that:

$$
\Lambda_1(C_1) \land \Lambda_2(C_2) > c_0 > 0.
$$

Similarly, we assume that several quantities are uniformly bounded by some constant.

**Assumption 5.2.** The following quantities are uniformly bounded:

$$
\| X_1 \|_\infty \lor \| X_2 \|_\infty \lor \| \Delta_2(X_2) \| \lor \max_{S_2 \in \mathcal{M}_2(C_2)} | \Delta_{1,S_2}(X_1) | \leq C.
$$

The following assumption requires certain rates on estimation of the nuisance parameters.

**Assumption 5.3.** The cross-fitting setup is used for some fixed $K > 1$ and the cross-fitted learners achieve the following rates:

$$
\| \hat{\mu}_{1A} - \mu_{1A0} \|_{P_{0,2}} = o_p(n^{-1/2})
$$

$$
\| \hat{\mu}_{2A} - \mu_{2A0} \|_{P_{0,2}} = o_p(n^{-1/4})
$$

$$
\| \hat{\mu}_{2Y} - \mu_{2Y0} \|_{P_{0,2}} = o_p(1)
$$

$$
\| \hat{\mu}_{2A} - \mu_{2A0} \|_{P_{0,2}} = o_p(n^{-1/2})
$$

$$
\| \hat{\mu}_{2Y} - \mu_{2Y0} \|_{P_{0,2}} = o_p(n^{-1/4})
$$

$$
\| \hat{\mu}_{1Y}S_2 - \mu_{1YS_20} \|_{P_{0,2}} = o_p(1)
$$

$$
\| \hat{\mu}_{1A} - \mu_{1A0} \|_{P_{0,2}} = o_p(n^{-1/2}).
$$

15
We draw attention to the fact that in a randomized trial setting, the propensity model is known. Consequently, the first line of the assumption is automatically satisfied, as the propensities for each individual can either be estimated with certainty, or with the parametric rate \( O_p(n^{-1/2}) \). In this case, the third and fifth lines of the above system are trivially satisfied under the second and fourth conditions. As such, application of these ideas in a randomized trial only requires consistency of the conditional expectations for the outcomes. This is a relatively mild condition satisfied by several types of nonparametric learners.

In the first-stage estimation problem, a general model selection technique may involve arbitrary second-stage models, and could possibly choose a least-favorable \( S_2 \) in terms of Stage 1 coverage. Dealing with this possibility could require generalizing the UPoSI procedure to hold simultaneously over models from both stages. Assumption 5.4 instead requires the second-stage selected model \( \hat{S}_2 \) to “settle” in some sense. This allows us to treat the variation added by \( \hat{S}_2 \) to be of a lower order than the variation added by the selection of \( \hat{S}_1 \).

**Assumption 5.4.** The second-stage selected model \( \hat{S}_2 \) takes values in \( M_2(C_2) \) and converges to some \( S^*_2 \in M_2(C_2) \) in the sense \( P(\hat{S}_2 = S^*_2) \rightarrow 1 \). The first-stage selected model \( \hat{S}_1 \) takes values in \( M_1(C_1) \).

Finally, we require an assumption ensuring regular behavior. An alternative assumption on the unknown distribution (Ertefaie et al., 2021) or method modifications (Fan et al., 2019; Laber et al., 2014; Chakraborty et al., 2010) also address the nonregularity occurring in the first stage. We focus on this assumption to focus the presentation.

**Assumption 5.5.** The targeted rule in Stage 2 yields unique treatment decisions almost surely, in the sense that \( \bar{X}_2 \) satisfies \( P(\bar{X}^0 \top \theta_{20}, \hat{S}_2 = 0) = 0 \).

With the assumptions in place, we may state a theorem on the validity of the proposed regions. It features the asymptotic version of the post-selection converge criterion discussed in Appendix B in (B.1). The proof of the following theorem appears in Appendix D.1.

**Theorem 5.1 (Validity of the confidence regions).** Under Assumptions 5.1–5.5, the confidence regions (33) and (34) satisfy:

\[
\lim_{n \to \infty} \inf P(\theta_{10, \hat{S}_1, \hat{S}_2} \in \hat{R}_{1n, \hat{S}_1, \hat{S}_2}) \geq 1 - \alpha, \tag{38}
\]

\[
\lim_{n \to \infty} \inf P(\theta_{20, \hat{S}_2} \in \hat{R}_{2n, \hat{S}_2}) \geq 1 - \alpha. \tag{39}
\]

These coverage statements (38) and (39) involve covering the full vector of the parameter, essentially treating each element of the selected parameter as part of a family and controlling the Family-Wise Coverage Rate. One consequence is that the False Coverage Rate (FCR) is controlled by our proposed regions, which follows from standard arguments regarding Family-Wise Error Rate and False Discovery Rate.

Next, we show that the perturbation bootstrap approach to estimating the quantiles of the distribution is valid. To do so, recall the definitions of the UPoSI random variables in (31) as well as their bootstrap analogues in (32). The proof of this theorem appears in Appendix D.2.
Theorem 5.2 (Validity of the perturbation bootstrap). Under the conditions of Theorem 5.1, the following distributional approximations hold:

\[
\sup_{a,b \geq 0} \left| P \left( \sqrt{n} \hat{D}_{2n}^G \leq a, \sqrt{n} \hat{D}_{2n}^H \leq b \right) - P \left( \sqrt{n} \hat{D}_{2n}^{Gb} \leq a, \sqrt{n} \hat{D}_{2n}^{Hb} \leq b \right) \right| \to 0
\]

\[
\sup_{a,b \geq 0} \left| P \left( \sqrt{n} \hat{D}_{1,n,\hat{S}_2}^G \leq a, \sqrt{n} \hat{D}_{1,n,\hat{S}_2}^H \leq b \right) - P \left( \sqrt{n} \hat{D}_{1,n,\hat{S}_2}^{Gb} \leq a, \sqrt{n} \hat{D}_{1,n,\hat{S}_2}^{Hb} \leq b \right) \right| \to 0.
\]

This distributional approximation is useful for obtaining the appropriate quantiles for the UPoSI regions. For example, RHS of the inequality in (34) depends on \(C_{2n}^G(\alpha) + C_{2n}^H(\alpha)\|\hat{\theta}_{2,n,\hat{S}_2}\|_1\).

Using Theorem 5.2, fix some \(c > 0\) and set \(a = c, b = \|\hat{\theta}_{2,n,\hat{S}_2}\|_1c\) inside the sup norm. Then we may treat the quantity \(\hat{D}_{2n} := \hat{D}_{2n}^H + \|\hat{\theta}_{2,n,\hat{S}_2}\|_1\hat{D}_{2n}^G\) as a univariate random variable and be assured that its quantiles are uniformly approximated by \(\hat{D}_{2n}^b := \hat{D}_{2n}^{Hb} + \|\hat{\theta}_{2,n,\hat{S}_2}\|_1\hat{D}_{2n}^{Gb}\). This approach has two benefits in that it: (1) makes it computationally simple to obtain the bivariate quantiles; and (2) selects bivariate quantiles that are the smallest for a given realization of \(\|\hat{\theta}_{2,n,\hat{S}_2}\|_1\).

Finally, we demonstrate that our proposed confidence intervals are valid post-selection, in that they satisfy a similar simultaneous coverage condition to (38) and (39).

Theorem 5.3 (Validity of the confidence intervals). Under the conditions of Theorem 5.1,

\[
\liminf_{n \to \infty} P \left( \bigcap_{j=1,\ldots,|\hat{S}_2|} \left| e_j^T (\hat{\theta}_{2,n,\hat{S}_2} - \theta_{20,\hat{S}_2}) \right| \leq \hat{L}_{2j,\hat{S}_2} \right) \geq 1 - \alpha \quad (40)
\]

\[
\liminf_{n \to \infty} P \left( \bigcap_{j=1,\ldots,|\hat{S}_1|} \left| e_j^T (\hat{\theta}_{1,n,\hat{S}_1,\hat{S}_2} - \theta_{10,\hat{S}_1,\hat{S}_2}) \right| \leq \hat{L}_{1j,\hat{S}_1,\hat{S}_2} \right) \geq 1 - \alpha. \quad (41)
\]

An interesting feature of these coordinate-wise confidence intervals is that the family of constructed intervals are simultaneously correct at the coverage rate \(1 - \alpha\). An analyst might view the method as an alternative to Scheffé, except that these apply to individual coefficients rather than contrasts, and naturally accommodate model selection.

The proof of this last theorem appears in Appendix D.3. Although we do not pursue it further in our presentation, we remark in Appendix D.4 that the construction of these confidence intervals implies an alternative set of UPoSI regions. These regions are uniformly smaller than the original versions and result in uniformly more powerful hypothesis tests.

5.4 Discussion of Population-level Inference

Since the design is explicitly acknowledged to be random in the setting of dynamic treatments, the previous presentation arguably represents the most natural way to formulate the target parameters and a method for inference about them. However, certain aspects of the problem make the behavior of the UPoSI regions undesirable. For instance, the deterministic inequalities (29) and (30) which inform the size of the regions both depend on the \(\ell_1\) norm of the unknown parameter. This is problematic for two reasons:
1. The size of the UPoSI regions is not equivariant under scaling transformations.

2. The uncertainty grows with the strength of the underlying associations.

This first deficiency could be ameliorated by first transforming the variables to some unitless representation—e.g., scaling each column by the standard deviation. The second problem is less-easily handled. In practice, this behavior can result in the regions being much too conservative in exactly the situations where analysts might expect high power.

The opposite is also true: we could imagine a hypothesis-testing scenario using the region \( \mathcal{R}_{1n,\hat{S}_1\hat{S}_2} \) where we wish to test the hypothesis that our selected rule space is completely spurious. This could be formalized through a test of \( H_0 : \theta_{10,\hat{S}_1\hat{S}_2} = 0 \). In this setting, we could replace the estimated parameter \( \hat{\theta}_{1n,\hat{S}_1\hat{S}_2} \) by its hypothesized value \( 0 \). This would remove the second term on the RHS of the inequality, so that the size of the region is completely determined by \( C_{1n,\hat{S}_2}(\alpha) \). The resulting region would then become the acceptance region for the test, which rejects if \( \| \hat{H}_{2n}(\hat{S}_1)\hat{\theta}_{1n,\hat{S}_1\hat{S}_2} \|_\infty > C_{1n,\hat{S}_2}(\alpha) \). In our simulations, we have found that this test has relatively high power, even if the regions yield very wide confidence intervals due to issue #2 above. In the next section, we present an alternative formulation of the UPoSI regions which is more advantageous in terms of region size.

6 Conditioning on the Design

6.1 Conditional vs. Population Inference

In the previous exposition, we’ve explicitly acknowledged the random nature of the histories \( \bar{X}_1, \bar{X}_2 \) in each stage. In the OLS problem that was handled therein, Kuchibhotla et al. (2020) noticed similar phenomena to those discussed in Section 5.4, and argued along similar lines to propose fixed-design UPoSI regions that were smaller than the population versions, although an explicit derivation for the conditional perspective in a random setting was not provided. As we demonstrate later in Section 6.3 viewing the inference problem conditionally upon the design elements in our setting can also result in smaller confidence regions. Alternative methods dealing with inference after selection are typically derived from with this inferential viewpoint, considering the design to be either deterministic or conditionally fixed (Berk et al., 2013; Lee et al., 2016; Tian and Taylor, 2017). Buja et al. (2019) warned that misspecification of the regression model results in a lack of ancillarity between the regressors and the target parameter; consequently, the target changes based on the observed values of the regressors. Nonetheless, such “conditional” approaches provide interesting comparisons in terms of power or confidence interval length, as well as false coverage rates.

6.2 Defining the Conditional Targets

In (13) and (18) the targets were defined implicitly by taking expectations of the random quantities involved in the first-order equations like (12). The linear working model in Stage \( \ell \) has a design which depends on both the history variable \( \bar{X}_\ell \) as well as the treatment \( A_\ell \) for each subject (c.f. equations (3) and (8)). Fixing these design elements can be achieved by
conditioning on all of these variables. Define the set of the design elements at Stage \( \ell \):

\[
\mathcal{D}_{\ell n} := \{X_{\ell 1}, A_{\ell 1}, \ldots, X_{\ell n}, A_{\ell n}\}.
\]

In order to obtain the design-conditional target Stage 2, first notice that \( \bar{H}_{2n} \) is fixed given \( \mathcal{D}_{2n} \) and define \( G_{2n}^{\text{cond}} := \mathbb{E}(G_{2n}|\mathcal{D}_{2n}) \). Next, take expectations conditioned upon \( \mathcal{D}_{2n} \) on both sides of equation (10) and minimize to determine the conditional target \( \theta_{2n,S_2}^{\text{cond}} \):

\[
0 = G_{2n}^{\text{cond}}(S_2) - \bar{H}_{2n}(S_2)\theta_{2n,S_2}^{\text{cond}}.
\]  

(42)

A similar argument may be used in the first stage as well. Noticing that \( \bar{H}_{1n} \) is fixed given \( \mathcal{D}_{1n} \), define \( G_{1n,S_2} := \mathbb{E}(G_{1n,S_2}|\mathcal{D}_{1n}) \); take the conditional expectations of both sides of equation (16) and minimize to arrive at the first-stage target, \( \theta_{1n,S_1,S_2}^{\text{cond}} \), defined through the relation

\[
0 = G_{1n,S_2}(S_2) - \bar{H}_{2n}(S_2)\theta_{1n,S_1,S_2}^{\text{cond}}.
\]  

(43)

We subscript the targets \( \theta_{2n,S_2}^{\text{cond}} \) and \( \theta_{1n,S_1,S_2}^{\text{cond}} \) by \( n \) in order to remind the reader that these quantities depend on the underlying data through the design elements, which are understood to be random both through \( \mathcal{D}_{\ell n} \).

One important difference from the conditional targets yielded by parametric Q-learning is that the role of confounding has been significantly diminished with the use of Robust Q-learning. Specifically, these targets are the coefficients yielded from the (weighted) projection of the evaluated \( \Delta_2 \) and \( \Delta_{1,S_2} \) functions rather than projections of the Q-functions. We might view these targets as noisy representations of the population-level targets. Because these \( \Delta_2 \) and \( \Delta_{1,S_2} \) functions are unrelated to the observed treatment, conditioning on the treatment when defining the targets does not lead to confounding bias in the same way that might occur when defining similar targets based on the parametric Q-learning algorithm (e.g., [Schulte et al.] 2014 Sec. 5.3).

On the other hand, these conditional targets differ from the population targets through a potential dependence on the conditioning set \( \mathcal{D}_{\ell n} \). As discussed in [Buja et al.] (2019), this opens up the possibility that the parameters may vary for different realizations of \( \mathcal{D}_{1n} \) and \( \mathcal{D}_{2n} \). This work further demonstrates that such issues are avoided when the models being considered contain the true model. Translating this to our setting, such a result might occur if, e.g. \( \Delta_2(\bar{X}_2) \equiv \bar{X}_2^\top \theta_{20,S_2} \) for some \( S_2 \) and the randomly-selected model \( S_2 \) contains \( S_2 \). In this case, the population parameter \( \theta_{20,S_2} \) and the conditional target \( \theta_{2n,S_2}^{\text{cond}} \) are equivalent. Conversely, misspecifications could occur either due to the fact that the true function does not lie in any linear span of the design variables, or that \( S_2 \) does not contain any true \( S_2 \).

### 6.3 Confidence Regions for Conditional Targets

Regions for these conditional targets may be derived using similar arguments to those in Section 5.1. The following inequalities hold deterministically:

\[
\|\bar{H}_{2n}(S_2)\{\hat{\theta}_{2n,S_2} - \theta_{2n,S_2}^{\text{cond}}\}\|_{\infty} \leq D_{2n}^{\text{cond}}
\]

(44)

\[
\|\bar{H}_{1n}(S_1)\{\hat{\theta}_{1n,S_1,S_2} - \theta_{1n,S_1,S_2}^{\text{cond}}\}\|_{\infty} \leq D_{1n,S_2}^{\text{cond}}.
\]

(45)
where the random variables \( D_{2n}^{\text{cond}} \) and \( D_{1n,S_2}^{\text{cond}} \) are defined as

\[
D_{2n}^{\text{cond}} := \| \hat{G}_{2n} - G_{2n}^{\text{cond}} \|_\infty \quad \quad D_{1n,S_2}^{\text{cond}} := \| \hat{G}_{1n,S_2} - G_{1n,S_2} \|_\infty.
\]

We can illustrate this using (44) as an example. Taking the first-order equation for \( \hat{\theta}_{2n,S_2} \) and subtracting (42) we obtain

\[
\hat{H}_{2n}(S_2)\{\theta_{2n,S_2} - \theta_{2n,S_2}^{\text{cond}}\} = \{\hat{G}_{2n} - G_{2n}^{\text{cond}}\}(S_2).
\]

Now apply the \( \ell_\infty \) norm to both sides and apply the inequality \( \|v(S_2)\|_\infty \leq \|v\|_\infty \) for any \( p_2 \)-dimensional vector \( v \) and submodel \( S_2 \) to arrive at (44). Let \( C_{2n}^{\text{cond}}(\alpha) \) and \( C_{1n,S_2}^{\text{cond}}(\alpha) \) represent the upper \( 1 - \alpha \) quantile of the random variables on the RHS of (44) and (45), respectively. Consequently, the following regions contain their respective targets at the appropriate rates, simultaneously over all \( S_1 \in \mathcal{M}_1, S_2 \in \mathcal{M}_2 \):

\[
\hat{R}_{1n,S_1S_2}^{\text{cond}} := \left\{ \theta \in \mathbb{R}^{|S_1|} : \| \hat{H}_{1n}(S_1)\{\hat{\theta}_{1n,S_1S_2} - \theta\} \|_\infty \leq C_{2n}^{\text{cond}}(\alpha) \right\}, \quad (46)
\]

\[
\hat{R}_{2n,S_2}^{\text{cond}} := \left\{ \theta \in \mathbb{R}^{|S_2|} : \| \hat{H}_{2n}(S_2)\{\hat{\theta}_{2n,S_2} - \theta\} \|_\infty \leq C_{1n,S_2}^{\text{cond}}(\alpha) \right\}. \quad (47)
\]

**Theorem 6.1 (Validity of the conditional regions).** Under the conditions of Theorem 5.1,

\[
\lim \inf_{n \to \infty} P \left( \theta_{1n,S_1S_2}^{\text{cond}} \in \hat{R}_{1n,S_1S_2}^{\text{cond}} \mid \mathcal{D}_{1n} \right) \geq 1 - \alpha, \quad (48)
\]

\[
\lim \inf_{n \to \infty} P \left( \theta_{2n,S_2}^{\text{cond}} \in \hat{R}_{2n,S_2}^{\text{cond}} \mid \mathcal{D}_{2n} \right) \geq 1 - \alpha. \quad (49)
\]

**Proof.** This follows from Theorem B.1 along with the simultaneity of (46) and (47) \( \square \)

### 6.4 Perturbation Bootstrap for Conditional Regions

A natural question is whether the bootstrap distributions of \( \hat{D}_{2n}^{Gb} \) and \( \hat{D}_{1n,S_2}^{Gb} \) are valid approximations to those of \( D_{2n}^{\text{cond}} \) and \( D_{1n,S_2}^{\text{cond}} \), respectively, on the relevant conditioning sets. This is the case, as stated in the following theorem, proved in Appendix D.5.

