# Inference on Strongly Identified Functionals of Weakly Identified Functions

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#### Abstract

In a variety of applications, including nonparametric instrumental variable (NPIV) analysis, proximal causal inference under unmeasured confounding, and missing-not-at-random data with shadow variables, we are interested in inference on a continuous linear functional (e.g., average causal effects) of nuisance function (e.g., NPIV regression) defined by conditional moment restrictions. These nuisance functions are generally weakly identified, in that the conditional moment restrictions can be severely ill-posed as well as admit multiple solutions. This is sometimes resolved by imposing strong conditions that imply the function can be estimated at rates that make inference on the functional possible. In this paper, we study a novel condition for the functional to be strongly identified even when the nuisance function is not; that is, the functional is amenable to asymptotically-normal estimation at  $\sqrt{n}$ -rates. The condition implies the existence of debiasing nuisance functions, and we propose penalized minimax estimators for both the primary and debiasing nuisance functions. The proposed nuisance estimators can accommodate flexible function classes, and importantly they can converge to fixed limits determined by the penalization regardless of the identifiability of the nuisances. We use the penalized nuisance estimators to form a debiased estimator for the functional of interest and prove its asymptotic normality under generic high-level conditions, which provide for asymptotically valid confidence intervals. We also illustrate our method in a novel partially linear proximal causal inference problem and a partially linear instrumental variable regression problem.

## 1 Introduction

Many causal or structural parameters of interest can be expressed as linear functionals of unknown functions that satisfy conditional moment restrictions. For example, in a nonparametric instrumental variable (NPIV) model, parameters such as average policy effects, weighted average derivatives, and average partial effects are all linear functionals of the NPIV regression, which is characterized by a conditional moment equation given by the exclusion restriction [Newey and Powell, 2003]. Similarly, in proximal causal inference under unmeasured confounding [Tchetgen Tchetgen et al., 2020], the average treatment effect and various policy effects can be expressed as linear functionals of a bridge function defined as a solution to some conditional moment restrictions [Cui et al., 2022, Kallus et al., 2021]. Similarly, in missing-not-at-random data problems with shadow variables, some parameters for the missing subpopulation can be also written as linear functionals of

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an unknown density ratio function that solves a certain conditional moment restriction [Li et al., 2022, Miao et al., 2015].

In this paper, we tackle the commonplace problem that the conditional moment restrictions only weakly identify the nuisance functions that define the target parameter. That is, the conditional moment restrictions can be severely ill-posed as well as admit multiple solutions, so that the nuisance functions are not uniquely identified and are not stable as underlying distributions vary. This problem can easily occur in many applications. For example, the identification of NPIV regressions requires the so-called "completeness condition," and stronger conditions yet are needed to control ill-posedness in nonparametric settings. These conditions can be easily violated if the instrumental variables are not very strong, as is common in practice [e.g., Andrews and Stock, 2005, Andrews et al., 2019]. Even with additional restrictions on the function space, Santos [2012] shows that NPIV regressions are unidentifiable in a variety of of models. Moreover, Canay et al. [2013] argues that completeness conditions are generally not testable, so the unidentifiability problem may not be diagnosable. Similar phenomena are also common in proximal causal inference and missing data problems with shadow variables (see Examples 2 and 3 in Section 2).

Fortunately, even when the nuisance functions are not identifiable, the linear functionals of interest can still be identifiable. In particular, these functionals often capture some identifiable aspects of the unidentifiable nuisance functions. For example, in proximal causal inference, merely the existence – but not uniqueness – of bridge functions is sufficient for identification of the average treatment effect and some policy effects [Miao and Tchetgen, 2018, Cui et al., 2022, Kallus et al., 2021]. But even if the functional is identifiable, the ill-posedness of the conditional moment restrictions that define it can raise significant challenges for statistical inference. In this setting, without conditions that limit ill-posedness, common nuisance estimators may be unstable and resulting estimators for the functional may not be  $\sqrt{n}$ -consistent and asymptotically normal.

**Setup and Main Results.** To tackle this challenge in generality, we study continuous linear functionals of nuisance functions characterized by linear conditional moment restrictions. Our parameter of interest is a functional of some unknown nuisance function  $h^* \in \mathcal{H} \subseteq \mathcal{L}_2(S)$ :

$$\theta^* = \mathbb{E}[m(W; h^*)],\tag{1}$$

where  $\mathcal{H}$  is a closed linear space (i.e. Hilbert space) and m is a given function such that  $h \mapsto \mathbb{E}[m(W;h)]$  is a continuous linear functional over  $\mathcal{H}$ . For example,  $\mathcal{H}$  can be the whole  $\mathcal{L}_2(S)$  space, or some other structured class like a partially linear function class or an additive function class. We posit that  $h^*$  solves the following linear conditional moment restriction in h:

$$\mathbb{E}[g_1(W)h(S) \mid T] = \mathbb{E}[g_2(W) \mid T], \tag{2}$$

for some given functions  $g_1 \in \mathcal{L}_2(W)$  and  $g_2 \in \mathcal{L}_2(W)$ , where S = S(W) and T = T(W) are two W-measurable variables (usually, potentially-overlapping subsets of the components of the vector W). This general formulation includes a wide variety of problems, including NPIV, proximal causal inference, and missing data with shadow variable (see Examples 1 to 3 in Section 2). To distinguish  $h^*$  from other nuisance functions introduced later, we refer to  $h^*$  as the *primary nuisance*.

Note that h(S) in Equation (2) is a function of variables S that may not appear in the conditioning variable T. Thus, solving Equation (2) is generally an ill-posed inverse problem: it may not have a unique solution and its solutions may depend on the data distributions discontinuously [Carrasco et al., 2007]. We here allow the conditional moment restrictions to be severely ill-posed and have nonunique solutions. However, we introduce a novel general condition that ensures strong identification of the linear functional, regardless of the identification of the nuisance functions

given by the conditional moment restrictions. Under this condition we develop estimation and inference methods, when given access to n independent and identically distributed data samples  $W_1, \ldots, W_n \sim W$ , with guarantees that are robust to the weak identification of  $h^*$ . This provides a general and unified solution to a wide range of applications where concerns regarding weakly identified nuisances arise naturally.

Specifically, we define the linear functional to be *strongly identified* if a certain minimization problem admits a solution.