**Theorem 6.2 (Validity of the conditional distribution of the perturbation bootstrap).** Under the conditions of Theorem 5.1, the following distributional results hold:

\[
\sup_{a \geq 0} \left| P \left( \sqrt{n} D_{2n}^{\text{cond}} \leq a \mid \mathcal{D}_{2n} \right) - P \left( \sqrt{n} \hat{D}_{2n}^{Gb} \leq a \mid \mathcal{D}_{2n} \right) \right| \to 0 \quad (50)
\]

\[
\sup_{a \geq 0} \left| P \left( \sqrt{n} D_{1n,S_2}^{\text{cond}} \leq a \mid \mathcal{D}_{1n} \right) - P \left( \sqrt{n} \hat{D}_{1n,S_2}^{Gb} \leq a \mid \mathcal{D}_{1n} \right) \right| \to 0. \quad (51)
\]

### 6.5 Confidence Intervals for Individual Parameters

Similar changes can be made in the case of confidence intervals for the conditional targets as well, by replacing the rightmost braced quantities in (36) and (37) by \( C_{2n}^{\text{cond}}(\alpha) \) and \( C_{1n,S_2}^{\text{cond}}(\alpha) \),
Theorem 5.1

We generated 1000 datasets simulated from various settings. The following models were used:

\[ X \]

Theorem 6.3

A, B, and C make the previously-described modifications for the first-stage parameters, \( \gamma \). This allows the identification of \( \Delta \).

The errors \( \eta \) represent half-lengths of our proposed confidence intervals; e.g., an interval for \( \eta \) may be constructed by centering it at \( \hat{\eta} \) and using a half-length of \( \hat{\Delta} \) in the sense that all of the constructed intervals are simultaneously valid at the 1 - \( \alpha \) confidence level. The proof is omitted, as it follows nearly identically to that of Theorem 5.3.

\[ \lim \inf_{n \to \infty} P \left( \bigcap_{j=1, \ldots, |S_2|} \left| e_j^\top (\hat{\theta}_{2n, S_2} - \theta_{2n, S_2}^{\text{cond}}) \right| \leq \hat{L}_{2j, S_2}^{\text{cond}} \bigg| \mathcal{H}_{2n} \right) \geq 1 - \alpha \] (52)

These represent half-lengths of our proposed confidence intervals; e.g., an interval for \( e_j^\top \theta_{2n, S_2}^{\text{cond}} \) may be constructed by centering it at \( e_j^\top \hat{\theta}_{2n, S_2} \) and using a half-length of \( \hat{\Delta}_{2j, S_2} \). In the first stage, an interval for the \( j \)th coordinate of the conditional target \( \theta_{1n, S_1, S_2}^{\text{cond}} \) may be constructed by centering it at \( \hat{\theta}_{1n, S_1, S_2} \) and using a half-length of \( \hat{\Delta}_{1j, S_1, S_2} \).

The following theorem states the simultaneous validity of these conditional confidence intervals, in the sense that all of the constructed intervals are simultaneously valid at the 1 - \( \alpha \) confidence level. The proof is omitted, as it follows nearly identically to that of Theorem 5.3.

**Theorem 6.3 (Validity of the conditional confidence intervals).** Under the conditions of Theorem 5.1

\[ \lim \inf_{n \to \infty} P \left( \bigcap_{j=1, \ldots, |S_1|} \left| e_j^\top (\hat{\theta}_{1n, S_1, S_2} - \theta_{1n, S_1, S_2}^{\text{cond}}) \right| \leq \hat{L}_{1j, S_1, S_2}^{\text{cond}} \bigg| \mathcal{H}_{1n} \right) \geq 1 - \alpha \] (53)

7 Simulation Study

We generated 1000 datasets simulated from various settings. The following models were used:

\[ Y = \eta_1(X_1) + A_1 \delta_1(X_1) + \eta_2(X_2) + A_2 \delta_2(X_2) + \epsilon \]
\[ A_k \sim \text{Bern}[\text{expit}\{\psi_A(X_k)\}] \text{ for } k = 1, 2, \]

where different functional forms were specified for \( \eta_1, \eta_2, \delta_1, \delta_2, \) and \( \psi_A \). The covariates \( X_1 \in \mathbb{R}^{p_1} \) and \( U \in \mathbb{R}^{p_1} \) were generated as \( U(-1, 1) \) random variables, with \( X_2 = X_1 + \gamma A_1 + U \). The errors \( \epsilon \) were specified as i.i.d. standard Normal variates. Due to this specification, we may make the identification \( \Delta_2 \equiv \delta_2 \). However, it is generally difficult to obtain an analytic form for \( \Delta_{1S_2} \). To simplify the problem, we focus on inference for the first stage parameters under settings in which we make the simplification \( \delta_2(X_2) \equiv 1 \), which automatically satisfies Assumption 5.5. Further, the coefficient \( \gamma \) is set to 0 in this scenario, so that \( X_2 \perp \perp A_1 | X_1 \). This allows the identification of \( \Delta_{1S_2} \equiv \delta_1 \), since the third and fourth terms of the outcome model have the same expectations conditional on \( \{X_1, A_1 = a\} \) when \( a = 0 \) and \( a = 1 \). Due to the simple identification of \( \Delta_2 \), we may provide inference results for all settings in Stage 2, but only the modified settings allow simplifications for Stage 1.

We report the results of six simulation scenarios at four different sample sizes. Scenarios A, B, and C make the previously-described modifications for the first-stage parameters,
while scenarios D, E, and F do not. We summarize the configurations in Table 1. Here, we list different functional forms considered: linear function \(f_l\), quadratic function \(f_q\), a highly-nonlinear function with interactions \(f_n\), and the constant functions 1 and 0. Specific forms for these functions are given in Appendix A. Because the true \(\Delta\) functions in each stage are linear, the conditional targets and unconditional targets are very similar. In fact, the two parameters are equivalent as long as the selected model contains the true model. In our simulations, the two versions of these parameters had very small differences, but the size of the \(\hat{R}^i\) intervals were much larger when compared to those of \(\hat{R}^{\text{cond}}\).

We constructed confidence intervals with both with the standard UPoSI method—i.e. the confidence intervals of form (35) which we call “UPoSI” in the simulations—as well as our proposed confidence intervals of the form (36) and (37) which we label as “UPoSI-coord”. As baselines, we compare these with the selective intervals (“SI”) constructed based on polyhedral inference, as well as naive confidence intervals which ignore the selection process by applying the perturbation bootstrap as if the model were not data-driven (“Naive”). To examine the conservativeness of the intervals, we examine the median confidence interval length of each method at each sample size; to understand the False Coverage properties of the intervals, we use the False Coverage Rate (FCR). We choose this metric because the SI procedure controls FCR under known nuisance parameters, and both variations of the UPoSI intervals strongly control FCR through (48) and (49). Summarizing length with the median instead of the mean avoids the infinite length characteristics of SI (Kivaranovic and Leeb, 2020) which would otherwise dominate the plots.

The nuisance parameters were estimated with super learning implemented in the R package SuperLearner (Polley et al., 2019). We used two different methods for model selection: the least angle regression (LAR) and forward selection (FS) algorithms with a fixed model size of five, both implemented in the selectiveInference R package. The SI intervals were then created based on this software package. Consequently, we use the conditional-design framework of Section 6 throughout our simulations, as the corresponding polyhedral inference methods that account for the random design have not yet been developed or implemented, to the authors’ knowledge. The SI methods are used as implemented—we note that heteroskedasticity is generally present in Stage 1, which is unhandled by the current software.

The results are presented in Figures 1 and 2. We can immediately see that the Naive intervals are quite small compared to the other methods. However, they do not control the FCR and are therefore invalid in the presence of selection. The SI intervals tend to be larger than the corresponding conditional UPoSI intervals, although there are a few situations in which the SI intervals are smaller on median. The SI median interval length may be infinite; to render these situations on the plot, we cap the median lengths at 16 to make visual comparisons possible. Finally, the UPoSI intervals strongly control FCR through the more stringent criterion (48) and (49). Of the two variants, the proposed coordinate-wise intervals are smaller and have the same level of control over FCR. The UPoSI methods strongly control FCR when used with both the LAR and FS model selection methods. The LAR method tends to perform better than the analogous FS SI method in terms of FCR control. Our simulation results appear to suggest that the selective intervals for FS are sensitive to the estimated nuisance parameters compared to those associated with LAR.
Table 1: Simulation scenarios studied in Section 7. The Stage 1 scenarios have been modified for simple identification of $\Delta_{1\delta_2}$.

| Stage | Scenario | $\eta_1$ | $\delta_1$ | $\eta_2$ | $\delta_2$ | $\psi_A$ | $\gamma$ |
|-------|----------|---------|---------|---------|---------|---------|---------|
| A     | $f_q$    | $f_i$   | $f_i$   | $f_i$   | $f_i$   | $f_i$   | $f_i$   |
| B     | $f_q$    | $f_i$   | $f_i$   | $f_i$   | $f_n$   | $f_n$   | $f_i$   |
| C     | $0$      | $f_i$   | $0$     | $1$     | $0$     | $0$     | $0$     |
| D     | $f_i$    | $f_i$   | $f_q$   | $f_i$   | $f_i$   | $f_i$   | $f_i$   |
| E     | $f_i$    | $f_i$   | $f_q$   | $f_i$   | $f_i$   | $f_n$   | $f_i$   |
| F     | $0$      | $0$     | $0$     | $0$     | $1$     | $1$     | $1$     |

8 Conclusion

Accounting for selection in adaptive strategy estimation is an important task, as demonstrated in our simulations. However, several challenges present themselves when one is allowed to choose the decision rule space. We presented a method based on the Universal Post-Selection Inference framework, which strongly controls the probability that the selective target does not belong to a confidence region. This method was shown to be valid even in the presence of nuisance parameters estimated data-adaptively under some conditions, and a bootstrap procedure was shown to complement this procedure and lead to asymptotically valid inference. An improvement to the UPoSI framework was demonstrated by constructing less conservative confidence intervals for each parameter.

Several challenges still remain. These results were proved in a fixed-dimensional asymptotic regime. We conjecture that many theoretical properties would also hold if the dimensions $\log p_1$, $\log p_2$ diverge slower than $n^c$ for some $c < 1/2$. Additionally, although the SI intervals suffer from under-coverage in this setting, it is unclear if these issues would be ameliorated if the design were not considered fixed in the inference procedure. More theoretical work should be done to examine selective inference with a random design. The UPoSI-based intervals can be large compared to naive intervals, especially when the design is considered random rather than fixed. Our proposed improvement to the intervals assists with this drawback, but more work may need to be done to improve inferential power.
Figure 1: Confidence interval performance for each method, grouped by the stage of Robust Q-learning and sample size when using LAR. Top: Median confidence interval length; Bottom: False coverage rates.
Figure 2: Confidence interval performance for each method, grouped by the stage of Robust Q-learning and sample size when using FS. Top: Median confidence interval length; Bottom: False coverage rates
References

Benjamini, Y. (2020) Selective inference: The silent killer of replicability. *Harvard Data Science Review, 2*.

Berk, R., Brown, L., Buja, A., Zhang, K., Zhao, L. et al. (2013) Valid post-selection inference. *Annals of Statistics, 41*, 802–837.

Bian, Z., Moodie, E. E. M., Shortreed, S. M. and Bhatnagar, S. (2021) Variable selection in regression-based estimation of dynamic treatment regimes. *Biometrics, 00*, 1–12.

Buja, A., Brown, L., Berk, R., George, E., Pitkin, E., Traskin, M., Zhang, K. and Zhao, L. (2019) Models as Approximations I: Consequences Illustrated with Linear Regression. *Statistical Science, 34*, 523–544.

Butler, E. L., Laber, E. B., Davis, S. M. and Kosorok, M. R. (2018) Incorporating patient preferences into estimation of optimal individualized treatment rules. *Biometrics, 74*, 18–26.

Chakraborty, B. and Moodie, E. (2013) *Statistical Methods for Dynamic Treatment Regimes*. Springer.

Chakraborty, B., Murphy, S. and Strecher, V. (2010) Inference for non-regular parameters in optimal dynamic treatment regimes. *Statistical Methods in Medical Research, 19*, 317–343.

Chernozhukov, V., Chetverikov, D., Demirer, M., Duflo, E., Hansen, C., Newey, W. and Robins, J. (2018) Double/debiased machine learning for treatment and structural parameters. *The Econometrics Journal, 21*, C1–C68.

Das, D., Gregory, K. and Lahiri, S. N. (2019) Perturbation bootstrap in adaptive Lasso. *Annals of Statistics, 47*, 2080–2116.

Ertefaie, A., McKay, J. R., Oslin, D. and Strawderman, R. L. (2021) Robust Q-Learning. *Journal of the American Statistical Association, 116*, 368–381.

Fan, J. and Li, R. (2001) Variable Selection via Nonconcave Penalized Likelihood and its Oracle Properties. *Journal of the American Statistical Association, 96*, 1348–1360.

Fan, Y., He, M., Su, L. and Zhou, X.-H. (2019) A smoothed Q-learning algorithm for estimating optimal dynamic treatment regimes. *Scandinavian Journal of Statistics, 46*, 446–469.

Fithian, W., Sun, D. and Taylor, J. (2014) Optimal inference after model selection. *arXiv preprint arXiv:1410.2597*.

Flores, M., Glusman, G., Brogaard, K., Price, N. D. and Hood, L. (2013) P4 medicine: How systems medicine will transform the healthcare sector and society. *Personalized Medicine, 10*, 565–576.
Horn, R. A. and Johnson, C. R. (2012) *Matrix Analysis*. Cambridge University Press, second edn.

Kivaranovic, D. and Leeb, H. (2020) On the Length of Post-Model-Selection Confidence Intervals Conditional on Polyhedral Constraints. *Journal of the American Statistical Association, 116*, 845–857.

Kuchibhotla, A. K., Brown, L. D., Buja, A., Cai, J., George, E. I. and Zhao, L. H. (2020) Valid post-selection inference in model-free linear regression. *Annals of Statistics, 48*, 2953–2981.

Laber, E. B., Lizotte, D. J., Qian, M., Pelham, W. E. and Murphy, S. A. (2014) Dynamic treatment regimes: Technical challenges and applications. *Electronic Journal of Statistics, 8*, 1225.

Lee, J. D., Sun, D. L., Sun, Y. and Taylor, J. E. (2016) Exact post-selection inference, with application to the lasso. *Annals of Statistics, 44*, 907–927.

Leeb, H. and Pötscher, B. M. (2005) Model Selection and Inference: Facts and Fiction. *Econometric Theory, 21*, 21–59.

— (2008) Sparse estimators and the oracle property, or the return of Hodges’ estimator. *Journal of Econometrics, 142*, 201–211.

Lu, W., Zhang, H. H. and Zeng, D. (2013) Variable selection for optimal treatment decision. *Statistical Methods in Medical Research, 22*, 493–504.

Minnier, J., Tian, L. and Cai, T. (2011) A Perturbation Method for Inference on Regularized Regression Estimates. *Journal of the American Statistical Association, 106*, 1371–1382.

Murphy, S. A. (2003) Optimal dynamic treatment regimes. *Journal of the Royal Statistical Society: Series B (Statistical Methodology), 65*, 331–355.

Nahum-Shani, I., Qian, M., Almirall, D., Pelham, W. E., Gnagy, B., Fabiano, G. A., Waxmonsky, J. G., Yu, J. and Murphy, S. A. (2012) Q-learning: A data analysis method for constructing adaptive interventions. *Psychological Methods, 17*, 478.

Polley, E., LeDell, E., Kennedy, C. and van der Laan, M. (2019) *SuperLearner: Super Learner Prediction*.

Robins, J. (1986) A new approach to causal inference in mortality studies with a sustained exposure period—application to control of the healthy worker survivor effect. *Mathematical Modelling, 7*, 1393–1512.

Robins, J., Orellana, L. and Rotnitzky, A. (2008) Estimation and extrapolation of optimal treatment and testing strategies. *Statistics in Medicine, 27*, 4678–4721.

Robins, J. M. (1989) The analysis of randomized and non-randomized AIDS treatment trials using a new approach to causal inference in longitudinal studies. *Health service research methodology: a focus on AIDS*, 113–159.
Robins, J. M., Rotnitzky, A. and Scharfstein, D. O. (2000) Sensitivity Analysis for Selection bias and unmeasured Confounding in missing Data and Causal inference models. In Statistical Models in Epidemiology, the Environment, and Clinical Trials (eds. M. E. Halloran and D. Berry), 1–94. New York, NY: Springer New York.

Robinson, P. M. (1988) Root-n-consistent semiparametric regression. Econometrica, 56, 931–954.

Rubin, D. B. (1978) Bayesian Inference for Causal Effects: The Role of Randomization. Annals of Statistics, 6, 34–58.

Schulte, P. J., Tsiatis, A. A., Laber, E. B. and Davidian, M. (2014) Q-and A-learning methods for estimating optimal dynamic treatment regimes. Statistical Science, 29, 640.

Speckman, P. (1988) Kernel Smoothing in Partial Linear Models. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 50, 413–436.

Stewart, G. W. (1969) On the continuity of the generalized inverse. SIAM Journal on Applied Mathematics, 17, 33–45.

Takeuchi, K. (1976) The distribution of information statistics and the criterion of goodness of fit of models. Mathematical Science, 153, 12–18.

Tian, X. and Taylor, J. (2017) Asymptotics of selective inference. Scandinavian Journal of Statistics, 44, 480–499.

Tibshirani, R. (1996) Regression shrinkage and selection via the lasso. Journal of the Royal Statistical Society: Series B (Statistical Methodology), 58, 267–288.

Tibshirani, R. J., Rinaldo, A., Tibshirani, R. and Wasserman, L. (2018) Uniform asymptotic inference and the bootstrap after model selection. Annals of Statistics, 46, 1255–1287.

Van de Geer, S., Bühlmann, P., Ritov, Y. and Dezeure, R. (2014) On asymptotically optimal confidence regions and tests for high-dimensional models. Annals of Statistics, 42, 1166–1202.

van der Laan, M. J. and Luedtke, A. R. (2015) Targeted learning of the mean outcome under an optimal dynamic treatment rule. Journal of Causal Inference, 3, 61–95.

Wallace, M. P. and Moodie, E. E. (2015) Doubly-robust dynamic treatment regimen estimation via weighted least squares. Biometrics, 71, 636–644.

Wallace, M. P., Moodie, E. E. M. and Stephens, D. A. (2019) Model selection for G-estimation of dynamic treatment regimes. Biometrics, 75, 1205–1215.

Watkins, C. J. and Dayan, P. (1992) Q-learning. Machine Learning, 8, 279–292.
Zhang, B., Tsiatis, A. A., Davidian, M., Zhang, M. and Laber, E. (2012) Estimating optimal treatment regimes from a classification perspective. *Stat*, 1, 103–114.

Zhang, C.-H. (2010) Nearly unbiased variable selection under minimax concave penalty. *Annals of Statistics*, 38, 894–942.

Zhang, C.-H. and Zhang, S. S. (2014) Confidence intervals for low dimensional parameters in high dimensional linear models. *Journal of the Royal Statistical Society: Series B (Statistical Methodology)*, 76, 217–242.

Zhao, P. and Yu, B. (2006) On Model Selection Consistency of Lasso. *Journal of Machine Learning Research*, 7, 23.

Zhao, Y., Zeng, D., Rush, A. J. and Kosorok, M. R. (2012) Estimating individualized treatment rules using outcome weighted learning. *Journal of the American Statistical Association*, 107, 1106–1118.

Zhao, Y.-Q., Zeng, D., Laber, E. B. and Kosorok, M. R. (2015) New statistical learning methods for estimating optimal dynamic treatment regimes. *Journal of the American Statistical Association*, 110, 583–598.

Zou, H. (2006) The adaptive lasso and its oracle properties. *Journal of the American Statistical Association*, 101, 1418–1429.
A Simulation Addedum

Each of these functions only depend on the first five elements (at most) of the argument. Let \( X(\{1\}) \) represent the first element, \( X(\{2\}) \) the second, and so on. Without loss of generality, let these functions be defined as functions of a vector \( X \in \mathbb{R}^5 \), understanding that the higher-dimensional functions be mapped to these functions through the first five coordinates. Then letting \( \beta = (2, 2, 1,.1,.1) \), we define

\[
\begin{align*}
    f_1(X) &= X^\top \beta \\
    f_2(X) &= 0.5 \{X^\top \text{diag}(\beta) X + X^\top \beta - 2\} \\
    f_n(X) &= 0.5 \sin \left[ \pi X(\{1\}) X(\{2\}) \right] + 2 \left[ X(\{3\}) - .5 \right]^2 - 1,
\end{align*}
\]

and the “constant functions” are represented by 0 and 1, which take the stated value over their ranges.

A.1 Stage 1 Blip Function

Under the simulation model, there is some subtlety in calculating \( \Delta_{1S_2}(\bar{X}_1) \) for each \( S_2 \). We restate the model below:

\[
Y = \eta_1(X_1) + A_1 \delta_1(X_1) + \eta_2(X_2) + A_2 \delta_2(X_2) + \epsilon \\
A_k \sim \text{Bern}[\expit\{\psi_A(X_k)\}] \quad \text{for } k = 1, 2,
\]

The \( \Delta_{1S_2}(\bar{X}_1) \) function is identified as the contrast in \( Y_{1S_2} \), given \( \bar{X}_1 \) and two different values of \( A_1 \):

\[
\Delta_{1S_2}(\bar{X}_1) = \mathbb{E}(Y_{1S_2} \mid \bar{X}_1, A_1 = 1) - \mathbb{E}(Y_{1S_2} \mid \bar{X}_1, A_1 = 0).
\]

Using the simulation model for \( Y \) and the definition of \( Y_{1S_2} \), we can write

\[
Y_{1S_2} = \eta_1(X_1) + A_1 \delta_1(X_1) + \eta_2(X_2) + 1 \{X_2^0(S_2)^\top \theta_{20,S_2} > 0\} X_2^0(S_2)^\top \theta_{20,S_2} + \epsilon \\
+ A_2 \{ \delta_2(X_2) - X_2^0(S_2)^\top \theta_{20,S_2} \}. \tag{A.1}
\]

If the conditional independence \( X_2 \perp A_1 \mid X_1 \) holds (\( \gamma = 0 \)), then

\[
\mathbb{E}[\{A.1\} \mid \bar{X}_1, A_1 = 0] - \mathbb{E}[\{A.1\} \mid \bar{X}_1, A_1 = 0] = \delta_1(X_1).
\]

We wish to derive conditions to make a similar contrast for the second line equal zero; this would imply that \( \Delta_{1S_2}(\bar{X}_1) \equiv \delta_1(X_1) \).

For the second line [A.2], we can also derive

\[
\mathbb{E}[\{A.2\} \mid X_1, A_1 = a] = \mathbb{E}[\mathbb{E}[\{A.2\} \mid X_1, A_1 = a, X_2] \mid X_1, A_1 = a] \\
= \mathbb{E}[\{ \delta_2(X_2) - X_2^0(S_2)^\top \theta_{20,S_2} \}] \mathbb{E}(A_2 \mid \bar{X}_1, A_1 = a, X_2) \mid \bar{X}_1, A_1 = a]
\]

Under the simulation setup, \( \mathbb{E}(A_2 \mid \bar{X}_1, A_1 = a, X_2) = \mathbb{E}(A_2 \mid X_2) \). Consequently, if the model \( S_2 \) is correctly-specified, then \( \delta_2(X_2) - X_2^0(S_2)^\top \theta_{20,S_2} = 0 \). When \( \delta_2(X_2) \equiv 1 \), then any model containing the intercept is correctly-specified.
An alternative is if \( \bar{X}_0(S_2) \) only depends upon \( X_2 \) under the previous conditional independence. In that case, all the random variation inside the conditional expectation depends only on \( X_2 \), so that using the independence assumption results in

\[
E \{ (A.2) \mid X_1, A_1 = 1 \} - E \{ (A.2) \mid X_1, A_1 = 0 \} = 0.
\]

A way to enforce this is through using a Markov modeling assumption, so that the transformation \( \bar{X}_0 \) is a function only of \( X_2 \). This does not restrict \( \delta_2 \).

### B Equivalence of Post-Selection Inference and Simultaneous Inference

This result was proved in [Kuchibhotla et al. (2020)](https://example.com). We restate the result here and give a bit of exposition around how this fits in with the additional complications arising from multiple stages of model decisions. The post-selection inference problem is defined for general parameters and confidence region construction methods, although it could also be viewed through the lens of hypothesis testing; we mostly focus on the former throughout.

Let us consider a coverage event for a general parameter, which may be allowed to vary with \( n \), represented by \( \bar{\theta}_{n,S} \), where \( \bar{\theta}_{n,S} \) is subscripted by \( S \) in order to reflect that the definition of the parameter varies by the index \( S \) taking its values in \( M \). When this index is chosen from \( M \) based on the data, we obtain some \( \hat{S} \) and then focus on a particular \( \bar{\theta}_{n,\hat{S}} \).

The goal of post-selection inference is to construct a confidence region \( \bar{R}_{n,\hat{S}} \) which contains this selected parameter at the desired confidence level. Mathematically, this may be stated:

\[
P \left( \bar{\theta}_{n,\hat{S}} \notin \bar{R}_{n,\hat{S}} \right) \leq \alpha. \tag{B.1}
\]

The following theorem, proved in [Kuchibhotla et al. (2020)](https://example.com), establishes the equivalence between this criterion and a simultaneous inference result.

**Theorem B.1.** ([Kuchibhotla et al. (2020), Thm. 3.1]) Let \( \{ \bar{R}_{n,S} \} \) be a family of confidence regions for a family of parameters \( \bar{\theta}_{n,S} \), with both the regions and parameters indexed by the model \( S \in M \). Let \( \hat{S} \) be a data-dependent model taking values almost surely in \( M \). Then \( \tag{B.1} \) is equivalent to

\[
P \left( \bigcap_{S \in M} \bar{\theta}_{n,S} \in \bar{R}_{n,\hat{S}} \right) \geq 1 - \alpha. \tag{B.2}
\]

Let us consider how this applies to the population targets defined in Section 3.2 in each of the two stages in Robust Q-learning. In the second stage, the set of parameters is given by \( \bar{\theta}_{20,S_2} \) as defined in (13). These parameters are indexed by \( S_2 \) taking values in \( M_2 \), and the parameters are fixed with \( n \). The post-selection parameter is then \( \bar{\theta}_{n,S} \equiv \bar{\theta}_{20,S_2} \).

By Assumption 5.4, the random parameters are chosen from \( M_2(C_2) \), so that we can set \( M \equiv M_2(C_2) \).

In the first stage, the set of parameters is \( \bar{\theta}_{10,S_1,S_2} \), as defined in (18). This parameter is also fixed with \( n \), although there are now two models involved: \( S_1 \in M_1 \) and \( S_2 \in M_2 \). The
post-selection parameter is \( \theta_{10,\tilde{S},\tilde{S}_2} \). Using Assumption 5.4, the pair of models \((\hat{S}_1, \hat{S}_2)\) are contained in \( \mathcal{M}_1(C_1) \times \mathcal{M}_2(C_2) \) almost surely. Consequently, we can set \( \hat{S} := (\hat{S}_1, \hat{S}_2) \) and \( \mathcal{M} := \mathcal{M}_1(C_1) \times \mathcal{M}_2(C_2) \), which gives a parameter \( \theta_{n,\hat{S}} \equiv \theta_{10,\tilde{S},\tilde{S}_2} \) of the required form.

Also by Assumption 5.4, the pair of models \((\hat{S}_1, \hat{S}_2)\) take values in \( \mathcal{M}^\dagger := \mathcal{M}_1(C_1) \times \{\tilde{S}_2\} \) with probability converging to one. We can choose \( \mathcal{M} \equiv \mathcal{M}^\dagger \) to obtain an asymptotic version of these probability statements that hold in in the limit. To see why this is the case, simply apply the following relationships:

\[
0 \leq P(A) - P(A, B) = P(A, B^c) \leq P(B^c),
\]

to the events \( A \equiv \{ \hat{\theta}_{n,\hat{S}} \notin \tilde{R}_{n,\hat{S}} \} \) and \( B \equiv \{ \hat{S} \in \mathcal{M}^\dagger \} \). The rightmost inequality vanishes.

### C Prerequisites for the Proofs

#### C.1 Some Additional Notation

Let the “positive part” function be defined as \( (a)_+ := a \mathbb{1}(a > 0) \). For a real matrix \( A \), let \( \|A\|_{2,2} \) represent its maximal singular value. This definition is used to make it clear that it is the operator norm mapping \( \ell_2 \) to \( \ell_2 \)—i.e., for any vector \( v \in \mathbb{R}^n \) and \( A \in \mathbb{R}^{m \times n} \), the norm satisfies \( \|Av\|_2 \leq \|A\|_{2,2} \|v\|_2 \). We will also make use of the \( L_2(P_0) \) norm for vector-valued random functions: if \( h = (h_1, \ldots, h_d)^\top \) is a vector-valued random function, then let \( \|h\|_{P_0,2} = \max_{j=1,\ldots,d} \|h_j\|_{P_0,2} \).

Unless otherwise specified, the notation of \( o_p(1) \) will be used to represent “little-o in probability” with respect to the \( \ell_\infty \) norm for vector-valued random variables. That is, for vectors \( V, U \), we use the expression \( U = V + o_p(r_n) \) to represent the statement \( r_n^{-1} \|U - V\|_\infty \xrightarrow{p} 0 \). Similarly, the \( U = V + O_p(r_n) \) notation will be used to represent \( r_n^{-1} \|U - V\|_\infty = O_p(1) \). Some random quantities defined in Section 3.4 depend on both the random sample from \( P_0 \) as well as random multipliers \( G \) from a bootstrap distribution \( P_\omega \). The notation \( O_p(r) \) and \( o_p(r) \) will represent similar probability statements with respect to the product measure of the observed data and random multipliers, \( P_0 \times P_\omega \).

We also recall that the function \( \| \cdot \|_\infty \) for matrices is not itself a proper matrix norm; however, for a \( m \times m \) matrix \( A \), the quantity \( m\|A\|_\infty \) is a proper matrix norm (see (5.6.0.4) in Horn and Johnson [2012]). We also have the property \( \|A\|_\infty \leq \|A\|_{2,2} \leq m\|A\|_\infty \). This fact will be useful in some of the future arguments.

To simplify the notation, we will subscript conditional expectations and their estimates by \( i \) to represent the evaluation of the function at the \( i^{th} \) value. For example, if \( i \in I_k \), we will write \( \mu_{2Y_0}(\tilde{X}_{2i}; D_{I_k}) - \mu_{2Y}(X_{2i}; D_{I_k}) \) in the more compact form \( \mu_{2Y_{0i}} - \mu_{2Y_i} \) and similarly we will write \( \mu_{1A_0}(\tilde{X}_{1i}; D_{I_k}) - \mu_{1A}(X_{1i}; D_{I_k}) \) as \( \mu_{1A_{0i}} - \mu_{1Ai} \). It will be understood that these function estimates are the product of cross-fitting, although this fact will not be explicitly notated except when necessary. For example, we will often write

\[
\frac{1}{n} \sum_{i=1}^{n} (\mu_{1A_{0i}} - \mu_{1Ai})
\]

instead of the double-sum over both \( k = 1, \ldots, K \) and \( i \in I_k \). The arguments involving cross-fitting more directly will draw attention to this nested structure.
Finally, several quantities were defined in the main text. To provide a more concrete reference, we list several of these quantities and relationships here.

\[
H_{10} = E \left[ \left\{ A_\ell - \mu_{A0}(X_\ell) \right\}^2 (X_\ell^0)^\otimes 2 \right]
\]

\[
\hat{H}_{1n} = \frac{1}{n} \sum_{i=1}^{n} (A_{i\ell} - \hat{\mu}_{A0i})^2 (X_\ell^0)^\otimes 2
\]

\[
\hat{H}_{2n} = \frac{1}{n} \sum_{i=1}^{n} (A_{i\ell} - \hat{\mu}_{A0i})^2 (X_\ell^0)^\otimes 2
\]

\[
G_{20} = E \left[ \left\{ A_2 - \mu_{2A0}(X_2) \right\}^2 \Delta_2(X_2)X_2^0 \right]
\]

\[
\hat{G}_{2n} = \frac{1}{n} \sum_{i=1}^{n} (A_{2i} - \hat{\mu}_{2A0i})(Y - \hat{\mu}_{2Y0i})X_2^0
\]

\[
G_{10S_2} = E \left[ \left\{ A_1 - \mu_{1A0}(X_1) \right\}^2 \Delta_{1S_2}(X_1)X_1^0 \right]
\]

\[
\hat{G}_{1nS_2} = \frac{1}{n} \sum_{i=1}^{n} (A_{1i} - \hat{\mu}_{1A0i})(Y_{1S2i} - \hat{\mu}_{1YS20i})X_{1i}^0
\]

\[
\hat{G}_{1nS_2} = \frac{1}{n} \sum_{i=1}^{n} (A_{1i} - \hat{\mu}_{1A0i})(Y_{1S2i} - \hat{\mu}_{1YS20i})X_{1i}^0
\]

Each of the terms involving sums also have a perturbation bootstrap version, which is superscripted with \( b \) and involves \( \omega_i \) multiplying the \( i^{th} \) term in the sum. For example,

\[
\hat{G}_{2n}^b = \frac{1}{n} \sum_{i=1}^{n} \omega_i (A_{2i} - \hat{\mu}_{2A0i})(Y - \hat{\mu}_{2Y0i})X_{2i}^0.
\]

The target parameters in the first and second stages, respectively, are

\[
\theta_{10,S_1S_2} = H_{10}(S_1)^{-1}G_{10S_2}(S_1)
\]

\[
\theta_{20,S_2} = H_{20}(S_2)^{-1}G_{20}(S_2)
\]

\[\text{(C.2)}\]

and have estimators leveraging the quantities in \( \text{(C.1)} \)

\[
\hat{\theta}_{1nS_1S_2} = \hat{H}_{1n}(S_1)^{-1}\hat{G}_{1nS_2}(S_1)
\]

\[
\hat{\theta}_{1nS_1S_2} = \hat{H}_{1n}(S_1)^{-1}\hat{G}_{1nS_2}(S_1)
\]

\[
\hat{\theta}_{2nS_2} = \hat{H}_{2n}(S_2)^{-1}\hat{G}_{2n}(S_2)
\]

\[
\hat{\theta}_{2nS_2} = \hat{H}_{2n}(S_2)^{-1}\hat{G}_{2n}(S_2).
\]

\[\text{(C.3)}\]

Bootstrapped versions of these estimators may be created by using the bootstrapped versions of each of the quantities appearing here. As an illustrative example, the bootstrap analogue of \( \hat{\theta}_{1nS_1S_2} \) is given by

\[
\hat{\theta}_{1nS_1S_2}^b = \hat{H}_{1n}(S_1)^{-1}\hat{G}_{1nS_2}^b(S_1).
\]
C.2 Defining Different Pseudo-Outcomes

We previously defined the relevant part of the Stage 1 Q-function in terms of an ideal pseudo-outcome $Y_{1,S_2}$. We will unify some notation around these pseudo outcomes by delineating the different levels of knowledge and estimation required for each. For any particular Stage 2 model $S_2 \in \mathcal{M}_2$, define:

$$Y_{1,S_2} = Y + \xi \{ A_2, \bar{X}_2^0(S_2); \theta_{20,S_2} \}$$ \hspace{1cm} (C.4)

$$\tilde{Y}_{1,S_2} = Y + \xi \{ A_2, \bar{X}_2^0(S_2); \tilde{\theta}_{2n,S_2} \}$$ \hspace{1cm} (C.5)

$$\hat{Y}_{1,S_2} = Y + \xi \{ A_2, \bar{X}_2^0(S_2); \hat{\theta}_{2n,S_2} \}$$ \hspace{1cm} (C.6)

where $\xi$ is defined in (6). The first pseudo-outcome leverages perfect knowledge of the $\Delta_2$ function along with its projection onto a linearized model. That of (C.5) requires perfect knowledge of the $\mu_{2A_0}, \mu_{2Y_0}$ functions in order to create the estimate $\tilde{\theta}_{2n,S_2}$. The final pseudo-outcome (C.6) is based entirely on the data using cross-fitting.