**Assumption 1** (Functional Strong Identification). We say  $\theta^*$  is strongly identified if

$$\Xi_0 \neq \emptyset, \quad \text{where} \quad \Xi_0 := \underset{\xi \in \mathcal{H}}{\operatorname{argmin}} \frac{1}{2} \mathbb{E} \Big[ \mathbb{E}[g_1(W)\xi(S) \mid T]^2 \Big] - \mathbb{E}[m(W; \xi)].$$
 (3)

Then, not only do we have  $\theta^* = \mathbb{E}[m(W; h_0)]$  for any solution  $h_0$  to the conditional moment equations in Eq. (2) (i.e.,  $\theta^*$  is identified even though  $h^*$  is not), but we also have that if we let  $\xi_0 \in \Xi_0$  be any solution to Eq. (3) and if we set  $q^{\dagger}(T) := \mathbb{E}[g_1(W)\xi_0(S) \mid T]$ , then  $\theta^*$  further admits the following de-biased or Neyman orthogonal representation (Theorem 1 in Section 4):

$$\theta^* = \mathbb{E}\Big[\psi(W; h_0, q^{\dagger})\Big] \qquad \qquad \psi(W; h, q) := m(W; h) + q(T)(g_2(W) - g_1(W)h(S)), \tag{4}$$

where we call  $q^{\dagger}$  the debiasing nuisance. Crucially, for this representation, the estimation error rates can be expressed solely based on "weak" metrics that avoid dependence on any ill-posedness measure (Lemma 1). For illustration, with  $g_1(W) = 1$ , for any  $\hat{h} \in \mathcal{H}$  and any  $\hat{\xi} \in \mathcal{H}$ , letting  $\tilde{q}(T) = \mathbb{E}[\hat{\xi}(S) \mid T]$ , we have

$$\left| \mathbb{E} \left[ \psi(W; \hat{h}, \tilde{q}) \right] - \theta^* \right|^2 \le \mathbb{E} \left[ \mathbb{E} \left[ \hat{h}(S) - h_0(S) \mid T \right]^2 \right] \cdot \mathbb{E} \left[ (\tilde{q}(S) - q^{\dagger}(S))^2 \right]$$
 (5)

$$= \mathbb{E}\left[\mathbb{E}\left[\hat{h}(S) - h_0(S) \mid T\right]^2\right] \cdot \mathbb{E}\left[\mathbb{E}\left[\hat{\xi}(S) - \xi_0(S) \mid T\right]^2\right]. \tag{6}$$

The fact that both estimation metrics project the functions onto T allows us to argue convergence rates for both of these functions without invoking any measure of ill-posedness of the corresponding inverse problems that defines them. In particular,  $\mathbb{E}[\mathbb{E}[\hat{h}(S) - h_0(S) \mid T]^2]$  exactly corresponds to the average squared slack in  $\hat{h}$  satisfying the moment restrictions in Eq. (2), and this does not involve how such slack translates to the distance from an exact solution. This is one of the key ingredient that enables our main results and it hinges on our key assumption that a solution to the minimization problem in Eq. (3) exists. Note that Eqs. (5) and (6) are meant only for illustration, and, in practice, given  $\hat{\xi}$  we will still need to estimate its projection  $\tilde{q}$ .

To demystify Assumption 1, we further examine its equivalent formulations based on the structure of the Riesz representer of the functional, *i.e.*, the function  $\alpha$  that satisfies

$$\mathbb{E}[m(W;h)] = \mathbb{E}[\alpha(S)h(S)] \quad \forall h \in \mathcal{H}, \tag{7}$$

whose existence is guaranteed by  $h \mapsto \mathbb{E}[m(W;h)]$  being linear and continuous [Luenberger, 1997, Section 5.3]. When  $h_0$  corresponds to the solution of an exogenous regression problem (i.e., S = T), weak identification of  $h^*$  is not a concern and Assumption 1 is automatic with  $\Xi_0 = \{\alpha\}$ . In our setting, the solution  $\xi_0$  is no longer the Riesz representer, but is closely related to it. For instance, when the function space  $\mathcal{H} = \mathcal{L}_2(S)$  and  $g_1(W) = 1$ , then  $\mathbb{E}[\mathbb{E}[\xi_0(S) \mid T] \mid S] = \alpha(S)$ , and our Assumption 1 is equivalent to the existence of  $\xi_0 \in \mathcal{H}$  satisfying the latter equality. Note that we can still write a representation as in Eq. (5) if we only assume the existence of some  $q_0$  solving

 $\mathbb{E}[q_0(T) \mid S] = \alpha(S)$  as, for example, assumed in Severini and Tripathi [2012], even if it is not of the form  $q_0 = \mathbb{E}[\xi_0(S) \mid T]$ . However, crucially, the resulting error in Eq. (5) then would not reduce to estimation errors of projections as in Eq. (6), therefore requiring control on ill-posedness. While the existence of (arbitrarily approximate) solutions to  $\mathbb{E}[q_0(T) \mid S] = \alpha(S)$  is equivalent to mere identification of  $\theta^*$  (Lemma 2), Assumption 1 provides the added regularity for strong identification of  $\theta^*$ . We in fact show that Assumption 1 holds if and only if the Riesz representer  $\alpha$  lies in a relatively smooth sub-space of the function space  $\mathcal{H}$ . This can be expressed as a "source condition" on the Riesz representer. Prior work on nonparametric inference for ill-posed inverse problems typically places such "source conditions" on the primary nuisance function  $h^*$ . Thus, our assumption can be viewed as a dual approach, imposing source conditions only on objects related to the functional.

Armed with our Assumption 1, we turn to the task of estimating the nuisance functions that can be plugged into the debiased representation in Eq. (4) and control the projected-error bound in Eq. (6). We propose minimax (adversarial) estimators  $\hat{h}, \hat{q}$  for the primary and debiasing nuisances. These estimators are generic and admit highly flexible function classes like reproducing kernel Hilbert space (RKHS) and neural networks. Moreover, our estimators do not require deriving the closed form of the functional Riesz representer  $\alpha$ , just like the automatic debiased machine learning methods (see a review in Section 3). We leverage  $L_2$ -norm penalization for primary-nuisance estimation, so as to ensure  $\hat{h}$  converges to some fixed limit  $h^{\dagger}$  in  $L_2$ -norm even when  $h^*$  is in general not identified and Eq. (2) admits many solutions (Theorem 4). Conversely, our debiasing-nuisance estimator converges to a fixed limit even without penalization, because  $\mathbb{E}[g_1(W)\xi_0(S) \mid T] = q^{\dagger}(T)$  is shown to be unique for all  $\xi_0 \in \Xi_0$  satisfying Equation (3) (Lemma 3 and Theorem 5).

We derive a novel analysis yielding finite-sample convergence rates for our nuisance estimators  $\hat{h}$  and  $\hat{q}$ , bounding the weak metric for the primary nuisance,  $\epsilon_n^2 = \mathbb{E}[\mathbb{E}[g_1(W)(\hat{h}(S) - h_0(S)) \mid T]^2]$ , and the strong metric for the debiasing nuisance  $\kappa_n^2 = \mathbb{E}[(\hat{q}(S) - q^{\dagger}(S))^2]$ . Our bounds rely solely on the critical radius  $r_n$  (a well-studied and typically tight notion of statistical complexity of a function space) of approximating function spaces  $\mathcal{H}_n$ ,  $\mathcal{Q}_n$  for the nuisance estimators  $\hat{h}$ ,  $\hat{q}$  and their approximation error  $\delta_n$ . Both finite sample-rates do not involve any measures of ill-posedness. The intuition behind the strong-metric result for  $q^{\dagger}$  is that it essentially corresponds to a weak-metric convergence for  $\xi_0$ , for which we can provide ill-posedness-free rates. For the primary nuisance function, we derive fast estimation rates of the order of  $\epsilon_n \sim r_n + \delta_n$ , due to the fact that it corresponds to a conditional moment problem. For the de-biasing nuisance function we derive slow rates of the order of  $\kappa_n \sim \sqrt{r_n} + \delta_n$ , since it roughly corresponds to a minimum distance problem, but not a conditional moment problem.