For completeness, we also define some of the bootstrap pseudo-outcome quantities used in the arguments in Section 3.4:

$$\tilde{Y}_{1,S_2}^b = Y + \xi( A_2, \bar{X}_2^0(S_2); \tilde{\theta}_{2n,S_2}^b )$$ \hspace{1cm} (C.7)

$$\hat{Y}_{1,S_2}^b = Y + \xi( A_2, \bar{X}_2^0(S_2); \hat{\theta}_{2n,S_2}^b )$$ \hspace{1cm} (C.8)

these quantities differ from those of (C.5) and (C.6) through the bootstrapped second-stage estimates, which are minimizers of the bootstrapped functions defined in Section 3.4.

C.3 Overview of the Proofs

Because of the complexity of the multi-stage Robust Q-learning process, there are several intermediate results that are necessary before getting to the main theorems. Here we will provide an overview of some of the results.

To prove Theorem 5.1, we make use of only a few results: a simple result for stochastic processes with a random index in Lemma E.1, an analogue of Lemma 4.1 in Kuchibhotla et al. (2020) stated as Lemma E.7, and a result on the negligibility of cross-fitting in Lemma E.9.

For the proof of Theorem 5.2, we use these results along with Lemmas E.14 and E.16. The first ensures that cross fitting and the second-stage model selection event do not impact the quantities being studied up to a $n^{-1/2}$ rate. The second ensures that the term has an influence function function representation up to this same level of approximation, in probability.

The final proof of Theorem 5.3 is relatively straightforward, only involving a matrix argument.

D Proofs of Theorems

D.1 Proof of Theorem 5.1

By Theorem 3.1 in Kuchibhotla et al. (2020), coverage for a random-model parameter is equivalent to simultaneous coverage over all models. We consider the Stage 1 case here, with
The understanding that the arguments for the stage 2 case are similar.

The deterministic inequality (30) which holds for any pair of models $S_1 \in M_1$, $S_2 \in M_2$, forms the basis for the Stage 1 UPoSI region (33). The only difference between the RHS of (30) and that of the inequality within (33) is the use of an estimator $\hat{\theta}_{1, S_1, S_2}$ for the unknown quantity. By Assumption 5.4 and Lemma E.1 $\|\theta_{10, S_1, S_2} - \theta_{10, S_1, S_2}\|_1 = o_p(n^{-1/2})$.

Using the triangle inequality, and re-arranging terms, we can bound

$$\frac{|\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}| - 1}{|\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}|} = \frac{\hat{D}^H_{1n, S_2} + \hat{D}^H_{1n, S_2}}{|\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}|} \left\{ \frac{\|\theta_{10, S_1, S_2} - \theta_{10, S_1, S_2}\|_1}{\Lambda_1(C_1) - C_1 \hat{D}^H_{1n}} + \|\theta_{10, S_1, S_2} - \theta_{10, S_1, S_2}\|_1 \right\}.$$ 

Examining the final equality, the second term in curly braces is $o_p(n^{-1/2})$ by Lemma E.1. Then we may use this fact along with Lemma E.7 to bound

$$\leq \frac{\hat{D}^H_{1n, S_2} + \hat{D}^H_{1n, S_2}}{|\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}|} \left\{ \frac{|S_1| (\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2})}{\Lambda_1(C_1) - C_1 \hat{D}^H_{1n}} + \|\theta_{10, S_1, S_2} - \theta_{10, S_1, S_2}\|_1 \right\} \leq \frac{\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}}{|\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}|} \left\{ \frac{C_1 \hat{D}^H_{1n}}{\Lambda_1(C_1) - C_1 \hat{D}^H_{1n}} + o_p(n^{-1/2}) \right\}.$$ 

Under Assumption 5.1, $1/\Lambda_1(C_1) \leq c_0^{-1}$. Further, for fixed $p_1$, $\hat{D}^H_{1n} = O_p(n^{-1/2})$, since by Lemma E.9 this quantity behaves up to $o_p(n^{-1/2})$ like the maximum deviation of a fixed number of mean-zero sample averages. Consequently, the second fraction on the RHS converges to zero in probability. Finally, we apply Lemma E.1 to the stochastic process defined by

$$\left\{ \frac{\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}}{|\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n, S_2}|} - 1 : S_2 \in M_2(C_2) \right\}$$

in the Euclidean metric space to conclude that the RHS is $o_p(1)$.

The coverage statement (39) follows similarly, without handling the additional random model.

**D.2 Proof of Theorem 5.2**

Let us consider the first stage, as the arguments are similar in the second stage but with fewer additional technicalities. Using the definitions of the $\hat{D}$ variables along with Lemmas E.14...
and \[E.16\] we may write
\[
\sqrt{n} \left\| G_{1n,S_2}^b - \hat{G}_{1n,S_2} \right\|_\infty = \left\| n^{-1/2} \sum_{i=1}^n (\omega_i - 1) \text{Inf}_{1GS_2^i} \right\|_\infty + o_p(1)
\]
\[
\sqrt{n} \left\| \hat{G}_{1n,S_2} - G_{10,S_2} \right\|_\infty = \left\| n^{-1/2} \sum_{i=1}^n \text{Inf}_{1GS_2^i} \right\|_\infty + o_p(1),
\]
with \(\mathbb{E}(\omega_i - 1) = 0\) and \(\mathbb{E}(\omega_i - 1)^2 = 1\). Consequently, these obey a central limit theorem and converge weakly to the same asymptotic distribution. For example,
\[
n^{-1/2} \sum_{i=1}^n \text{Inf}_{1GS_2^i} \xrightarrow{d} N(0, \Sigma_1)
\]
where \(\Sigma_1 := \mathbb{E}(\text{Inf}_{1GS_2^2})\). Similarly, conditional on \(O_1, \ldots, O_n\), the Lindeberg-Feller CLT ensures the bootstrap term converges in distribution:
\[
n^{-1/2} \sum_{i=1}^n (\omega_i - 1) \text{Inf}_{1GS_2^i} \xrightarrow{d} N(0, \Sigma_{1n}),
\]
where \(\Sigma_{1n} := n^{-1} \sum_{i=1}^n \text{Inf}_{1GS_2^i} \xrightarrow{a.s.} \Sigma_1\) by the Law of Large Numbers. Similarly, we can use \[\text{Lemma E.9}\] to conclude
\[
\sqrt{n} \left\| \hat{H}_{1n}^i - \hat{H}_{1n} \right\|_\infty = \sqrt{n} \left\| \hat{H}_{1n}^i - \hat{H}_{1n} \right\|_\infty + o_p(1)
\]
\[
\sqrt{n} \left\| \hat{H}_{1n} - \hat{H}_{10} \right\|_\infty = \sqrt{n} \left\| \hat{H}_{1n} - \hat{H}_{10} \right\|_\infty + o_p(1)
\]
where each of the non-remainder terms on the RHS are constructed from sample means of i.i.d. terms, with the bootstrap portion having a similar composition as above. Consequently, the CLT and LLN ensure that the bootstrap quantities converge to the same asymptotic distribution as the observed-data quantities.

**D.3 Proof of Theorem 5.3**

Recall the following property of least-squares estimators: if \(\hat{\theta}_{2n,S_2}\) minimizes the least squares objective function, and \(\theta_{2n,S_2}^\nu\) minimizes the objective function under the additional restriction \(v^T \hat{\theta}_{2n,S_2}^\nu = t\) for some \(t \in \mathbb{R}\), then we may represent the quantity
\[
\hat{H}_{2n}(S_2)(\theta_{2n,S_2}^\nu - \hat{\theta}_{2n,S_2}) = v \left\{ v^T \hat{H}_{2n}(S_2)^{-1}v \right\}^{-1} (t - v^T \hat{\theta}_{2n,S_2}).
\]

Consider the restricted least-squares estimator \(\hat{\theta}_{2n,S_2}^r\), which is the least-squares estimator under the restriction \(\hat{\theta}_{2n,S_2}(\{j\}) = t\) for some value \(t \in \mathbb{R}\). Using this property of restricted least-squares estimators with the identity \(\hat{\theta}_{2n,S_2}(\{j\}) = e_j^T \hat{\theta}_{2n,S_2}^r\), we may represent
\[
\left\| \hat{H}_{2n}(S_2)(\hat{\theta}_{2n,S_2}^r - \hat{\theta}_{2n,S_2}) \right\|_\infty = \left\| e_j \left\{ e_j^T \hat{H}_{2n}(S_2)^{-1}e_j \right\}^{-1} (t - e_j^T \hat{\theta}_{2n,S_2}) \right\|_\infty
\]
\[
= \left\{ e_j^T \hat{H}_{2n}(S_2)^{-1}e_j \right\}^{-1} |t - e_j^T \hat{\theta}_{2n,S_2}|.
\]

Now, suppose that the restriction corresponds to a null hypothesis, i.e. a null hypothesis $e_j^T \theta_{20,S_2} = t$. Under such a hypothesis, we may write the $\ell_\infty$ norm of the RHS as

$$
\left\| e_j \left\{ e_j^T \hat{H}_{2n}(S_2)^{-1} e_j \right\}^{-1} e_j^T \left( \theta_{20,S_2} - \hat{\theta}_{2n,S_2} \right) \right\|_\infty
$$

$$
= \left\| e_j \left\{ e_j^T \hat{H}_{2n}(S_2)^{-1} e_j \right\}^{-1} e_j^T \hat{H}_{2n}(S_2)^{-1} \hat{H}_{2n}(S_2) \left( \theta_{20,S_2} - \hat{\theta}_{2n,S_2} \right) \right\|_\infty
$$

$$
= \left\| \left\{ e_j^T \hat{H}_{2n}(S_2)^{-1} e_j \right\}^{-1} e_j e_j^T \hat{H}_{2n}(S_2)^{-1} \hat{H}_{2n}(S_2) \left( \theta_{20,S_2} - \hat{\theta}_{2n,S_2} \right) \right\|_\infty.
$$

The second equality used the fact that the term in curly braces is a scalar, and so may commute with other terms. To see the $\text{diag}(e_j)$ equality, notice that $e_j e_j^T \hat{H}_{2n}(S_2)^{-1}$ is a matrix of zeroes with a nonzero $j^{th}$ diagonal element, which takes its value from the $j^{th}$ diagonal element of $\hat{H}_{2n}(S_2)^{-1}$. The multiplicative inverse of this component is represented by the preceding term. Consequently, the final line may be succinctly written as the absolute value of the scalar quantity,

$$
\left| e_j^T \hat{H}_{2n}(S_2) \left( \theta_{20,S_2} - \hat{\theta}_{2n,S_2} \right) \right|
$$

which is bounded from above by $\| \hat{H}_{2n}(S_2) \left( \theta_{20,S_2} - \hat{\theta}_{2n,S_2} \right)\|_\infty$. The deterministic inequality (29) provides a further bound for the term.

Recalling the expression of the test statistic (D.1) as well as the upper bound (29), we have demonstrated that under the null hypothesis $H_0 : e_j^T \theta_{20,S_2} = t$,

$$
\left\{ e_j^T \hat{H}_{2n}(S_2)^{-1} e_j \right\}^{-1} |t - e_j^T \hat{\theta}_{2n,S_2}| \leq D_G^{\text{G}} + D_H^{\text{H}} \| \theta_{20,S_2} \|_1
$$

holds almost-surely. Notice that this almost-sure bound is free of both $S_2$ and the coordinate $j$. Consequently, this bound is simultaneous over $S_2 \in M_2$, $j = 1, \ldots, |S_2|$. Using a similar argument as in the proof of Theorem 5.1, we may show that estimating $\theta_{20,S_2}$ provides error of smaller order than the RHS. This establishes

$$
\liminf_{n \to \infty} P \left( \bigcap_{S_2 \in M_2} \bigcap_{j=1,\ldots,|S_2|} \left\{ |e_j^T (\hat{\theta}_{2n,S_2} - \theta_{20,S_2})| \leq \hat{L}_{2jS_2} \right\} \right) \geq 1 - \alpha.
$$

A similar arguments can be used in the first stage, handling the random second stage model as in Theorem 5.1 for the quantity $\hat{L}_{1jS_1S_2}$ defined in (37).

**D.4 A Corollary: Alternative Confidence Regions**

Technically, the development of the previous section proved that

$$
\left\| \text{diag} \left\{ \hat{H}_{2n}(S_2)^{-1} \right\}^{-1} (\hat{\theta}_{2n,S_2} - \theta_{20,S_2}) \right\|_\infty \leq \| \hat{H}_{2n}(S_2) (\hat{\theta}_{2n,S_2} - \theta_{20,S_2}) \|_\infty.
$$
or that the test statistic which estimates the remaining parameters in each dimension is more powerful that the omnibus test. However, we still use the UPoSI inequality on the RHS to provide quantiles. We could then create the confidence region

\[
\mathcal{R}^*_{2n,S_2} := \left\{ \theta_2 \in \mathbb{R}^{|S_2|} : \left\| \text{diag} \left\{ H_{2n}(S_2)^{-1} \right\}^{-1} (\theta_{2n,S_2} - \theta_{20,S_2}) \right\|_\infty \leq C_{2n}^G(\alpha) + C_{2n}^H(\alpha) \| \theta_{2n,S_2} \|_1 \right\},
\]

with a similar region also for the stage 1 parameter. The development of the previous section has shown that this is also a valid \(1 - \alpha\) confidence region for \(\theta_{20,S_2}\), and that \(\mathcal{R}^*_{2n,S_2}\) is uniformly smaller than \(\mathcal{R}^*_{2n,S_2}\) in Lebesgue measure.

### D.5 Proof of Theorem 6.2

We will show the first-stage perturbation bootstrap result (51) with the understanding that the second-stage result (50) follows similarly. In Appendix D.2 we arrived at the asymptotically linear representations

\[
\sqrt{n} \left\| \hat{G}_{1n,S_2}^b - \hat{G}_{1n,S_2} \right\|_\infty = \left\| n^{-1/2} \sum_{i=1}^{n} (\omega_i - 1) \text{Inf}_{1GS_2}^{cond} \right\|_\infty + o_p(1)
\]

\[
\sqrt{n} \left\| \hat{G}_{1n,S_2} - \hat{G}_{10,S_2} \right\|_\infty = \left\| n^{-1/2} \sum_{i=1}^{n} \text{Inf}_{1GS_2}^{cond} \right\|_\infty + o_p(1).
\]

The conditional weak convergence result would follow by the Lindeberg-Feller CLT if a similar linearization holds when replacing \(G_{10,S_2}\) with \(G_{1n,S_2}\). Identical arguments as those in the proof of Lemma E.14 can be made to show that

\[
\left\| \hat{G}_{1n,S_2} - \hat{G}_{1n,S_2}^* \right\|_\infty = \left\| \hat{G}_{1n,S_2} - \hat{G}_{1n,S_2}^* \right\|_\infty + o_p(n^{-1/2}).
\]

At this point, analogous arguments to those made in Appendix E.4.3 can be made to show that an asymptotically linear representation holds for \(G_{1n,S_2}^* - G_{1n,S_2}\) when conditioning upon the first-stage design elements \(\mathcal{D}_{1n}\). Such arguments would lead to an influence function for each realization of \(\mathcal{D}_{1n}\), \(\text{Inf}_{1GS_2}^{cond}(\mathcal{D}_{1n})\). On sets with such realizations, we could write

\[
\sqrt{n} \left\| \hat{G}_{1n,S_2}^b - \hat{G}_{1n,S_2} \right\|_\infty = \left\| n^{-1/2} \sum_{i=1}^{n} (\omega_i - 1) \text{Inf}_{1GS_2}^{cond}(\mathcal{D}_{1n}) \right\|_\infty + o_p(1)
\]

\[
\sqrt{n} \left\| \hat{G}_{1n,S_2} - \hat{G}_{10,S_2} \right\|_\infty = \left\| n^{-1/2} \sum_{i=1}^{n} \text{Inf}_{1GS_2}^{cond}(\mathcal{D}_{1n}) \right\|_\infty + o_p(1).
\]

Let \(\epsilon_{2i}^{cond}\) and \(\epsilon_{1S_2}^{cond}\) be the errors in models defined similarly to (3) and (8) except replacing \(\theta_{20,S_2}\) with \(\theta_{2n,S_2}\) and \(\theta_{10,S_1,S_2}\) with \(\theta_{1n,S_1,S_2}\). We define the quantities

\[
\text{Inf}_{2S_2}^{cond} := \bar{X}_{1i}(A_{2i} - \mu_2A_{0i})\epsilon_{2i}^{cond}
\]

\[
\bar{B}_{S_2}^{cond} := 1(\bar{X}_2^0(S_2)^\top \theta_{2n,S_2} > 0) - A_2
\]

\[
\bar{M}^{cond} := \bar{B}_{S_2}^{cond} \left\{ A_1 - \mu_1A_0(\bar{X}_1) \right\} \bar{X}_2^0 \bar{X}_2^0(S_2)^\top,
\]

\[
\text{Inf}_{1GS_2}^{cond} := \bar{X}_{1i}(A_{11} - \mu_1A_{0i})\epsilon_{1S_2}^{cond} + \bar{E}(\bar{M}^{cond} \mid \mathcal{D}_{1n}) \text{Inf}_{2S_2}^{cond}.
\]
Notice that both $\text{Inf}_{2S_2}^\text{cond}$ and $\text{Inf}_{1G S_2}^\text{cond}$ have expectation zero when conditioning on the $\mathcal{D}_{1n}$. We can see the first through the tower property: since the set $\mathcal{D}_{1n}$ is contained within $\mathcal{D}_{2n}$,

$$E(\text{Inf}_{2S_2}^\text{cond} \mid \mathcal{D}_{1n}) = E \left\{ E(\text{Inf}_{2S_2}^\text{cond} \mid \mathcal{D}_{2n}) \mid \mathcal{D}_{1n} \right\}.$$ 

The second follows from the first, along with the property $E(\epsilon_{1S_2}^\text{cond} \mid \mathcal{D}_{1n}) = 0$.

Finally, we check Lindeberg’s condition for this first-stage influence function. If the following two conditions hold, then (51) follows from the Lindeberg-Feller CLT:

$$\frac{1}{n} \sum_{i=1}^{n} E \left( \| \text{Inf}_{1G S_2}^\text{cond} \|_2 \mid \mathcal{D}_{1n} \right) 1 \left( \| \text{Inf}_{1G S_2}^\text{cond} \|_2 > \gamma \sqrt{n} \right) \rightarrow 0, \text{ for all } \gamma > 0 \quad (D.3)$$

$$\frac{1}{n} \sum_{i=1}^{n} E \left( \text{Inf}_{1G S_2}^\text{cond} \mid \mathcal{D}_{1n} \right) \otimes^2 \rightarrow \Sigma_1. \quad (D.4)$$

Since all of the terms involved in $\text{Inf}_{1G S_2}^\text{cond}$ have finite variance, it is straightforward to verify that (D.3) and (D.4) hold with arbitrary probability over the conditioning set. The first condition follows from Chebyshev’s inequality, while the second follows from the LLN.

The result for the second-stage result (50) follows very similarly, establishing the influence function $\text{Inf}_{2S_2}^\text{cond}$ reported above. Instead, we would modify the arguments of Appendix E.4.1 and use the Lindeberg-Feller CLT.

E Proofs of Lemmas

E.1 General Lemmas

First, we state some general lemmas. The first is a simple result about random indices, which will be useful for handling random vectors that depend on a random model.

Lemma E.1. Let $\{X_s : s \in \mathcal{S}\}$ be a stochastic process with indexing set $\mathcal{S}$. Suppose $X_s$ takes its values in a normed metric space $\mathcal{X}, \| \cdot \|$, where $\| \cdot \|$ is a norm. Let $\hat{s}$ be an $\mathcal{S}$-valued random variable defined on the same probability space as the stochastic process. Then, for any fixed point $s' \in \mathcal{S}$, and any $\varepsilon \geq 0$,

$$P \left\{ \| X_{\hat{s}} - X_{s'} \| > \varepsilon \right\} \leq P (\hat{s} \neq s').$$

Proof. Since the stochastic process and random index are measurable on the same probability space, we may decompose the LHS probability as

$$P \left\{ \| X_{\hat{s}} - X_{s'} \| > \varepsilon \right\} = P \left\{ \| X_{\hat{s}} - X_{s'} \| > \varepsilon, \hat{s} = s' \right\} + P \left\{ \| X_{\hat{s}} - X_{s'} \| > \varepsilon, \hat{s} \neq s' \right\}.$$

The first term is zero, since the event $\{\hat{s} = s'\}$ ensures that $\| X_{\hat{s}} - X_{s'} \| = 0$ almost surely. The second term is bounded by $P (\hat{s} \neq s')$, completing the proof.

The following lemma is a standard result for matrices (e.g., Stewart, 1969).
Lemma E.2. Let $\hat{M}$ and $M$ be two matrices and $\| \cdot \|$ be any proper matrix norm. Suppose (i) both $M^{-1}$ and $\hat{M}^{-1}$ exist with $0 < c_0 < \| M^{-1} \| < c_1 < \infty$ for constants $c_0$ and $c_1$, and (ii) $\| \hat{M} - M \| \leq (2\| M^{-1} \|)^{-1}$. Then,

$$\| \hat{M}^{-1} - M^{-1} \| \leq 2c_0^2\| \hat{M} - M \|. $$

Next is a useful lemma for handling the sum of a product of random variables.

Lemma E.3. Let $X_i, Y_i$ for $i = 1, \ldots, n$ be random variables on a common probability space, although not necessarily i.i.d. Let

$$\frac{1}{n} \sum_{i=1}^{n} |X_i| \xrightarrow{p} \mu,$$

and suppose $\max_{i=1,\ldots,n} |Y_i| = o_p(n^{-1/2})$. Then

$$n^{-1/2} \sum_{i=1}^{n} X_i Y_i \xrightarrow{p} 0.$$

Proof. By hypothesis, for any $\epsilon, \delta > 0$ there exists $N \equiv N(\epsilon, \delta)$ such that

$$P \left( \max_{i=1,\ldots,n} |Y_i| < \epsilon n^{-1/2} \right) \geq 1 - \delta$$

for all $n \geq N$. Let $\Omega_1$ represent the sets on which the the condition inside the probability statement holds. By definition, $P(\Omega_1) \geq 1 - \delta$. For $n \geq N$ on $\Omega_1$, we have

$$\left| n^{-1/2} \sum_{i=1}^{n} X_i Y_i \right| \leq n^{-1/2} \sum_{i=1}^{n} |X_i| \epsilon n^{-1/2}$$

$$= \epsilon n^{-1} \sum_{i=1}^{n} |X_i|. \quad (E.1)$$

By the hypothesis, for any $\gamma > 0$ the sample average in $[E.1]$ converges to $\mu$ with probability no less than $1 - \gamma$. Let $\Omega_2$ represent the sets satisfying this condition. Then on $\Omega_1 \cap \Omega_2$, the average in $[E.1]$ converges to $\epsilon \mu$. By Frechet’s inequality, $P(\Omega_1 \cap \Omega_2) \geq 1 - \delta - \gamma$ with $\delta, \gamma$ arbitrary. Since $\epsilon$ is also arbitrary, the proof is complete.

Finally, we state this slight variation on Lemma 6.1 in Chernozhukov et al. (2018).

Lemma E.4. Let $X_n$ and $Z_n$ be a sequence of random vectors defined on the same probability space. Suppose $\| X_n \| = O_p(r_n)$ conditionally on $Z_n$, for a sequence of positive constants $r_n$. Then $\| X_n \| = O_p(r_n)$ unconditionally as well.
E.2 Lemmas for Cross-fitted Functions

Lemma E.5. Suppose \((W_i, X_i)\) are \(O_i\)-measurable random variables, where \(O_i\) are i.i.d. from some distribution \(P_0\) and \(W_i \in \mathbb{R}^d\). Suppose for \(i = 1, \ldots, n\) that \(\mathbb{E}(W_i \mid X_i) = 0 \in \mathbb{R}^d\) and \(\|\mathbb{E}(W_i \circ X_i)\|_\infty \leq C_W < \infty\). Let \(h(X_i; D_{I_k})\) for any \(k = 1, \ldots, K\) and \(i \in I_k\) be a cross-fitted function. If \(\|h\|_{P_0,2} = o_p(r_n)\) for some sequence \(r_n\), then

\[
\left\| n^{-1} \sum_{k=1}^K \sum_{i \in I_k} W_i h(X_i; D_{I_k}) \right\|_\infty = o_p(n^{-1/2} r_n),
\]

where the constant does not depend on the dimension of \(W\) or \(X\). Furthermore, if \(\omega_1, \ldots, \omega_n\) are random multipliers independent of \(O_1, \ldots, O_n\) with \(\mathbb{E}(\omega_i^2) < \infty\), then the previous result holds with \(W_i\) replaced by \(\omega_i W_i\).

Proof. Consider the \(j^{th}\) element of the sum inside the max-norm:

\[
S_{njk} := \sum_{i \in I_k} W_i \{j\} h(X_i; D_{I_k}).
\]

Let \(P_K := \{I_k\}_{k=1, \ldots, K}\) represent a particular random partition of the indices \(1, \ldots, n\) into \(K\) disjoint and set with a roughly-equivalent size. As in \cite{Ertefaie et al. 2021}, we have \(\mathbb{E}(S_{njk}) = 0\) and conditional variance

\[
\mathbb{E}(S_{njk}^2 \mid D_{I_k}; P_K) \leq n_k C_W \mathbb{E}\{h^2(X_i; D_{I_k}) \mid D_{I_k}, P_K\},
\]

provided by the Cauchy-Schwarz inequality. By Chebyshev’s Inequality, we have

\[
P\left( |S_{njk}| > \varepsilon \sqrt{n} \mid D_{I_k}; P_K \right) \leq \varepsilon^{-2} n^{-1} n_k C_W \mathbb{E}\{h^2(X_i; D_{I_k}) \mid D_{I_k}, P_K\}.
\]

Since \(P_K\) is independent of the data, this conditional expectation is equal to \(\|h\|_{P_0,2}^2\). Next, make the substitution \(n^{-1} n_k = K^{-1} + o(1)\), where the \(o(1)\) term is uniform over the index \(k\) due to the finite number of folds \(K\). By hypothesis,

\[
P\left( |S_{njk}| > \varepsilon \sqrt{n} \right) \leq \{K^{-1} + o(1)\} \varepsilon^{-2} C_W o_p(r_n).
\]

Now, use the upper bound \(\sum_{k=1}^K S_{njk} \leq K \max_{k=1, \ldots, K} |S_{njk}|\) and sub-additivity of the probability measures:

\[
P\left( \sum_{k=1}^K S_{njk} > \varepsilon \sqrt{n} \right) \leq P\left( K \max_{k=1, \ldots, K} |S_{njk}| > \varepsilon \sqrt{n} \right)
= P\left( \bigcup_{k=1, \ldots, K} \{ |S_{njk}| > \varepsilon \sqrt{n} / K \} \right)
\leq \sum_{k=1}^K P\left( |S_{njk}| > \varepsilon \sqrt{n} / K \right)
\leq \{1 + o(1)\} K^2 \varepsilon^{-2} C_W \mathbb{E}(\|h\|_{P_0,2}^2).
\]

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The displayed result in the lemma statement follows as $C_W$ is a uniform bound on the variance over the index $j = 1, \ldots, d$. An application of the sub-additivity of probability measures again demonstrates that

$$P \left( \max_{1 \leq j \leq d} \left| \sum_{K=1}^{K} S_{njk} \right| > \varepsilon \sqrt{n} \right) \leq d \{1 + o(1)\} K^2 \varepsilon^{-2} C_W \mathbb{E}(\|h\|^2_{F_0,2}).$$

An application of Lemma E.4 completes the proof.

The result for random multipliers holds by similar arguments. To see this, let $S_{njk}^b$ be the analogous sum with random multipliers. By independence, $\mathbb{E}(\omega_i \mathbf{W}_i \mid \mathbf{X}_i) = 0$ and $\text{Var}(\omega_i \mathbf{W}_i \mid \mathbf{X}_i) = \mathbb{E}(\omega_i^2)\mathbb{E}(\mathbf{W}_i \otimes \mathbf{W}_i)$. The bound $C_W$ can then be replaced by $C'_W = \mathbb{E}(\omega_i^2)C_W$. The analogue of (E.2) resulting from this is

$$\mathbb{E}(S_{njk}^b \mid \mathbf{D}_{k}^{\ell}; \mathcal{P}_K) \leq C'_W n_k \|h\|^2_{F_0,2},$$

from which the remainder of the proof follows as before.

\[ \square \]

**Lemma E.6.** Suppose the setup of the previous lemma holds. Let $h_1$ and $h_2$ be two vector-valued cross-fitting functions such that for $k = 1, \ldots, K$, $i \in I_k$, and $j = 1, 2$, $h_j(X_i; D_{k})$ takes values in $\mathbb{R}^d$. Let these functions satisfy $\|h_j\|_{F_0,2} = o_p(r_{nj})$ for the sequences $r_{n1}$ and $r_{n2}$. Then for both $v = 1$ and $v = 0$,

$$\left\| n^{-1} \sum_{k=1}^{K} \sum_{i \in I_k} \omega_i^v h_1(X_i; D_{k}) h_2(X_i; D_{k}) \right\|_{\infty} = O_p(r_{n1} r_{n2}),$$

where the constant does not depend on the dimension of $\mathbf{W}$ or $\mathbf{X}$.

**Proof.** Start with the $(j, \ell)^{th}$ element of the sum inside the max-norm:

$$S_{nj\ell k} := \sum_{i \in I_k} \omega_i^v h_{1j}(X_i; D_{k}) h_{2\ell}(X_i; D_{k}),$$

where we let $h_{ab}$ be the $i^{th}$ coordinate of the $h_a$ function, $a = 1, 2$, $b = 1, \ldots, d_a$. Apply the Cauchy-Schwarz inequality to this term to find

$$n_k^{-1}|S_{nj\ell k}| \leq \left\{ \frac{1}{n_k} \sum_{i \in I_k} \omega_i^{2v} h_{1j}^2(X_i; D_{k}) \right\}^{1/2} \left\{ \frac{1}{n_k} \sum_{i \in I_k} h_{2\ell}^2(X_i; D_{k}) \right\}^{1/2}.$$  \hspace{1cm} (E.3)

For the second factor in curly braces, apply Markov’s Inequality to find

$$P \left( \sum_{i \in I_k} h_{2\ell}^2(X_i; D_{k}) > a \mid D_{k}^{\ell}, \mathcal{P}_K \right) \leq \frac{1}{a} \mathbb{E}\{h_{2\ell}^2(X_i; D_{k}) \mid D_{k}^{\ell}, \mathcal{P}_K\}$$

Integrating both sides over the distribution of $D_{k}^{\ell}$ and $\mathcal{P}_K$, the expectation on the RHS simplifies to $\mathbb{E}(\|h_{2\ell}\|^2_{F_0,2})$. If $v = 0$, then this same argument may be made for the first term in curly braces as well. This shows that

$$n_k^{-1}|S_{nj\ell k}| = O_p\left\{ \mathbb{E}(\|h_{2\ell}\|^2_{F_0,2}) \mathbb{E}(\|h_{1j}\|_{F_0,2}) \right\};$$

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which is $o_p(r_{n1}r_{n2})$ by Lemma E.4, uniformly in the indices $j$ and $\ell$. The number of folds $K$ and the dimensions $d_1, d_2 < \infty$ are fixed. Further, our notation $\|h_1\|_{p,2}$ represents the maximum of the $\|\cdot\|_{p,2}$ norm over the coordinates of $h_1$. Following similar arguments as in the proof of Lemma E.5, we have

$$
P \left( \left| \sum_{k=1}^{K} S_{nj\ell k} \right| > a \right) \leq \{ 1 + o(1) \} \frac{K}{a} o_p(r_{n1}r_{n2}).$$

Taking the maximum over $d_1 \times d_2$ elements in the resulting matrix, and using the uniformity of the previous bound in $j$ and $\ell$, use the expression below to complete the $v = 0$ case:

$$
P \left( \max_{j \leq d_1, \ell \leq d_2} \left| \sum_{k=1}^{K} S_{nj\ell k} \right| > a \right) \leq d_1d_2 \{ 1 + o(1) \} \frac{K}{a} o_p(r_{n1}r_{n2}).$$

To handle the $v = 1$ case, we need only handle the first curly-braced term in (E.3). Apply the Markov’s inequality argument and leverage the independence $\omega_i \perp \perp O_i$, to find

$$
P \left( \frac{1}{n_k} \sum_{i \in I_k} \omega_i^2 h^2_{ij}(X_i; D_{1k}) > a \right) | D_{1k}, \mathcal{P}_K \right) \leq \frac{1}{a} \mathbb{E} (\omega^2_i) \mathbb{E} \left\{ h^2_{ij}(X_i; D_{1k}) \right\}. D_{1k}, \mathcal{P}_K \right).$$

Since $\mathbb{E} (\omega^2_i) < \infty$, the rest follows as in the $v = 0$ case, completing the proof. \qed

### E.3 Lemmas Required for the Proof of Theorem 5.1

**Lemma E.7** (Analogue of Lemma 4.1 in Kuchibhotla et al. (2020)). Suppose Assumption 5.1 holds. For all models $S_1 \in \mathcal{M}_1(C_1)$, $S_2 \in \mathcal{M}_2(C_2)$, and a data-dependent $S_2 \in \mathcal{M}_2$,

$$
\begin{align*}
\|\hat{\theta}_{2n, S_2} - \theta_{20, S_2}\|_1 & \leq \frac{|S_2| (\hat{D}^G_{2n} + \hat{D}^H_{2n} \|\theta_{20, S_2}\|_1)}{\Lambda_2(C_2) - C_2 \hat{D}^H_{2n}} \\
\|\hat{\theta}_{1n, S_1, S_2} - \theta_{10, S_1, S_2}\|_1 & \leq \frac{|S_1| (\hat{D}^G_{1n, S_2} + \hat{D}^H_{1n} \|\theta_{10, S_1, S_2}\|_1)}{\Lambda_1(C_1) - C_1 \hat{D}^H_{1n}}.
\end{align*}
$$

**Proof.** These follow using the same arguments of Kuchibhotla et al. (2020). We will follow the more complex case given by the second inequality.