Putting everything together, we develop a complete estimation and inference pipeline for parameters defined by Eqs. (1) and (2) that avoids dependence on ill-posedness measures or point-identification assumptions on the nuisance functions, where our main assumptions are Assumption 1 and high-level conditions on the complexity and approximability of general function classes. We construct de-biased estimators for the functional of interest by plugging our penalized nuisance estimates, estimated in a cross-fitting manner, into the debiased representation in Eq. (4). We prove that the resulting functional estimator is asymptotically linear and has an asymptotic normal distribution (Theorem 6) under Assumption 1, some regularity conditions, and assuming the critical radii and approximation errors decay fast enough in that  $r_n^{3/2}$ ,  $\sqrt{r_n}\delta_n$ ,  $\delta_n^2$  are all  $o(n^{-1/2})$ . In particular, these constraints apply to many non-parametric function spaces of interest.

We illustrate the application of our proposed method to partially linear proximal causal inference (Section 7.2) and partially linear IV estimation (Section 7.1). This semiparametric proximal causal inference settings is new as, to our knowledge, existing literature on proximal causal inference

focus on either parameteric or fully nonparametric estimation. In particular, we characterize when the primary nuisance function in proximal causal inference is a partially linear function (Proposition 3) and discuss how to apply our proposed method to estimate the linear coefficients. Our method can be similarly applied to partially linear IV estimation problems, extending the existing literature that either assumes the unique identification of IV regression [Chernozhukov et al., 2018a, Florens et al., 2012, Ai and Chen, 2003] or allows under-identified IV regression but focus on linear-sieve estimation [Chen, 2021]. Finally, we extend our results to a generalized framework where the primary nuisance function is weakly identified by orthogonality conditions (Section 8). This framework encompasses a wider variety of nuisance functions than our basic setup. We show that our identification, estimation, and inferential results extend to this generalized framework.

Roadmap. The rest of this paper is organized as follows. We first review examples of our setup in Section 2 as well as related literature in Section 3. We then further characterize the strong identification of linear functionals of weakly identified nuisances in Section 4, interpreting Assumption 1 in Section 4.1, instantiating the condition in concrete examples in Section 4.2, and discussing the statistical challenges raised by weakly identified nuisances in Section 4.3. Then we propose our minimax nuisance estimators in Section 5, considering the primary nuisance in Section 5.1 and the debiasing nuisance in Section 5.2. We further construct debiased functional estimators, establish their asymptotic normality, and discuss variance estimation and confidence intervals in Section 6. In Section 7, we illustrate the application of our method in partially linear IV estimation and partially linear proximal causal inference. In Section 8, we present a more general framework and accordingly extend all results in Sections 4 to 6. Finally, we conclude this paper and discuss future directions in Section 9.

**Notation.** For a generic random vector  $W \in \mathcal{W}$ , we use  $\mathcal{L}_2(W)$  to denote the space of square integrable functions of W with respect to the probability distribution of W. For any  $f(W), g(W) \in$  $\mathcal{L}_2(W)$ , we denote the  $L_2$ -norm by  $||f||_2 = \sqrt{\mathbb{E}[f^2(W)]}$  and inner product by  $\langle f, g \rangle = \mathbb{E}[f(W)g(W)]$ . We denote the empirical  $L_2$ -norm with respect to data  $W_1, \ldots, W_n$  by  $||f||_n = \sqrt{\sum_{i=1}^n f^2(W_i)/n}$ . We let  $\mathbb{P}(f(W)) = \int f(w) d\mathbb{P}(w)$  be the expectation with respect to W alone. We differentiate this from  $\mathbb{E}[f(W; W_1, \dots, W_n)]$ , which we use to denote full expectation with respect to both W and data  $W_1, \ldots, W_n$ . Thus if  $\hat{h}$  depends on the data  $W_1, \ldots, W_n$ , then  $\mathbb{P}(f(W; \hat{h}))$  remains a function of  $\tilde{h}$  (and thus the data) but  $\mathbb{E}[f(W;\tilde{h})]$  is a nonrandom scalar. We use both  $\mathbb{E}_n$  and  $\mathbb{P}_n$  to denote the empirical expectation with respect to W given data  $W_1, \ldots, W_n$ :  $\mathbb{E}_n(f(W)) = \mathbb{P}_n(f(W)) = \mathbb{P}_n(f(W))$  $\frac{1}{n}\sum_{i=1}^n f(W_i)$ . We further define the empirical process  $\mathbb{G}_n$  by  $\mathbb{G}_n(f) = \sqrt{n}(\mathbb{P}_n - \mathbb{P})(f)$ . For any linear operator  $L: \mathcal{A} \mapsto \mathcal{B}$  where  $\mathcal{A}$  and  $\mathcal{B}$  are Hilbert spaces, we denote its range space by  $\mathcal{R}(L) = \{La : a \in \mathcal{A}\} \subseteq \mathcal{B}$  and its null space by  $\mathcal{N}(L) = \{a : La = 0\} \subseteq \mathcal{A}$ . Unless otherwise stated, the default norm for the  $\mathcal{L}_2(W)$  space is  $\|\cdot\|_2$ . Thus, the convergence of functions in  $\mathcal{L}_2(W)$ , the compactness of subsets of  $\mathcal{L}_2(W)$ , and the continuity of functionals defined on  $\mathcal{L}_2(W)$ are all understood in terms of the norm  $\|\cdot\|_2$ , and the default inner product is  $\langle\cdot,\cdot\rangle$ . Furthermore, for vector-valued square-integrable functions, we use the notation  $||f||_{2,2} = \mathbb{E}[f(W)^{\top}f(W)]^{1/2}$  for the  $L_2$  with the euclidean norm as the base vector norm, and we generalize the above conventions using this as the default norm when not stated.

For any set D, we denote its closure as cl(D) and its interior as int(D). We say that D is star-shaped if for any  $d \in D$  and  $\alpha \in [0,1]$ , we have  $\alpha d \in D$ . The star hull of D is defined as  $\{\alpha d : d \in D, \alpha \in [0,1]\}$ . For a function class  $\mathcal{G} \subseteq \mathcal{L}_2(W)$ , we say it is b-uniformly bounded if  $|g(W)| \leq b$  almost surely for any  $g \in \mathcal{G}$ . The localized Rademacher complexity of a function class  $\mathcal{G}$  is defined as  $\mathcal{R}_n(\delta;\mathcal{G}) = \mathbb{E}[\sup_{g \in \mathcal{G}, ||g||_2 \leq \delta} \left| \frac{1}{n} \sum_{i=1}^n \epsilon_i g(W_i) \right|]$ , where  $W_1, \ldots, W_n, \epsilon_1, \ldots, \epsilon_n$  are

independent with  $W_i \sim W$  and  $\epsilon_i$  taking values in  $\{-1,1\}$  equiprobably. The critical radius  $\eta_n$  of the function class  $\mathcal{G}$  is defined as any solution to the inequality  $\mathcal{R}_n(\delta;\mathcal{G}) \leq \delta^2$ . We use  $|\mathcal{G}|$  to denote the cardinality of  $\mathcal{G}$  up to equality almost everywhere. For real-valued sequences  $a_n, b_n$ , we use the standard "big-O" notations  $a_n = o(b_n)$  to denote that  $a_n/b_n \to 0$  as  $n \to \infty$ , and  $a_n = \omega(b_n)$  to denote that  $a_n/b_n \to \infty$  as  $n \to \infty$ .