For a particular $S_1 \in \mathcal{M}_1(C_1)$, we have

$$
\hat{\theta}_{1n, S_1, S_2} - \theta_{10, S_1, S_2} = \{ \hat{H}_{1n}(S_1) \}^{-1} \left[ \{ \hat{G}_{1n, S_2} - G_{10, S_2} \}(S_1) - \{ \hat{H}_{1n} - H_{10} \}(S_1) \theta_{10, S_1, S_2} \right],
$$

which results from the normal equations. Examining the $\ell_2 \mapsto \ell_2$ operator norm, we can bound

$$
\|\hat{H}_{1n}(S_1) - H_{10}(S_1)\|_{2,2} \leq |S_1| \hat{D}^H_{1n}, \tag{E.4}
$$
Assumptions 5.2 and 5.3 hold, then
\[ \|\hat{H}_{1n}(S_1)^{-1}\|_{2,2} \leq \frac{\|H_{10}(S_1)^{-1}\|_{2,2}}{1 - \|H_{10}(S_1)^{-1}\left\{\hat{H}_{1n}(S_1) - H_{10}(S_1)\right\}\|_{2,2}} \leq \left\{1/\|H_{10}(S_1)^{-1}\|_{2,2} - C_1\hat{D}_{in}^H\right\}^{-1} \leq \left\{\Lambda_1(C_1) - C_1\hat{D}_{in}^H\right\}^{-1}, \]

where the second inequality uses the sub-multiplicativity of the $\ell_2 \mapsto \ell_2$ operator norm along with (E.4) and the final inequality uses the definition of $\Lambda_1(C_1)$. Consequently, for $C_1$ satisfying $\Lambda_1(C_1) - C_1\hat{D}_{in}^H > 0$, we may bound
\[ \|\hat{\theta}_{1n,S_1\hat{S}_2} - \theta_{10,S_1\hat{S}_2}\|_2 \leq \frac{\|G_{1n,\hat{S}_2} - G_{10,\hat{S}_2}\|_2 + \|\hat{H}_{1n} - H_{10}\|_2}{\Lambda_1(C_1) - C_1\hat{D}_{in}^H} \leq \left|S_1\right|^{1/2}(\hat{D}_{in}^G + \hat{D}_{in}^H\|\theta_{10,S_1\hat{S}_2}\|_1) \leq \frac{\|S_1\|_2\|\hat{\theta}_{1n,S_1\hat{S}_2} - \theta_{10,S_1\hat{S}_2}\|_2}{\Lambda_1(C_1) - C_1\hat{D}_{in}^H}. \]

The stated result follows by applying
\[ \|\hat{\theta}_{1n,S_1\hat{S}_2} - \theta_{10,S_1\hat{S}_2}\|_1 \leq \|\hat{\theta}_{1n,S_1\hat{S}_2} - \theta_{10,S_1\hat{S}_2}\|_2. \]

**Proposition E.8.** Let $Z_\ell = A_\ell\bar{X}_\ell^0$ with $\mu_{\ell Z0} = \mu_{\ell A0}(\bar{X}_\ell)\bar{X}_\ell^0$ and $\hat{\mu}_{\ell Z} = \hat{\mu}_{\ell A}(\bar{X}_\ell)\bar{X}_\ell^0$. If Assumptions 5.2 and 5.3 hold, then
\[ \|\hat{\mu}_{\ell Z} - \mu_{\ell Z0}\|_{P_{0,2}} = o_p(n^{-1/4}) \]
\[ \|\hat{\mu}_{\ell Z} - \mu_{\ell Z0}\|_{P_{0,2}} \|\hat{\mu}_{\ell Y} - \mu_{\ell Y0}\|_{P_{0,2}} = o_p(n^{-1/2}) \]
\[ \|\hat{\mu}_{\ell Z} - \mu_{\ell Z0}\|_{P_{0,2}} \|\hat{\mu}_{\ell Y} - \mu_{\ell Y0}\|_{P_{0,2}} = o_p(n^{-1/2}), \]

where the norm $\|v\|_{P_{0,2}} = \max_{j=1,...,d} \|v(\{j\})\|_{P_{0,2}}$ for $d$-dimensional $v$.

**Proof.** Simple inequalities show that
\[ \|\hat{\mu}_{\ell Z} - \mu_{\ell Z0}\|_{P_{0,2}} = \|(\hat{\mu}_{\ell A} - \mu_{\ell A0})(\bar{X}_\ell)\bar{X}_\ell^0\|_{P_{0,2}} \leq C \|\hat{\mu}_{\ell A} - \mu_{\ell A0}\|_{P_{0,2}}. \]

Consequently, the stated rates follow directly from Assumption 5.3. \qed

**Lemma E.9.** If Assumptions 5.2 and 5.3 hold, then:
\[ \|\hat{H}_{1n} - H_{1n}\|_\infty = o_p(n^{-1/2}) \]
\[ \|\hat{H}_{1n}^p - H_{1n}^p\|_\infty = o_p(n^{-1/2}) \]
\[ \max_{S_\ell \in M_\ell} \|\hat{H}_{1n}(S_\ell)^{-1} - H_{1n}(S_\ell)^{-1}\|_\infty = o_p(n^{-1/2}) \]
\[ \max_{S_\ell \in M_\ell} \|\hat{H}_{1n}(S_\ell)^{-1} - H_{1n}(S_\ell)^{-1}\|_\infty = o_p(n^{-1/2}) \]


Proof. We begin by defining the difference
\[ \varphi^H_{\ell i} := (Z_{\ell i} - \hat{\mu}_{\ell Zi})^2 - (Z_{\ell i} - \mu_{\ell Z0i})^2 \]
for \( i = 1, \ldots, n \). By adding and subtracting terms, we may express this as
\[ \varphi^H_{\ell i} = (\hat{\mu}_{\ell Zi} - \mu_{\ell Z0i})^2 + (\hat{\mu}_{\ell Zi} - \mu_{\ell Z0i})(Z_{\ell i} - \mu_{\ell Z0i})^T + (Z_{\ell i} - \mu_{\ell Z0i})(\hat{\mu}_{\ell Zi} - \mu_{\ell Z0i})^T. \]
(E.9)

To prove (E.5) and (E.6), re-express the differences as
\[ \hat{H}_{\ell n} - \tilde{H}_{\ell n} = \frac{1}{n} \sum_{i=1}^{n} \varphi^H_{\ell i} \]
\[ \hat{H}^b_{\ell n} - \tilde{H}^b_{\ell n} = \frac{1}{n} \sum_{i=1}^{n} \omega_i \varphi^H_{\ell i}. \]

Since Lemmas E.5 and E.6 apply either in the presence or absence of these random multipliers, we focus on the argument for (E.5). Of the three terms comprising (E.9), the first satisfies the conditions of Lemma E.6 while the final two satisfy those of Lemma E.5. Consequently,
\[ \frac{1}{n} \sum_{i=1}^{n} \{(\hat{\mu}_{\ell Zi} - \mu_{\ell Z0i})(Z_{\ell i} - \mu_{\ell Z0i})^T + (Z_{\ell i} - \mu_{\ell Z0i})(\hat{\mu}_{\ell Zi} - \mu_{\ell Z0i})^T\} = o_p(n^{-3/4}) \]
\[ \frac{1}{n} \sum_{i=1}^{n} (\hat{\mu}_{\ell Zi} - \mu_{\ell Z0i})^2 = o_p(n^{-1/2}) \]
under Assumptions 5.2 and 5.3 which establishes the first two equations.

Equation (E.7) follows from (E.5) along with Lemma E.2. Specifically, Assumption 5.1 and the arguments in the proof of Lemma E.7 ensure that
\[ \|\hat{H}_{\ell n}(S_\ell)^{-1}\|_\infty \leq \left\{A_\ell(C_\ell) - C_\ell \|\hat{H}_{\ell n} - \tilde{H}_{\ell n}\|_\infty\right\}^{-1}, \]
since \( \|A\|_\infty \leq \|A\|_2 \) for a matrix \( A \). Condition (ii) follows from this fixed bound along with the previously established rates. Consequently, the \( o_p(n^{-1/2}) \) results established previously ensure that the inverses also obey this rate. Using the result of Lemma E.2 we obtain the first of the following series of inequalities:
\[ \|\hat{H}_{\ell n}(S_\ell)^{-1} - \hat{H}_{\ell n}(S_\ell)^{-1}\|_\infty \leq \frac{2\|\hat{H}_{\ell n}(S_\ell) - \hat{H}_{\ell n}(S_\ell)\|_\infty}{\left\{A_\ell(C_\ell) - C_\ell \|\hat{H}_{\ell n} - \tilde{H}_{\ell n}\|_\infty\right\}^2} \leq \frac{2\|\hat{H}_{\ell n}(S_\ell) - \hat{H}_{\ell n}(S_\ell)\|_\infty}{\left\{c_0 - C_\ell \|\hat{H}_{\ell n} - \tilde{H}_{\ell n}\|_\infty\right\}^2} \leq \frac{2\|\hat{H}_{\ell n} - \tilde{H}_{\ell n}\|_\infty}{\left\{c_0 - C_\ell \|\hat{H}_{\ell n} - \tilde{H}_{\ell n}\|_\infty\right\}^2}, \]
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where the final two inequalities follow from the lower bound $c_0$ on $\Lambda_f(C_\ell)$, and the upper bound $\|H_0(S_\ell) - \hat{H}_0(S_\ell)\|_\infty \leq \|H_{fn} - \hat{H}_{fn}\|_\infty$, respectively. In this final expression, the denominator converges to $c_2^2$ in probability and the numerator is $o_p(n^{-1/2})$, which both follow from (E.5). Consequently, the entire expression is $o_p(n^{-1/2})$. A similar argument establishes the final result (E.8) using (E.6).

E.4 Lemmas Required for the Proof of Theorem 5.2

This section includes several results needed to prove the main lemmas used in the proof of Theorem 5.2. To organize these results, we focus on three sets:

1. those used to show that the stage 2 estimators have an influence function representation uniformly over the stage 2 models $S_2 \in M_2(C_2)$ (Appendix E.4.1),

2. those used to establish the asymptotic negligibility of cross-fitting in stage 1 (Appendix E.4.2); and

3. those used to show that the stage 1 estimators have an influence function representation uniformly over the stage 1 models $S_1 \in M_1(C_1)$ (Appendix E.4.3).

E.4.1 Results Establishing an Influence Function in the Second Stage

Proposition E.10. Under Assumptions 5.2 and 5.3,

$$\|\hat{G}_{2n} - \tilde{G}_{2n}\|_\infty = o_p(n^{-1/2})$$

(E.10)

$$\|\hat{G}_{2n}^b - \tilde{G}_{2n}^b\|_\infty = o_p^*(n^{-1/2}).$$

(E.11)

Proof. As in the proof of Lemma E.9, begin by writing (E.10) and (E.11) as

$$\hat{G}_{2n} - \tilde{G}_{2n} = \frac{1}{n} \sum_{i=1}^{n} \varphi_{G_{2i}}^G,$$

$$\hat{G}_{2n}^b - \tilde{G}_{2n}^b = \frac{1}{n} \sum_{i=1}^{n} \omega_i \varphi_{G_{2i}}^G,$$

where we define for $i = 1, \ldots, n$, the term inside the sum as

$$\varphi_{G_{2i}}^G := (Z_{2i} - \hat{\mu}_{2Zi})(Y_i - \hat{\mu}_{2Yi}) - (Z_{2i} - \mu_{2Z0i})(Y_i - \mu_{2Y0i}).$$

By adding and subtracting terms, we arrive at the expression

$$\varphi_{G_{2i}}^G = (Z_{2i} - \mu_{2Z0i})(\mu_{2Y0i} - \hat{\mu}_{2Yi})$$

(E.12)

$$+ (\mu_{2Azi} - \hat{\mu}_{2Ai})\{\bar{X}_{2i}^0(Y_i - \mu_{2Y0i})\}$$

(E.13)

$$+ (\mu_{2Z0i} - \hat{\mu}_{2Zi})(\mu_{2Y0i} - \hat{\mu}_{2Yi}),$$

(E.14)

where we’ve substituted the identity $\mu_{2Z0i} - \hat{\mu}_{2Zi} = (\mu_{2Azi} - \hat{\mu}_{2Ai})\bar{X}_{2i}^0$ in (E.13).

As in the proof of Lemma E.9, we plan to use Lemmas E.5 and E.6 to show the results (E.10) and (E.11). Consequently, we focus only on the former result, as the random multiplier...
Consequently, under the conditions of Theorem 5.1, cross-fitting approximates the oracle estimators uniformly in probability over sparse models:

\[
\frac{1}{n} \sum_{i=1}^{n} \{(Z_{2i} - \mu_{2Z0i})(\mu_{2Y0i} - \hat{\mu}_{2Yi}) + (\mu_{2A0i} - \hat{\mu}_{2Ai})X_{2i}(Y_i - \mu_{2Y0i})\} = o_p(n^{-1/2}).
\]

For the final term (E.14), we may apply Proposition E.8 with Lemma E.6 to show

\[
\frac{1}{n} \sum_{i=1}^{n} (\mu_{2Z0i} - \hat{\mu}_{2Zi})(\mu_{2Y0i} - \hat{\mu}_{2Yi}) = o_p(n^{-1/2}),
\]

concluding the proof of (E.10). The result (E.11) follows similarly.

Lemma E.11. Under Assumptions 5.1 and 5.4, the following inequalities hold for any \( S_1 \in \mathcal{M}_1(C_1) \) and \( S_2 \in \mathcal{M}_2(C_2) \):

\[
\|\hat{\theta}_{2n,S_2} - \bar{\theta}_{2n,S_2}\|_1 \leq \frac{|S_2|((\|\bar{G}_{2n} - \bar{G}_{2n}\|_\infty + \|\bar{H}_{2n} - \bar{H}_{2n}\|_\infty)\|\hat{\theta}_{2n,S_2}\|_1)}{\Lambda_2(C_2) - C_2D_{2n}^H} + \|\hat{\theta}_{2n,S_2}\|_1,
\]

\[
\|\hat{\theta}_{1n,S_1S_2} - \bar{\theta}_{1n,S_1S_2}\|_1 \leq \frac{|S_1|((\|\bar{G}_{1n,S_2} - \bar{G}_{1n,S_2}\|_\infty + \|\bar{H}_{1n} - \bar{H}_{1n}\|_\infty)\|\hat{\theta}_{1n,S_1S_2}\|_1)}{\Lambda_2(C_2) - C_2D_{2n}^H} + \|\hat{\theta}_{1n,S_1S_2}\|_1.
\]

Consequently, under the conditions of Theorem 5.1, cross-fitting approximates the oracle estimators uniformly in probability over sparse models:

\[
\max_{S_2 \in \mathcal{M}_2(C_2)} \|\hat{\theta}_{2n,S_2} - \bar{\theta}_{2n,S_2}\|_1 = o_p(n^{-1/2})
\]

\[
\max_{S_1 \in \mathcal{M}_1(C_1)} \|\hat{\theta}_{1n,S_1S_2} - \bar{\theta}_{1n,S_1S_2}\|_1 = o_p(n^{-1/2}).
\]

Proof. We may prove this using a similar argument as in Lemma E.7. We sketch out a few relevant expressions in the argument for the inequality in Stage 1. First, use Lemma E.1 along with Assumption 5.4 to conclude that

\[
\|\hat{\theta}_{1n,S_1S_2} - \bar{\theta}_{1n,S_1S_2}\|_1 = \|\hat{\theta}_{1n,S_1S_2} - \bar{\theta}_{1n,S_1S_2}\|_1 + o_p(n^{-1/2}).
\]

The first-order equations ensure:

\[
\hat{\theta}_{1n,S_1S_2} - \bar{\theta}_{1n,S_1S_2} = \left(\hat{H}_{1n}(S_1)\right)^{-1} \left[\{\bar{G}_{1n,S_2} - \bar{G}_{1n,S_2}\}(S_1) - \{\bar{H}_{1n} - \bar{H}_{1n}\}(S_1)\right]_{1n,S_1S_2}.
\]

Similarly, the \(\ell_2 \mapsto \ell_2\) operator norm bound below follows:

\[
\|\hat{H}_{1n}(S_1) - \bar{H}_{1n}(S_1)\|_{2,2} \leq |S_1|\|\bar{H}_{1n} - \bar{H}_{1n}\|_{\infty}.
\]
Using the previously-established bound on $\|\widehat{H}_2n(S_2)^{-1}\|_{2,2}$, we can derive the expression

$$
\|\hat{\theta}_{1n,S_1} - \tilde{\theta}_{1n,S_1}\|_2 \leq |S_1|^{1/2} \frac{\|\bar{G}_{1n,S_1} - \bar{G}_{1n,S_2}\|_\infty + \|\tilde{H}_2n - \bar{H}_nn\|_\infty \|\hat{\theta}_{1n,S_1} - \hat{\theta}_{1n,S_2}\|_1}{A_1(C_1) - C_1\tilde{D}_{1n}^H},
$$

(E.15)

which allows us to establish the first result using the relationship between $\ell_1$ and $\ell_2$ norms.

Now we may establish the uniform rate on $\|\hat{\theta}_{1n,S_1} - \tilde{\theta}_{1n,S_1}\|_1$ using this inequality. The term $\max_{S_1 \in \mathcal{M}_1(C_1)} |\tilde{\theta}_{1n,S_1}| = O_p(1)$ using Lemma 4.1 in Kuchibhotla et al. (2020) and the two remaining terms in the numerator are $o_p(n^{-1/2})$ by Lemmas E.9 and E.13 uniformly over $\mathcal{M}_1(C_1)$. Finally, the denominator converges in probability to a term bounded from below by $c_0$ according to Assumption 5.1. The continuous mapping theorem implies that the RHS of (E.15) is $o_p(n^{-1/2})$, completing the proof. \hfill $\square$

**Lemma E.12.** Under the conditions for Lemmas E.9 and E.11, the following property holds for any $S_2 \in \mathcal{M}_2(C_2)$:

$$
\left\|\hat{\theta}_{2n,S_2} - \theta_{2n,S_2}\right\|_\infty = O_p\left(n^{-1/2}\right)
$$

(E.16)

$$
\left\|\hat{\theta}_{2n,S_2} - \theta_{2n,S_2}\right\|_\infty = o_p\left(n^{-1/2}\right)
$$

(E.17)

$$
\left\|\hat{\theta}_{2n,S_2} - \theta_{2n,S_2}\right\|_\infty = o_p\left(n^{-1/2}\right),
$$

(E.18)

where we define the function

$$
\text{Inf}_{2S_2i} = H_{2n}(S_2)^{-1}(A_{2i} - \mu_{2A0i})X_{2i}^0(S_2) \left\{Y_i - \mu_{2Y0i} - (A_{2i} - \mu_{2A0i})X_{2i}^0(S_2)^\top \theta_{20,S_2}\right\}.
$$

**Proof.** Begin with (E.16). Under Lemma E.11 we may replace $\hat{\theta}_{2n,S_2}$ in this expression by $\tilde{\theta}_{2n,S_2}$ without affecting the remainder. Doing so, we write

$$
\hat{\theta}_{2n,S_2} - \theta_{2n,S_2} = H_{2n}(S_2)^{-1}\bar{G}_{2n}(S_2) - \theta_{2n,S_2} = H_{2n}(S_2)^{-1}\left\{\bar{G}_{2n}(S_2) - \bar{H}_{2n}(S_2)\theta_{20,S_2}\right\}
$$

Next, we express the sum

$$
\frac{1}{n} \sum_{i=1}^n \text{Inf}_{2S_2i} = H_{2n}(S_2)^{-1}\left\{\bar{G}_{2n}(S_2) - \bar{H}_{2n}(S_2)\theta_{20,S_2}\right\},
$$

and hence $R_{n,S_2} = \hat{\theta}_{2n,S_2} - \theta_{2n,S_2} - \frac{1}{n} \sum_{i=1}^n \text{Inf}_{2S_2i}$ may be written

$$
R_{n,S_2} = \left\{\bar{H}_{2n}(S_2)^{-1} - H_{2n}(S_2)^{-1}\right\}\left\{\bar{G}_{2n}(S_2) - \bar{H}_{2n}(S_2)\theta_{20,S_2}\right\}.
$$

(E.19)

The $\ell_0$ norm of the second quantity in curly braces is bounded by $C_2$ by the definition of $\mathcal{M}_2(C_2)$. Using the relationship $\|Ab\|_\infty \leq \|A\|_\infty \|b\|_0 \|b\|_\infty$ for matrix $A$ and vector $b$, we may bound the remainder (E.19) by

$$
C_2\|\bar{H}_{2n}(S_2)^{-1} - H_{2n}(S_2)^{-1}\|_\infty \|\bar{G}_{2n}(S_2) - \bar{H}_{2n}(S_2)\theta_{20,S_2}\|_\infty.
$$

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Under Lemma E.2, the first normed quantity is $O_p(n^{-1/2})$ and so the proof will be complete if $\|\hat{G}_{2n}(S_2) - \hat{H}_{2n}(S_2)\theta_{20,S_2}\|_\infty = o_p(1)$. To this end, express the quantity

$$\hat{G}_{2n}(S_2) - \hat{H}_{2n}(S_2)\theta_{20,S_2} = \frac{1}{n} \sum_{i=1}^n (A_{2i} - \mu_{2A_0}) \hat{X}_2(S_2)e_{2,S_2},$$

which is a sample average of $|S_2|$-dimensional random variables having mean zero. Consequently, the above term is $O_p(n^{-1/2})$. Consequently, the remainder term is $O_p(n^{-1}) = o_p(n^{-1/2})$.

Next, we use similar arguments to handle (E.17). Again, we may replace $\hat{\theta}_{2n,S_2}^b$ by the oracle term $\hat{\theta}_{2n,S_2}^b$. Writing the bootstrap error

$$\hat{\theta}_{2n,S_2}^b - \theta_{20,S_2} = \hat{H}_{2n}(S_2)^{-1} \left\{ G_{2n}(S_2) - \hat{H}_{2n}(S_2)\theta_{20,S_2} \right\},$$

along with the desired influence function-based sample average:

$$\frac{1}{n} \sum_{i=1}^n \omega_i \text{Inf}_{2S_2i} = H_{20}(S_2)^{-1} \left\{ G_{2n}(S_2) - \hat{H}_{2n}(S_2)\theta_{20,S_2} \right\},$$

we can express their difference with a similar remainder term:

$$\hat{\theta}_{2n,S_2}^b - \theta_{20,S_2} - \frac{1}{n} \sum_{i=1}^n \omega_i \text{Inf}_{2S_2i}$$

$$= \left\{ \hat{H}_{2n}(S_2)^{-1} - H_{20}(S_2)^{-1} \right\} \left\{ G_{2n}(S_2) - \hat{H}_{2n}(S_2)\theta_{20,S_2} \right\}. $$

By similar arguments as in the (E.16) case, this remainder can be shown to be $o_p^*(n^{-1/2})$.

The final expression [E.18] is a direct consequence of the two previous expressions, along with the triangle inequality. □

### E.4.2 Results Establishing the Asymptotic Negligibility of Cross-fitting in the First Stage

**Lemma E.13.** Under Assumptions 5.1–5.3, the following rates hold:

$$\|\hat{G}_{1n,S_2}^G - \hat{G}_{1n,S_2}^b\|_\infty = o_p(n^{-1/2}) \tag{E.20}$$

$$\|\hat{G}_{1n,S_2}^b - \hat{G}_{1n,S_2}^b\|_\infty = o_p^*(n^{-1/2}). \tag{E.21}$$

**Proof.** We will follow the general strategy as in the proof of Proposition E.10, which demonstrated similar properties in the second stage. Additionally, we must handle complexities arising from the pseudo-outcomes. To establish (E.20), we first write the sums

$$\hat{G}_{1n,S_2}^G - \hat{G}_{1n,S_2}^b = \frac{1}{n} \sum_{i=1}^n \varphi_{1i}^G$$

$$\hat{G}_{1n,S_2}^b - \hat{G}_{1n,S_2}^b = \frac{1}{n} \sum_{i=1}^n \omega_i \varphi_{1i}^G,$$
where we define for \( i = 1, \ldots, n \), the term inside the sum as 
\[
\varphi^G_{i} := (Z_{ii} - \mu_{1Zi})(\hat{Y}_{1S^*_i} - \hat{\mu}_{1YS^*_i}) - (Z_{ii} - \mu_{1Z0i})(\hat{Y}_{1S^*_i} - \hat{\mu}_{1YS^*_0i}).
\]

Following along the previous proof, we expand the representation of \( \varphi^G_{i} \) to find 
\[
\varphi^G_{i} = (Z_{ii} - \mu_{1Z0i})(\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}) + (Z_{ii} - \mu_{1Z0i})(\mu_{1YS^*_0i} - \hat{\mu}_{1YS^*_i}) + (\mu_{1Z0i} - \mu_{1Zi})(\hat{Y}_{1S^*_i} - \hat{\mu}_{1YS^*_i}). \tag{E.22}
\]

This last line involves both the estimated conditional expectation as well as the estimated pseudo-outcome. Expand this problematic term into three summands:
\[
\hat{Y}_{1S^*_i} - \hat{\mu}_{1YS^*_i} = (\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}) + (\hat{Y}_{1S^*_i} - \mu_{1YS^*_0i}) + (\mu_{1YS^*_0i} - \hat{\mu}_{1YS^*_i}).
\]

Substituting this into (E.22), we obtain 
\[
\varphi^G_{i} = (Z_{ii} - \mu_{1Z0i})(\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}) \tag{E.23}
\]
\[
+ (\mu_{1Z0i} - \mu_{1Zi})(\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}) \tag{E.24}
\]
\[
+ (\mu_{1Z0i} - \mu_{1Zi})(\mu_{1YS^*_0i} - \hat{\mu}_{1YS^*_i}) \tag{E.25}
\]
\[
+ \{X^0_1(\mu_{1A0i} - \hat{\mu}_{1Ai})\} (\hat{Y}_{1S^*_i} - \mu_{1YS^*_0i}) \tag{E.26}
\]
\[
+ (\mu_{1Z0i} - \mu_{1Zi})(\mu_{1YS^*_0i} - \hat{\mu}_{1YS^*_i}). \tag{E.27}
\]

where we made the additional substitution \((\mu_{1Z0i} - \mu_{1Zi}) = X^0_1(\mu_{1A0i} - \hat{\mu}_{1Ai}) \) in (E.26).

Analogous to the proof of Proposition E.10, Lemma E.5 applies to (E.25) and (E.26), while Lemma E.6 applies to (E.27). Assumption 5.3 as well as Proposition E.8 ensure that (E.25) and (E.27) are \( o_p(n^{-1/2}) \) when averaged over \( i = 1, \ldots, n \). The outcome of these lemmas are not impacted by the random multipliers.

To examine the rates of (E.23) and (E.24), we re-write the expression 
\[
\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i} = -A_2X^0_2(\hat{\theta}_{2n,S^*_2} - \hat{\theta}_{2n,S^*_2}) + \{X^0_2(S^*_2)^\top \hat{\theta}_{2n,S^*_2}\}_+ - \{X^0_2(S^*_2)^\top \hat{\theta}_{2n,S^*_2}\}_+.
\]

Now we use the triangle inequality and the inequality \(|A_+ - B_+| \leq 2|A - B|\):
\[
|\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}| \leq |A_2X^0_2(S^*_2)^\top (\hat{\theta}_{2n,S^*_2} - \hat{\theta}_{2n,S^*_2})| + |\{X^0_2(S^*_2)^\top \hat{\theta}_{2n,S^*_2}\}_+ - \{X^0_2(S^*_2)^\top \hat{\theta}_{2n,S^*_2}\}_+| \\
\leq C\|\hat{\theta}_{2n,S^*_2} - \hat{\theta}_{2n,S^*_2}\| + 2C\|\hat{\theta}_{2n,S^*_2} - \hat{\theta}_{2n,S^*_2}\|1.
\]

This is a uniform rate over all the observed samples; as such, the maximum \( \max_{i=1,\ldots,n}|\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}| \) is uniformly bounded by some constant multiple of the difference \( \|\hat{\theta}_{2n,S^*_2} - \hat{\theta}_{2n,S^*_2}\|1 \). Use Lemma E.11 to conclude that \( \max_{i=1,\ldots,n}|\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}| = o_p(n^{-1/2}) \). Multiply the sample average of the terms in (E.23) by \( \sqrt{n} \) and take the modulus to obtain 
\[
\left|n^{-1/2}\sum_{i=1}^{n}(Z_{ii} - \mu_{1Z0i})(\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i})\right| \leq n^{-1/2}\sum_{i=1}^{n}\|Z_{ii} - \mu_{1Z0i}\|\infty |\hat{Y}_{1S^*_i} - \hat{Y}_{1S^*_i}| \tag{E.28}
\]

Because \( \|Z_{ii} - \mu_{1Z0i}\|\infty \leq C \) and the maximum is taken over finitely-many elements, its sample mean converges. Furthermore, the bound on the maximum of the remaining factor
of the RHS ensures that the conditions of Lemma E.3 are satisfied. Consequently, (E.28)
is \( o_p(1) \). The conclusion of this lemma likewise does not change in the presence of random
multipliers; to see this, notice that the average

\[
\frac{1}{n} \sum_{i=1}^{n} \omega_i \|Z_{1i} - \mu_{1Z0i}\|_\infty
\]

also converges in probability due to independence of \( \omega_i \) and the other term.

A very similar argument can be used for (E.24). Writing the desired term and applying
similar bounds as in (E.28) we need to show that

\[
n^{-1/2} \sum_{i=1}^{n} \left\| \mu_{1Z0i} - \hat{\mu}_{1Zi} \right\|_\infty |\tilde{Y}_{1S^*_i} - \tilde{Y}_{1S^*_i}|\n\]

converges in probability to zero, which would follow from Lemma E.3 if

\[
\frac{1}{n} \sum_{i=1}^{n} \left\| (\mu_{1A0i} - \hat{\mu}_{1Ai})X^0_{1i} \right\|_\infty \leq C \frac{1}{n} \sum_{k=1}^{K} \sum_{i \in I_k} |\mu_{1A0i} - \hat{\mu}_{1Ai}|
\]

converges in probability to some constant, where we have re-written the sum on the RHS to
draw attention to the fold structure. We can apply Markov’s inequality to each of the
\( K \) folds to ensure that this piece is \( o_p(1) \). This also holds in the presence of random multipliers: for the \( k^{th} \) fold, we have

\[
\frac{1}{n_k} \sum_{i \in I_k} |\omega_i| |\mu_{1A0i} - \hat{\mu}_{1Ai}| \xrightarrow{p^*} \mathbb{E}[G | \mathbb{E} \{ |\mu_{1A0} - \hat{\mu}_{1A} | \mid D_{1k} \}]
\]

where we recall that \( n_k := |I_k| \) and \( n_k/n = K + o_p(1) \). By Assumption 5.3 this last quantity
converges to zero.

We have handled each of the terms (E.23)–(E.27) when averaged over the \( n \) indices, also
accounting for the addition random multipliers. This completes the proof. \( \square \)

**Lemma E.14.** Under Assumptions 5.1–5.5, we have

\[
\begin{align*}
\|\hat{G}_{1n,S^*_2} - G_{10,S^*_2}\|_\infty &= \|\hat{G}_{1n,S^*_2} - G_{10,S^*_2}\|_\infty + o_p(n^{-1/2}) \\
\|\hat{G}^b_{1n,S^*_2} - \hat{G}_{1n,S^*_2}\|_\infty &= \|\hat{G}^b_{1n,S^*_2} - \hat{G}_{1n,S^*_2}\|_\infty + o_p(n^{-1/2})
\end{align*}
\]

**Proof.** Decompose the first term as

\[
\begin{align*}
\|\hat{G}_{1n,S^*_2} - G_{10,S^*_2}\|_\infty &= \|\hat{G}_{1n,S^*_2} - \hat{G}_{1n,S^*_2}\|_\infty + \|\hat{G}_{1n,S^*_2} - G_{1n,S^*_2}\|_\infty + \|G_{1n,S^*_2} - G_{10,S^*_2}\|_\infty.
\end{align*}
\]

We need to show that the first two terms are \( o_p(n^{-1/2}) \). Viewing \( \{G_{1n,S^2} : S^2 \in \mathcal{M}_2\} \) as a
stochastic process taking values in the norm-induced metric space \((\mathbb{R}^p, \| \cdot \|_\infty)\), notice that
it is measurable given the observed data \( O_1, \ldots, O_n \), the partition \( \mathcal{P}_K \), and any additional randomness in the machine learning procedures which yield cross-fitted estimates. Given
all of this information, the model selection procedure \( \hat{S}_2 \) is also measurable. Consequently, \[ \text{Lemma E.1} \] applies to show that

\[
P \left( \| \hat{G}_{1n,\hat{S}_2} - \hat{G}_{1n,S^*_2} \|_\infty > \varepsilon \sqrt{n} \right) \leq P \left( \| \hat{G}_{1n,\hat{S}_2} - \hat{G}_{1n,S^*_2} \|_\infty > 0 \right) 
\leq P \left( \hat{S}_2 \neq S^*_2 \right) \rightarrow 0.
\]

The second term is \( o_p(n^{-1/2}) \) by \[ \text{Lemma E.13} \] which gives the desired result.