## 2 Examples

Before proceeding we review important examples of parameters defined by Eqs. (1) and (2).

**Example 1** (Functionals of NPIV Regression). Consider a causal inference problem with an observed outcome  $Y \in \mathbb{R}$ , potentially endogenous variables  $X \in \mathbb{R}^{d_X}$ , and instrumental variables  $Z \in \mathbb{R}^{d_Z}$ . We are interested in the NPIV regression model [e.g., Newey and Powell, 2003, Darolles et al., 2011, Hall and Horowitz, 2005]:

$$Y = h^{\star}(X) + \epsilon$$
, where  $\mathbb{E}[\epsilon \mid Z] = 0$ ,  $h^{\star} \in \mathcal{H} = \mathcal{L}_2(X)$ .

The NPIV regression  $h^*$  solves the following conditional moment restriction:

$$\mathbb{E}[h(X) \mid Z] = \mathbb{E}[Y \mid Z],\tag{8}$$

which is an example of Equation (2) with  $g_1(W) = 1$ ,  $g_2(W) = Y$ , S = X, and T = Z.

We are interested in linear functionals of the IV regression  $h^*$  when  $h^*$  is not necessarily identifiable. One example is the coefficient of the best linear approximation to the IV regression function,  $\operatorname{argmin}_{\beta \in \mathbb{R}^{d_X}} \mathbb{E}\left[\left(h^*(X) - \beta^\top X\right)^2\right] = \left(\mathbb{E}\left[XX^\top\right]\right)^{-1}\theta^*$ , where

$$\theta^* = \mathbb{E}[\alpha(X)h^*(X)], \quad \alpha(X) = X. \tag{9}$$

Alternatively, we can consider other linear functionals of NPIV regressions, such as the weighted average derivatives described in Ai and Chen [2007], Chen and Pouzo [2015].

It is known that the IV regression  $h^*$  is identifiable if and only if a completeness condition on the distribution of  $X \mid Z$  is satisfied (Proposition 2.1 in Newey and Powell, 2003). However, as Severini and Tripathi [2006] showed, the completeness condition can be easily violated, especially when the instrumental variables are not very strong. Moreover, the completeness condition is impossible to test in general nonparametric models [Canay et al., 2013], so the failure of identifying  $h^*$  may not be detectable. Fortunately, even when the NPIV regression  $h^*$  is unidentifiable, the functional of interest can be still identifiable as we will discuss in Section 4.

Here we consider a general nonparametric IV model with  $\mathcal{H} = \mathcal{L}_2(X)$ . In Section 7.1, we will further study a partially linear IV model, where  $X = (X_a, X_b)$ , the function class  $\mathcal{H}$  is the direct sum of linear functions in  $X_a$  and of  $\mathcal{L}_2(X_b)$ , and  $\theta^*$  is the linear coefficient in  $X_a$ .

Example 2 (Proximal Causal Inference). Consider a causal inference problem with potential outcomes Y(a) that would be realized if the treatment assignment were equal to  $a \in \{0,1\}$ . We are interested in the average treatment effect,  $\theta^* = \mathbb{E}[Y(1) - Y(0)]$ . The actual treatment assignment is denoted as A, the corresponding observed outcome is Y = Y(A), and some additional covariates X are also observed, but these do not account for all confounders and there exist unmeasured confounders U. We consider the proximal causal inference framework [e.g., Tchetgen Tchetgen et al., 2020, Miao et al., 2018, Deaner, 2018] that requires two different sets of proxy variables <math>Z, V that strongly correlate with the unobserved confounders. The so-called negative control treatment Z

cannot directly affect the outcome Y, and the so-called negative control outcome V cannot be affected by either the treatment A or the negative control treatment Z (see Assumptions 4 to 7 in Cui et al., 2022 for formal statements).

If  $h^* \in \mathcal{H} = \mathcal{L}_2(V, X, A)$  is a so-called outcome bridge function satisfying

$$\mathbb{E}[Y - h^*(V, X, A) \mid U, X, A] = 0, \tag{10}$$

then our target parameter can be written as a linear functional of it:

$$\theta^* = \mathbb{E}[h^*(V, X, 1) - h^*(V, X, 0)] = \mathbb{E}[\alpha(V, X, A)h^*(V, X, A)],$$
where  $\alpha(V, X, A) = \frac{A - \mathbb{P}(A = 1 \mid V, X)}{\mathbb{P}(A = 1 \mid V, X)(1 - \mathbb{P}(A = 1 \mid V, X))}.$ 
(11)

Equation (10) involves unobserved variables, but under negative control assumptions, Equation (10) implies that  $h^*$  also solves the following (observable) conditional moment restriction

$$\mathbb{E}[Y - h(V, X, A) \mid Z, X, A] = 0. \tag{12}$$

When the negative control treatment Z consists of sufficiently strong proxies for the unmeasured confounders U (see Assumption 8 in Cui et al. [2022]), any solution to Equation (12) also solves Equation (10). As a result, our target parameter in Equation (11) can be also viewed as a linear functional of a solution to Equation (12), which is a special example of our general framework with  $g_1(W) = 1$ ,  $g_2(W) = Y$ ,  $S = (V^\top, X^\top, A)^\top$ , and  $T = (Z^\top, X^\top, A)^\top$ . Similarly, we can consider various average policy effects in the proximal causal inference framework, even with continuous treatments, as they can also be written as linear functionals of bridge functions [Kallus et al., 2021, Qi et al., 2021].

Kallus et al. [2021] points out that the solution to Equation (12) is very likely to be nonunique and gives various concrete examples. This particularly occurs in data-rich settings where there are more proxy variables than the unobserved confounders. Since the unobserved confounders are unknown in practice, it is generally impossible to know a priori whether bridge functions are unique or not. Fortunately, it is well known that even with nonunique bridge functions, any of them can still lead to the same average treatment effect or average policy effect under suitable conditions [Cui et al., 2022, Miao and Tchetgen, 2018, Kallus et al., 2021] (however, for inference, this literature still requires bridge functions to be unique, parametric, and/or satisfy restricted ill-posedness, all of which we will avoid). In Section 4, we will derive identification conditions for the target linear functionals.