This same argument establishes the result for the bootstrap version. \qed

### E.4.3 Results Establishing an Influence Function in the First Stage

Now, we need to show that the UPoSI bootstrap results apply in stage 1. To this end, recall the definition in Appendix C.2 of \( B_{S_2} := 1(\mathbf{X}^0_2(S_2)^\top \theta_{20,S_2} > 0) - A_2 \). First, we need the blip function to behave like a smooth function:

**Lemma E.15** (The blip function does not have unsmooth behavior). Let \( \omega_i \) be i.i.d. random multipliers as described in Section 3.4. Further, let the random variable \( M \in \mathbb{R}^{p_1 \times |S^*_2|} \) be defined according to the expression

\[
M := B_{S_2} \left\{ A_1 - \mu_{1A0}(\bar{X}_1) \right\} \mathbf{X}^0_1 \mathbf{X}^0_2(S^*_2)^\top,
\]

with \( M_i, i = 1, \ldots, n \) the observed realizations from \( O_1, \ldots, O_n \). For both \( v = 0 \) and \( v = 1 \) under Assumptions 5.4 5.5,

\[
\frac{1}{n} \sum_{i=1}^n \omega_i^n \mathbf{X}^0_1(A_{i1} - \mu_{1A0i}) \left[ \xi \left\{ A_{2i}, \mathbf{X}^0_2(S^*_2); \bar{\theta}_{2n,S^*_2} \right\} - \xi \left\{ A_{2i}, \mathbf{X}^0_2(S^*_2); \theta_{20,S^*_2} \right\} \right] = \frac{1}{n} \sum_{i=1}^n \omega_i^n M_i \left( \bar{\theta}_{2n,S^*_2} - \theta_{20,S^*_2} \right) + o_p(n^{-1/2}) \quad (E.29)
\]

\[
= \mathbb{E}(M) \frac{1}{n} \sum_{i=1}^n \text{Inf}_{2i} + o_p(n^{-1/2}). \quad (E.30)
\]

Similarly, the perturbation bootstrap version satisfies

\[
\frac{1}{n} \sum_{i=1}^n \omega_i^n \mathbf{X}^0_1(A_{i1} - \mu_{1A0i}) \left[ \xi \left\{ A_{2i}, \mathbf{X}^0_2(S^*_2); \bar{\theta}^b_{2n,S^*_2} \right\} - \xi \left\{ A_{2i}, \mathbf{X}^0_2(S^*_2); \theta_{20,S^*_2} \right\} \right] = \mathbb{E}(M) \frac{1}{n} \sum_{i=1}^n \omega_i \text{Inf}_{2i} + o_p(n^{-1/2}). \quad (E.31)
\]

**Proof.** The arguments for \[ (E.29) \] are exactly the same as those around equations (38) and (39) in the Supplement of \[ Ertefae et al. (2021). \]

Using the definitions of \( R_{ni} = 1(\mathbf{X}^0_2(S^*_2)^\top \theta_{2n,S^*_2} > 0) - 1(\mathbf{X}^0_2(S^*_2)^\top \theta_{20,S^*_2} > 0) \) and \( R_{ni} = 1\left\{ 0 \leq |\mathbf{X}^0_2(S^*_2)^\top \theta_{20,S^*_2}| \leq |\mathbf{X}^0_2(S^*_2)^\top (\bar{\theta}_{2n,S^*_2} - \theta_{20,S^*_2})| \right\}, \) which satisfies \( |\bar{R}_{ni}| \leq R_{ni}, \)
we expand the first term:

$$\frac{1}{n} \sum_{i=1}^{n} \omega_i^{v} \bar{X}_1^0(A_{1i} - \mu_{1,01}) \left[ \xi \left\{ A_{2i}, \bar{X}_2^0(S_2^\ast) ; \bar{\theta}_{2n,s_2} \right\} - \xi \left\{ A_{2i}, \bar{X}_2^0(S_2^\ast) ; \theta_{20,s_2} \right\} \right]$$

$$= \frac{1}{n} \sum_{i=1}^{n} \omega_i^{v} \bar{X}_1^0(A_{1i} - \mu_{1,01}) B_{S_2^0}^2 \bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2})$$  \hspace{1cm} (E.32)

$$+ \frac{1}{n} \sum_{i=1}^{n} \omega_i^{v} \bar{X}_1^0(A_{1i} - \mu_{1,01}) \bar{X}_2^0(S_2^\ast)^T \theta_{20,s_2} \bar{R}_{ni}$$  \hspace{1cm} (E.33)

$$+ \frac{1}{n} \sum_{i=1}^{n} \omega_i^{v} \bar{X}_1^0(A_{1i} - \mu_{1,01}) \bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2}) \bar{R}_{ni}.$$  \hspace{1cm} (E.34)

Equation (E.33) can be bounded using

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \omega_i^{v} \bar{X}_1^0(A_{1i} - \mu_{1,01}) \bar{X}_2^0(S_2^\ast)^T \theta_{20,s_2} \bar{R}_{ni} \right\|_{\infty} \leq C \frac{1}{n} \sum_{i=1}^{n} |\omega_i^{v}| |\bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2})| R_{ni},$$

which follows from the triangle inequality, \( \| \bar{X}_1^0(A_{1i} - \mu_{1,01}) \|_{\infty} \leq C \), and

\begin{align*}
|\bar{X}_2^0(S_2^\ast)^T \theta_{20,s_2} \bar{R}_{ni}| &\leq |\bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2})| R_{ni}.
\end{align*}

A similar argument bounds (E.34).

$$\left\| \frac{1}{n} \sum_{i=1}^{n} \omega_i^{v} \bar{X}_1^0(A_{1i} - \mu_{1,01}) \bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2}) \bar{R}_{ni} \right\|_{\infty} \leq C \frac{1}{n} \sum_{i=1}^{n} |\omega_i^{v}| |\bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2})| R_{ni}.$$

Apply the Cauchy-Schwarz inequality to find

$$\frac{1}{n} \sum_{i=1}^{n} |\omega_i^{v}| |\bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2})| R_{ni} \leq C \left[ \frac{1}{n} \sum_{i=1}^{n} |\omega_i^{v}| |\bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2})|^2 \right]^{1/2} \left[ \frac{1}{n} \sum_{i=1}^{n} R_{ni}^2 \right]^{1/2}.$$

Using Holder’s inequality, we can bound \( |\bar{X}_2^0(S_2^\ast)^T (\bar{\theta}_{2n,s_2} - \theta_{20,s_2})| \leq \| \bar{X}_2^0(S_2^\ast)^T \|_{\infty} \| \bar{\theta}_{2n,s_2} - \theta_{20,s_2} \|_1 \). Markov’s inequality and the independence of \( \omega_i \) and \( O_i \) can be used to show that the first bracketed quantity is \( O_p^\ast(\| \bar{\theta}_{2n,s_2} - \theta_{20,s_2} \|_1) \). By the arguments on page 14 of the supplement of Ertefaie et al. (2021), the second term is \( o_p^\ast(1) \). Consequently, the rate
We arrive at the result if we show the remainder satisfies \(E\) demonstrates that \((E.33), (E.34)\) are each \(o_p(n^{-1/2})\). This demonstrates the desired remainder term \((E.29)\).

Next, we establish \((E.30)\). We can write \((E.32)\) as an i.i.d. sum of a matrix-valued random variable \(M_i \in \mathbb{R}^{p_1 \times S_2^*}\) with \(\|M\|_\infty \leq C^2\):

\[
\left( n^{-1} \sum_{i=1}^n \omega_i^* M_i \right) \left( \tilde{\theta}_{2n,S_2^*} - \theta_{20,S_2^*} \right).
\]

Adding and subtracting \(E(\,G^*M) \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i,\) equation \((E.32)\) equals:

\[
\mathbb{E}(\,G^*M \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i) + R_{nG1S_2^*}.
\]

\[
R_{nG1S_2^*} := \left( n^{-1} \sum_{i=1}^n \omega_i^* M_i \right) \left( \tilde{\theta}_{2n,S_2^*} - \theta_{20,S_2^*} \right) - \mathbb{E}(\,G^*M \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i).
\]

We arrive at the result if we show the remainder satisfies \(\|R_{nG1S_2^*}\|_\infty = o_p(n^{-1/2})\). Expanding the remainder, we have

\[
R_{nG1S_2^*} = \left\{ n^{-1} \sum_{i=1}^n \omega_i^* M_i - \mathbb{E}(\,G^*M) \right\} \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i
\]

\[
+ \mathbb{E}(\,G^*M) \left( \tilde{\theta}_{2n,S_2^*} - \theta_{20,S_2^*} - \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i \right)
\]

\[
+ \left\{ n^{-1} \sum_{i=1}^n \omega_i^* M_i - \mathbb{E}(\,G^*M) \right\} \left( \tilde{\theta}_{2n,S_2^*} - \theta_{20,S_2^*} - \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i \right).
\]

Next, apply the triangle inequality to the \(\ell_\infty\) norm and use the property \(\|MV\|_\infty \leq \|M\|_\infty \|V\|_1 \leq \|M\|_\infty \|V\|_0 \|V\|_\infty\) for any matrix \(M\) and vector \(V\) to find

\[
\|R_{nG1S_2^*}\|_\infty = |S_2^*| \left\| n^{-1} \sum_{i=1}^n \omega_i^* M_i - \mathbb{E}(\,G^*M) \right\|_\infty \left\| \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i \right\|_\infty
\]

\[
+ |S_2^*| \|\mathbb{E}(\,G^*M)\|_\infty \left\| \tilde{\theta}_{2n,S_2^*} - \theta_{20,S_2^*} - \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i \right\|_\infty
\]

\[
+ |S_2^*| \left\| n^{-1} \sum_{i=1}^n \omega_i^* M_i - \mathbb{E}(\,G^*M) \right\|_\infty \left\| \tilde{\theta}_{2n,S_2^*} - \theta_{20,S_2^*} - \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i \right\|_\infty.
\]

By \(\text{Lemma E.12}\), \(\left\| \tilde{\theta}_{2n,S_2^*} - \theta_{20,S_2^*} - \frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i \right\|_\infty = o_p(n^{-1/2})\). By the law of large numbers, \(\frac{1}{n} \sum_{i=1}^n \text{Inf}_2S_2^* i = o_p(1)\). If \(\left\| n^{-1} \sum_{i=1}^n \omega_i^* M_i - \mathbb{E}(\,G^*M)\right\|_\infty = O_p(n^{-1/2})\), then \(\|R_{nG1S_2^*}\|_\infty = o_p(n^{-1/2})\). Since \(\|M\|_\infty \leq C^2\), the term being analyzed is the maximum over a finite number of sample means with expectation zero and finite variance. Consequently, the required rate holds, establishing \((E.30)\).
Under Assumptions 5.1–5.5, the remaining arguments follow as before, using the influence function representation of \( \delta > 0 \) which are defined similarly to the non-bootstrapped versions \( \tilde{R}_{ni}^b \) and \( R_{ni} \), respectively. The definitions of these bootstrap analogs, replace \( \theta_{ni} \), wherever it appears by \( \tilde{\theta}_{ni}^b \). Following through with the arguments, we merely need to show that
\[
\frac{1}{n} \sum_{i=1}^{n} R_{ni}^b = o_p(1).
\]

Using Markov’s inequality, this follows if \( \mathbb{E}(R_{n1}^b) \to 0 \). Given its definition,
\[
\mathbb{E}(R_{n1}^b) = P \left\{ 0 \leq |\tilde{X}_2^b(S^*_2)^\top \theta_{20,S^*_2}| \leq |\tilde{X}_2^b(S^*_2)^\top (\tilde{\theta}_{2n,S^*_2} - \theta_{20,S^*_2})| \right\}.
\]

By the influence function representation of Lemma E.12, \( \tilde{\theta}_{2n,S^*_2} - \theta_{20,S^*_2} = o_p(1) \). Consequently, if \( |\tilde{X}_2^b(S^*_2)^\top \theta_{20,S^*_2}| > 0 \) almost surely, then for any \( \delta > 0 \) we may find \( \gamma > 0 \) such that \( P \left( |\tilde{X}_2^b(S^*_2)^\top \theta_{20,S^*_2}| < \gamma \right) \leq \delta \). Notice that we are assured \( \gamma > 0 \) since \( |\tilde{X}_2^b(S^*_2)^\top \theta_{20,S^*_2}| > 0 \) almost surely. Then bound the expectation
\[
\mathbb{E}(R_{n1}^b) \leq P \left\{ 0 \leq |\tilde{X}_2^b(S^*_2)^\top \theta_{20,S^*_2}| \leq |\tilde{X}_2^b(S^*_2)^\top (\tilde{\theta}_{2n,S^*_2} - \theta_{20,S^*_2})|, |\tilde{X}_2^b(S^*_2)^\top \theta_{20,S^*_2}| \geq \gamma \right\} + \delta.
\]

The probability on the RHS is bounded by
\[
P \left\{ 0 \leq \gamma \leq |\tilde{X}_2^b(S^*_2)^\top (\tilde{\theta}_{2n,S^*_2} - \theta_{20,S^*_2})|, |\tilde{X}_2^b(S^*_2)^\top \theta_{20,S^*_2}| \geq \gamma \right\} \to 0,
\]
where the convergence results from the consistency of the bootstrap estimator. Since \( \delta > 0 \) is arbitrary, this ensures that \( \mathbb{E}(R_{n1}^b) \to 0 \).

Continuing along in the analogous argument, we have shown that the top line of (E.31) is equal to
\[
\left( n^{-1} \sum_{i=1}^{n} \omega_i^b M_i \right) \left( \tilde{\theta}_{2n,S^*_2}^b - \theta_{20,S^*_2} \right).
\]

The remaining arguments follow as before, using the influence function representation of \( n^{-1} \sum_{i=1}^{n} \omega_i \text{Inf}_{2S^*_2;i} \), resulting from Lemma E.12.

\[\square\]

Lemma E.16. Let the random variable \( M \) be defined as in Lemma E.15. Define the function
\[
\text{Inf}_{1GS^*_2;i} := \tilde{X}_1^0(A_{1i} - \mu_{1A}) \epsilon_{1S^*_2;i} + E(M) \text{Inf}_{2S^*_2;i}.
\]

Under Assumptions 5.1–5.5
\[
\tilde{G}_{1n,S^*_2} - G_{10,S^*_2} = \frac{1}{n} \sum_{i=1}^{n} \text{Inf}_{1GS^*_2;i} + o_p(n^{-1/2}) \quad \text{(E.35)}
\]
\[
\tilde{G}_{1n,S^*_2}^b - \tilde{G}_{1n,S^*_2} = \frac{1}{n} \sum_{i=1}^{n} (\omega_i - 1) \text{Inf}_{1GS^*_2;i} + o_p(n^{-1/2}) \quad \text{(E.36)}
\]
Proof. Represent the quantity $\tilde{G}_{1n,S_2} - G_{10,S_2}$ as a sum:

$$\tilde{G}_{1n,S_2} - G_{10,S_2} = \frac{1}{n} \sum_{i=1}^{n} X_{1i}^0 (A_{1i} - \mu_{1A0i}) \left\{ \epsilon_{1S_2^i} + (\bar{Y}_{1S_2^i} - Y_{1S_2^i}) \right\}. \quad (E.37)$$

The difference $\bar{Y}_{1S_2^i} - Y_{1S_2^i}$ can be represented as the difference in the blips:

$$\bar{Y}_{1S_2^i} - Y_{1S_2^i} = \xi \left\{ A_{2i} \tilde{X}_{2i}^0 (S_2^i); \tilde{\theta}_{2n,S_2} \right\} - \xi \left\{ A_{2i} \tilde{X}_{2i}^0 (S_2^i); \theta_{2n,S_2} \right\}. $$

The term resulting from this blip difference is analyzed in Lemma E.15, and results in (E.35). Similarly, we consider the bootstrap version

$$\tilde{G}_{1n,S_2} - G_{10,S_2} = \frac{1}{n} \sum_{i=1}^{n} \omega_i \tilde{X}_{1i}^0 (A_{1i} - \mu_{1A0i}) \left\{ \epsilon_{1S_2^i} + (\tilde{Y}_{1S_2^i} - Y_{1S_2^i}) \right\},$$

where the bootstrap pseudo-outcomes $\tilde{Y}_{1S_2^i} := Y + \xi (\tilde{X}_{2i}^0 (S_2^i); \tilde{\theta}_{2n,S_2})$ use the bootstrapped estimator $\tilde{\theta}_{2n,S_2}$. Subtracting off (E.37) from the previous display, we arrive at the representation

$$\tilde{G}_{1n,S_2} - \tilde{G}_{1n,S_2} = \frac{1}{n} \sum_{i=1}^{n} (\omega_i - 1) \tilde{X}_{1i}^0 (A_{1i} - \mu_{1A0i}) \epsilon_{1S_2^i} + \frac{1}{n} \sum_{i=1}^{n} \tilde{X}_{1i}^0 (A_{1i} - \mu_{1A0i}) \left\{ \omega_i (\tilde{Y}_{1S_2^i} - Y_{1S_2^i}) - (\bar{Y}_{1S_2^i} - Y_{1S_2^i}) \right\}. \quad (E.38)$$

In light of (E.30) in Lemma E.15 and using the definition of $M$ therein,

$$\frac{1}{n} \sum_{i=1}^{n} \tilde{X}_{1i}^0 (A_{1i} - \mu_{1A0i})(\bar{Y}_{1S_2^i} - Y_{1S_2^i}) = (EM) \frac{1}{n} \sum_{i=1}^{n} \inf_{2S_2^i} + o_p(n^{-1/2}).$$

Similarly, (E.31) in this same lemma ensures that

$$\frac{1}{n} \sum_{i=1}^{n} \omega_i \tilde{X}_{1i}^0 (A_{1i} - \mu_{1A0i})(\tilde{Y}_{1S_2^i} - Y_{1S_2^i}) = (EM) \frac{1}{n} \sum_{i=1}^{n} \omega_i \inf_{2S_2^i} + o_p(n^{-1/2}).$$

Subtracting these representations, we obtain

$$\frac{1}{n} \sum_{i=1}^{n} \tilde{X}_{1i}^0 (A_{1i} - \mu_{1A0i}) \left\{ \omega_i (\tilde{Y}_{1S_2^i} - Y_{1S_2^i}) - (\bar{Y}_{1S_2^i} - Y_{1S_2^i}) \right\} = (EM) \frac{1}{n} \sum_{i=1}^{n} (\omega_i - 1) \inf_{2S_2^i} + o_p(n^{-1/2}).$$

The result (E.36) can be found by plugging the above representation into (E.38). 