In Section 7.2, we will further study a partially linear proximal causal inference model. We will show that when the regression function  $\mathbb{E}[Y(a) \mid U, X]$  is partially linear in a, there always exists a bridge function  $h^*(V, X, A)$  partially linear in A. In this case, the partially linear coefficient is a causal parameter and it is also a linear functional of the bridge function.

**Example 3** (Missing-Not-at-Random Data with Shadow Variables). Consider a partially missing outcome Y and an indicator  $A \in \{0,1\}$  denoting whether Y is observed, so that we only observe V = AY. We are interested in the average missing outcome,  $\theta^* = \mathbb{E}[(1-A)Y]$  (which also gives the outcome mean via  $\mathbb{E}[Y] = \theta^* + \mathbb{E}[V]$ ). However, suppose that the outcome is *missing not at random*, namely, although we observed some covariates X, we generally allow that  $Y \not\perp A \mid X$ . Nonetheless, if  $h^*$  were the Y-conditional missingness propensity ratio  $h^*(X,Y) = \mathbb{P}(A = 0 \mid X,Y)/\mathbb{P}(A = 1 \mid X,Y)$ , then  $\theta^*$  is a linear functional of it, using only the observables  $W = (X^\top, V, A)^\top$ :

$$\theta^* = \mathbb{E}[\alpha(X, V)h^*(X, V)], \quad \alpha(X, V) = V. \tag{13}$$

Here we again consider a general nonparametric model with  $h^* \in \mathcal{H} = \mathcal{L}_2(X, V)$ .

Since the definition of  $h^*$  involves conditioning on unobservables, we cannot generally learn it. We therefore additionally consider so-called shadow variables Z satisfying  $Z \perp A \mid X, Y$  and  $Z \not\perp Y \mid X$  [e.g., Li et al., 2022, d'Haultfoeuille, 2010, Miao et al., 2015, Miao and Tchetgen Tchetgen, 2016]. These conditions are particularly relevant when the missingness is directly driven by the outcome Y and the shadow variables Z are strong proxies for the outcome Y. Under these conditions,  $h^*$  will necessarily satisfy the following conditional moment restriction [Li et al., 2022]:

$$\mathbb{E}[Ah(X,V) \mid X,Z] = \mathbb{E}[1-A \mid X,Z]. \tag{14}$$

This is an example of Equation (2) with  $g_1(W) = A$ ,  $g_2(W) = 1-A$ ,  $S = (X^\top, V)$ , and  $T = (X^\top, Z)$ . Again, the conditional moment restriction in Equation (14) admits multiple solutions (i.e., does not identify  $h^*$ ) unless a strong completeness condition on the distribution of  $V \mid X, Z$  holds. In Section 4, we will discuss conditions that ensure the identification of  $\theta^*$  even when  $h^*$  is not identified.

#### 3 Related Literature

Our paper is related to the literature on the estimation of and inference on point-identified (finitely and/or infinitely dimensional) parameters defined by conditional moment restrictions [e.g., Newey, 1990, Chamberlain, 1987, Newey and Powell, 2003, Ai and Chen, 2003, Blundell et al., 2007, Chen and Pouzo, 2012, 2009, Chen and Reiss, 2011, Hall and Horowitz, 2005, Darolles et al., 2011]. Some other literature study partial identification sets and inference thereon when unconditional or conditional moment restrictions underidentify the parameters [e.g., Andrews and Shi, 2013, 2014, Andrews and Barwick, 2012, Chernozhukov et al., 2007, Belloni et al., 2019, Canay and Shaikh, 2017, Bontemps and Magnac, 2017, Hong, 2017, Santos, 2012].

Our paper studies the estimation and inference of identifiable functionals of unknown nuisance functions satisfying certain conditional moment restrictions. We do not restrict the nuisance functions to be parametric and focus on inference after using flexible nonparametric estimation of nuisances. Existing literature usually study this problem when the nuisance function is pointidentified [e.g., Ai and Chen, 2007, 2012, Chen and Pouzo, 2015, Chen and Christensen, 2018, Brown and Newey, 1998, Newey and Stoker, 1993, Chen et al., 2021. Recently, a few works further consider functionals of partially identified nuisance functions. In particular, Severini and Tripathi [2006], Escanciano and Li [2013], Freyberger and Horowitz [2015] study the point identification and partial identification of continuous linear functionals of partially identified NPIV regressions. Severini and Tripathi [2012] discuss efficiency considerations for point-identified linear functionals of unidentified NPIV regressions. Some works also study the estimation of identifiable linear functionals of unidentifiable nuisances and derive their asymptotic distributions, either in the IV setting [Santos, 2011, Babii and Florens, 2017, Chen, 2021, Escanciano and Li, 2021] or in the shadow variable setting [Li et al., 2022]. These works are reviewed in more detail in Section 4. Our paper builds on these literature and develops them in several aspects. First, our paper proposes a unified solution to a wider variety of problems, including IV, shadow variables, and proximal causal inference [Tchetgen Tchetgen et al., 2020]. Second, these existing literature are restricted to series or kernel estimation for conditional moment models, while our paper adopts a minimax estimation framework to accommodate generic function classes and thus more flexible machinelearning models like RKHS and neural networks. Third, much of the existing literature directly restricts the ill-posedness of the conditional moment restrictions that define the nuisance functions (e.g., the NPIV regressions) for the target functional to be well estimable [e.g., Babii and Florens, 2017, Escanciano and Li, 2021, Santos, 2011, Li et al., 2022]. In contrast, we characterize an alternative condition for the target functional to be strongly identifiable, without controlling the level of ill-posedness of the conditional moment equations at all. We also reveal its close connection to ostensibly different conditions in Ai and Chen [2007], Ichimura and Newey [2022] (see Appendix A for an expanded discussion).

Our proposed estimation method is based on the minimax estimation framework formalized in Dikkala et al. [2020], Bennett and Kallus [2020]. Such minimax methods have been employed in average treatment effect estimation under unconfoundedness [Hirshberg and Wager, 2021, Kallus, 2020, Chernozhukov et al., 2020] and policy evaluation [Kallus, 2018, Feng et al., 2019, Yang et al., 2020, Uehara et al., 2021], but in these settings the nuisances are inherently unique regression functions. The minimax framework and its variants have also been successfully applied to causal inference under unmeasured confounding, including IV estimation [Lewis and Syrgkanis, 2018, Zhang et al., 2020, Liao et al., 2020, Bennett et al., 2019, Muandet et al., 2020] and proximal causal inference [Kallus et al., 2021, Ghassami et al., 2021, Mastouri et al., 2021], but this literature typically assumes that the unknown nuisance functions are uniquely identified whenever considering inference.

In contrast, our paper tackles the challenge of inference when the unknown functions are not unique solutions. To this end, we employ penalization to target certain unique nuisance function among all possible ones. Penalization is a common technique for solving ill-posed inverse problems [Carrasco et al., 2007, Engl et al., 1996], which has been in particular applied to series or kernel estimation for underidentified conditional moment models [Chen and Pouzo, 2012, Santos, 2011, Babii and Florens, 2017, Chen, 2021, Escanciano and Li, 2021, Li et al., 2022, Florens et al., 2011]. Our paper shows the effectiveness of penalization in the general minimax estimation framework and investigates the impact of penalization on the estimation of linear functionals.

Our paper is also related to the debiased machine learning literature [see Chernozhukov et al., 2018a, and the references therein]. This literature typically studies the estimation and inference of smooth functionals of certain regression functions that are inherently unique, in contrast to solutions of general moment restrictions. To alleviate the inherent bias of machine learning regression estimators, this literature leverages Nevman orthogonal estimating equations for functionals of interest, which requires estimating some Riesz representers first. The Riesz representers can be estimated by fitting regressions according to their analytic forms (like propensity scores in average treatment effect estimation) [e.q., Farrell, 2015, Farrell et al., 2021, Chernozhukov et al., 2017, 2018a, Semenova and Chernozhukov, 2021. Alternatively, some recent literature propose to estimate the Riesz representers by exploiting the representer property directly. These methods do not need to derive the analytic forms of Riesz representers on a case-by-case basis, and are therefore termed automatic debiased machine learning [Chernozhukov et al., 2020, 2018b, 2022c,b, 2021, 2022a. Our proposed method also avoids deriving Riesz representers explicitly and is therefore automatic in the same sense. However, existing automatic debiased machine learning methods focus on exogenous/unconfounded settings where nuisances are naturally well-posed and unique, while we focus on ill-posed nuisances. Interestingly, Equation (3) in our Assumption 1, when specialized to the exogenous setting with S=T, recovers the formulation used to learn Riesz representers in Chernozhukov et al. [2021, 2022a].

## 4 Functional Strong Identification

Defining the linear operator  $P: \mathcal{H} \to \mathcal{L}_2(T)$  by  $[Ph](T) = \mathbb{E}[g_1(W)h(S) \mid T]$ , the set of all solutions to Equation (2) is given by

$$\mathcal{H}_0 = \{ h \in \mathcal{H} : [Ph](T) = \mathbb{E}[g_2(W) \mid T] \} = h^* + \mathcal{N}(P). \tag{15}$$

Therefore, the conditional moment restriction in Equation (2) uniquely identifies the nuisance function  $h^*$  only when the linear operator P is injective so that  $\mathcal{N}(P) = \{0\}$ . As discussed in Section 1, this condition often fails.

Fortunately, even when the primary nuisance function  $h^*$  is not uniquely identified, the functional  $\theta^*$  can still be identifiable. In this paper, we impose Assumption 1 to enable both the identification of and estimation and inference on the functional. Assumption 1 requires the existence of solutions to the minimization problem in Equation (3), or, more succinctly,  $\Xi_0 \neq \emptyset$ . It turns out that this condition is non-trivial, and is equivalent to a smoothness condition on the Riesz representer  $\alpha$ , as will be explained in Section 4.1.

In the following theorem, we show that Assumption 1 immediately implies the identification of the target parameter  $\theta^*$ , and solutions  $\xi_0 \in \Xi_0$  in Assumption 1 can be used in the identification.

**Theorem 1.** If Assumption 1 holds, then for any  $h_0 \in \mathcal{H}_0$  and  $q^{\dagger} \in \{P\xi_0 : \xi_0 \in \Xi_0\}$ ,

$$\theta^* = \mathbb{E}[m(W; h_0)] = \mathbb{E}\Big[q^{\dagger}(T)g_2(W)\Big] = \mathbb{E}\Big[\psi(W; h_0, q^{\dagger})\Big],$$
where  $\psi(W; h, q) := m(W; h) + q(T)(g_2(W) - g_1(W)h(S)).$ 

We refer to the last identification formula, given by  $\psi$ , as the *doubly robust* identification formula. This is because this identification formula satisfies certain robustness properties, as described in the lemma below.

**Lemma 1.** If Assumption 1 holds, then for any  $h \in \mathcal{H}$ ,  $\xi \in \mathcal{H}$ ,  $q = P\xi$ ,  $h_0 \in \mathcal{H}_0$ ,  $\xi_0 \in \Xi_0$ , and  $q^{\dagger} = P\xi_0$ ,

$$|\mathbb{E}[\psi(W; h, q)] - \theta^*| = |\langle P(h - h_0), P(\xi - \xi_0) \rangle| \le ||P(h - h_0)||_2 ||P(\xi - \xi_0)||_2, \tag{16}$$

$$\frac{\partial}{\partial t} \mathbb{E} \left[ \psi(W; h_0 + th, q^{\dagger}) \right] \Big|_{t=0} = \frac{\partial}{\partial t} \mathbb{E} \left[ \psi(W; h_0, q^{\dagger} + tq) \right] \Big|_{t=0} = 0.$$
 (17)

Equation (16) shows that the doubly robust identification formula enjoys a mixed bias property. The mixed bias property in Equation (16) means that if we could plug estimates  $\hat{h}$  and  $\hat{\xi}$  into the doubly robust formula to estimate the target functional, then the estimation bias only depends on the product of their estimation errors, in terms of weak metrics  $||P(\cdot)||_2$ . Importantly, these weak-metric errors can be directly bounded without invoking any additional ill-posedness measure. In practice, we will need to estimate the debiasing nuisance  $q^{\dagger} = P\xi_0$ , so even with an estimator  $\hat{\xi}$  for  $\xi_0$ , we need to additionally approximate the operator P. But we will show in Section 5 that this does not change the implication of Equation (16): the estimation bias of the functional does not depend on any ill-posedness measure. Moreover, since the functional estimation bias only depends on the product of nuisance estimation errors, the bias can be asymptotically negligible even if each nuisance is estimated nonparametrically with a sub-root-n weak-metric-error convergence rate.

Equation (17) shows that the doubly robust formula satisfies the Neyman orthogonality property. It means that the doubly robust identification formula is insensitive to perturbations to the nuisances. Neyman orthogonality plays a pivotal role in the recent debiased machine learning

literature that has enabled the use of nuisances estimated by flexible machine learning methods [e.g., Chernozhukov et al., 2016, 2022b, 2021, 2022c]. Equation (17) is notable in that the Neyman orthogonality holds for underidentified nuisances.

In Section 6, we will estimate the target parameter by plugging nuisance estimators into the doubly robust identification formula. The robustness properties shown in Lemma 1 enable the  $\sqrt{n}$ -consistency and asymptotic normality of the resulting functional estimator, under generic high-level conditions that permit flexible nonparametric nuisance estimators. Interestingly, the doubly robust identification formula with the debiasing nuisance  $q^{\dagger} = P\xi_0$  recovers the influence function derived in Ichimura and Newey [2022] when specialized to our setup (see Appendix A.1).

We note that the results so far are based on a closed linear class  $\mathcal{H}$  for the primary nuisance  $h^*$ . It turns out that we can extend them to a closed and convex class  $\mathcal{H}$ . See Appendix B for details.

#### 4.1 Interpreting the Strong Identification Assumption

In this part, we aim to demystify our strong identification condition in Assumption 1 by showing that it implicitly restricts the Riesz representer  $\alpha$  of the target linear functional. We also compare Assumption 1 with many other assumptions in the existing literature.

#### 4.1.1 Restrictions on Riesz Representers

**Theorem 2.** Assumption 1 holds if and only if the Riesz representer  $\alpha$  in Equation (7) satisfies that  $\alpha \in \mathcal{R}(P^*P)$ . Moreover,  $\{\xi \in \mathcal{H} : P^*P\xi = \alpha\}$  is equal to the solution set  $\Xi_0$  in Assumption 1.

Theorem 2 shows that Assumption 1 requires the Riesz representer  $\alpha$  to lie in the range space of operator  $P^*P$ , where  $P^*: \mathcal{L}_2(T) \mapsto \mathcal{H}$  is the adjoint of P. It can be shown that  $P^*$  is given by  $[P^*q](S) = \Pi_{\mathcal{H}}[\mathbb{E}[g_1(W)q(T) \mid S] \mid S] = \Pi_{\mathcal{H}}[g_1(W)q(T) \mid S]$  for any  $q \in \mathcal{L}_2(T)$ , where  $\Pi_{\mathcal{H}}(\cdot \mid S)$  is the projection operator onto  $\mathcal{H}$ . Since  $\mathcal{H}$  is a closed linear space, this projection is well-defined [Theorem 1 of Section 3.12 in Luenberger, 1997].

Although Assumption 1 and Theorem 2 impose equivalent restrictions, the formulation in Assumption 1 is more amenable to estimation, as it involves only the functional  $\mathbb{E}[m(W;h)]$  but not the Riesz representer  $\alpha(S)$ . This obviates the need to derive the form of the Riesz representer  $\alpha(S)$ , which is in line with the spirit of the recent automatic debiased machine learning methods for functionals of exogenous regression functions [Chernozhukov et al., 2020, 2021, 2022c,a]. These methods propose ways to learn Riesz representers solely based on the functionals of interest, without needing to derive the form of the Riesz representers on a case-by-case basis. Our formulation in Assumption 1 has the same advantages.

**Example 4.** To understand Assumption 1 and Theorem 2, it is instructive to consider a compact linear operator P. Let  $\{\sigma_i, u_i, v_i\}_{i=1}^{\infty}$  denote singular value decomposition of the compact operator P, where  $\{u_i\}_{i=1}^{\infty}$ ,  $\{v_i\}_{i=1}^{\infty}$  are orthonormal bases in  $\mathcal{L}_2(T)$  and  $\mathcal{H} \subseteq \mathcal{L}_2(S)$  respectively, and  $\sigma_1 \geq \sigma_2 \geq \ldots$  are singular values. Then the adjoint operator  $P^*$  has the decomposition  $\{\sigma_i, v_i, u_i\}_{i=1}^{\infty}$  and  $P^*P$  has the decomposition  $\{\sigma_i^2, v_i, v_i\}_{i=1}^{\infty}$ . The Riesz representer  $\alpha \in \mathcal{H}$  in Equation (7) can be represented as  $\alpha = \sum_{i=1}^{\infty} \gamma_i v_i$  with  $\sum_{i=1}^{\infty} \gamma_i^2 < \infty$  and any  $\xi \in \mathcal{H}$  can be represented as  $\xi = \sum_{i=1}^{\infty} \beta_i v_i$  with  $\sum_{i=1}^{\infty} \beta_i^2 < \infty$ .

Note that  $P\xi = \sum_{i=1}^{\infty} \beta_i Pv_i = \sum_{i=1}^{\infty} \beta_i \sigma_i u_i$ , and  $\mathbb{E}[m(W;\xi)] = \mathbb{E}[\alpha(S)\xi(S)] = \sum_{i=1}^{\infty} \gamma_i \beta_i$ . Thus the optimization problem in Assumption 1 can be equivalently written as follows:

$$\min_{\beta_1, \beta_2, \dots} \sum_{i=1}^{\infty} \sigma_i^2 \beta_i^2 - 2 \sum_{i=1}^{\infty} \gamma_i \beta_i, \text{ subject to } \sum_{i=1}^{\infty} \beta_i^2 < \infty.$$
 (18)

The optimal interior solution is given by  $\beta_{0,i} = \gamma_i/\sigma_i^2$ , which corresponds to the solution  $\xi_0 = \sum_{i=1}^{\infty} \gamma_i v_i/\sigma_i^2$ . Then, Assumption 1 requires that  $\sum_{i=1}^{\infty} \beta_{0,i}^2 = \sum_{i=1}^{\infty} \gamma_i^2/\sigma_i^4 < \infty$ . This condition requires that  $\gamma_i$  must be zero on eigenfunctions for which  $\sigma_i = 0$  (i.e., basis functions for  $\mathcal{N}(P)$ ). This means that the Riesz representer  $\alpha$  must belong to  $\mathcal{N}(P)^{\perp}$ . Moreover, the condition imposes that the Riesz representer cannot be supported heavily on the lower part of the right eigenfunctions of the conditional expectation operator P. This means that the Riesz representer has to be smooth enough relative to the spectrum of the conditional expectation operator P. Theorem 2 states the solution  $\xi_0$  to Equation (18) can be also characterized as a root to  $\alpha = P^*P\xi_0$ . Indeed, for  $\xi_0 = \sum_{i=1}^{\infty} \beta_{0,i} v_i$  with  $\sum_{i=1}^{\infty} \beta_{0,i}^2 < \infty$ , we have  $P^*P\xi_0 = \sum_{i=1}^{\infty} \sigma_i^2 \beta_{0,i} v_i$ . Equating it to  $\alpha = \sum_{i=1}^{\infty} \gamma_i v_i$  gives  $\beta_{0,i} = \gamma_i/\sigma_i^2$  for all i, which recovers the solution to Equation (18). This verifies the conclusion of Theorem 2 in the special case of a compact linear operator P. But Theorem 2 holds more generally for non-compact linear operators as well, such as the operators in Examples 2 and 3.

#### 4.1.2 Strong Identification versus Identification

Example 4 shows that, for compact P, Assumption 1 automatically restricts the Riesz representer  $\alpha$  to the orthogonal complement of the null space of operator P. That is, it restricts to  $\alpha \in \mathcal{N}(P)^{\perp}$ . This can be shown to be the sufficient and necessary condition for the identification of the target parameter for general P, by slightly generalizing the analysis in Severini and Tripathi [2006].

**Lemma 2.** The parameter  $\theta^*$  is identifiable, i.e.,  $\theta^* = \mathbb{E}[m(W; h_0)]$  for any  $h_0 \in \mathcal{H}_0$ , if and only if  $\alpha \in \mathcal{N}(P)^{\perp} = \operatorname{cl}(\mathcal{R}(P^*))$ .

Lemma 2 gives the weakest condition for the identification of the target parameter  $\theta^*$  when the primary nuisance  $h^*$  can be underidentified. This condition trivially holds if the nuisance function  $h^*$  is identified to begin with, so that  $\mathcal{N}(P) = \{0\}$  and  $\operatorname{cl}(\mathcal{R}(P^*)) = \mathcal{H}$ . In fact, the converse is also true:  $h^*$  is identifiable if and only if every continuous linear functional of  $h^*$  is identifiable (see Lemma 6 in Appendix C). But for a given parameter of interest, Lemma 2 shows that the identifiability of  $h^*$  is not necessary for the identifiability of  $\theta^*$ , since  $\theta^*$  may capture identifiable parts of the nuisance  $h^*$ , provided that the corresponding Riesz representer is orthogonal to the null space of P.

Although the condition in Lemma 2 is enough for the identification of  $\theta^*$ , it alone does not suffice for inference on  $\theta^*$ . Thus, we impose the strong identification condition in Assumption 1. Assumption 1 is certainly always stronger than the identification condition in Lemma 2, since by Theorem 2 we know that Assumption 1 is equivalent to  $\alpha \in \mathcal{R}(P^*P)$ , and  $\mathcal{R}(P^*P) \subseteq \text{cl}(\mathcal{R}(P^*))$ . Thus our Assumption 1 requires the target functional to be not only identifiable, but also regular enough so that inference on it is possible.

#### 4.1.3 Relation to the Condition in Severini and Tripathi [2012]

Our Assumption 1 is also closely related to the condition  $\alpha \in \mathcal{R}(P^*)$  proposed in Severini and Tripathi [2012]. This condition is equivalent to the existence of  $q_0 \in \mathcal{L}_2(T)$  that solves

$$[P^*q](S) = \Pi_{\mathcal{H}}[g_1(W)q(T) \mid S] = \alpha(S), \tag{19}$$

or equivalently,

$$Q_0 \neq \emptyset$$
, where  $Q_0 := \{ q \in \mathcal{L}_2(T) : [P^*q](S) = \alpha(S) \}$  (20)

Compared to the identification condition in Lemma 2, this condition additionally rules out  $\alpha$  on the boundary of  $\mathcal{R}(P^*)$ . In the setting of NPIV regression, Severini and Tripathi [2012] argue that

this is a necessary condition for the  $\sqrt{n}$ -estimability of IV functionals. Deaner [2019] also shows that this condition is sufficient and necessary for the robust estimation of IV functionals when the IV exclusion restriction is misspecified.

However, the condition that  $\alpha \in \mathcal{R}(P^*)$ , or equivalently, that there exists  $q_0 \in \mathcal{Q}_0$ , is only a necesary condition for  $\sqrt{n}$ -estimability. Even when it is true, the target linear functional may not be  $\sqrt{n}$ -estimable, especially if the inverse problem in Equation (2) is severely ill-posed [Chen and Pouzo, 2015]. To overcome this challenge, we impose our strong identification condition in Assumption 1. Note that our condition  $\alpha \in \mathcal{R}(P^*P)$  further strengthens the condition  $\alpha \in \mathcal{R}(P^*)$ , since we always have  $\mathcal{R}(P^*P) \subseteq \mathcal{R}(P^*)$ . In particular,  $\mathcal{R}(P^*P)$  is a strict subset of  $\mathcal{R}(P^*)$  unless  $\mathcal{R}(P)$  is a closed set and the inverse problem in Equation (2) is well-posed [Carrasco et al., 2007]. We do not assume a closed  $\mathcal{R}(P)$  and therefore well-posedness. Instead, we restrict the Riesz representer  $\alpha$  to  $\mathcal{R}(P^*P)$ . This imposes a stronger restriction on the Riesz representer than the condition  $\alpha \in \mathcal{R}(P^*)$ , but it allows the inverse problem in Equation (2) for the primary nuisance function to be arbitrarily ill-posed.

Moreover, we find that the class of solution functions  $\Xi_0$  in Eq. (3) is actually closely related to  $\mathcal{Q}_0$  above. According to Theorem 2, we have  $P^*P\xi_0 = \alpha$ , which immediately implies that  $P\xi_0 \in \mathcal{Q}_0$  for any  $\xi_0 \in \Xi_0$ . Furthermore, for any  $q_0 \in \mathcal{Q}_0$  we have  $\mathcal{Q}_0 = q_0 + \mathcal{N}(P^*)$ ; that is,  $\mathcal{Q}_0$  is a closed affine space, and therefore must have a unique minimum-norm element. Then, since  $\mathcal{R}(P)$  is orthogonal to  $\mathcal{N}(P^*)$  for any linear operator P, these two observations provide an alternative interpretation for Assumption 1: it requires that the minimum-norm function in  $\mathcal{Q}_0$  belongs to  $\mathcal{R}(P)$ , which we formalize in the following lemma.

**Lemma 3.** Define 
$$q^{\dagger} = \operatorname{argmin}_{q \in \mathcal{Q}_0} \|q\|_2^2$$
. Let  $\xi_0 \in \mathcal{H}$ . Then,  $\xi_0 \in \Xi_0$  if and only if  $P\xi_0 = q^{\dagger}$ .

Lemma 3 shows that the debiasing nuisance  $q^{\dagger} = P\xi_0$  used in the doubly robust identification formula in Theorem 1 is the minimum-norm element of the class  $\mathcal{Q}_0$ . However, we can actually show that the doubly robust identification formula is valid, with robustness properties akin to Lemma 1, for any  $q_0 \in \mathcal{Q}_0$ , not just  $q^{\dagger}$ .

**Theorem 3.** If  $\alpha \in \mathcal{R}(P^*)$ , then the conclusions in Theorem 1 hold for any  $q_0 \in \mathcal{Q}_0$ . In particular,  $\theta^* = \mathbb{E}[\psi(W; h_0, q_0)]$  for any  $h_0 \in \mathcal{H}_0$  and  $q_0 \in \mathcal{Q}_0$ . Moreover, for any  $h \in \mathcal{H}$ ,  $q \in \mathcal{L}_2(T)$ ,  $h_0 \in \mathcal{H}_0$ , and  $q_0 \in \mathcal{Q}_0$ ,

$$|\mathbb{E}[\psi(W;h,q)] - \theta^*| = |\langle P(h-h_0), q - q_0 \rangle| = |\langle h - h_0, P^*(q - q_0) \rangle|$$

$$\leq \min\{ ||P(h-h_0)||_2 ||q - q_0||_2, ||h - h_0||_2 ||P^*(q - q_0)||_2 \}.$$
(21)

Additionally, for two fixed functions  $h_0 \in \mathcal{H}$  and  $q_0 \in \mathcal{L}_2(T)$ , we have  $h_0 \in \mathcal{H}_0$  and  $q_0 \in \mathcal{Q}_0$  if and only if

$$\frac{\partial}{\partial t} \mathbb{E}[\psi(W; h_0 + th, q_0)]\big|_{t=0} = \frac{\partial}{\partial t} \mathbb{E}[\psi(W; h_0, q_0 + tq)]\big|_{t=0} = 0, \quad \forall h \in \mathcal{H}, q \in \mathcal{L}_2(T). \tag{22}$$

Interestingly, Theorem 3 shows that  $h_0 \in \mathcal{H}_0$  and  $q_0 \in \mathcal{Q}_0$  is the sufficient and necessary condition for the Neyman orthogonality of the doubly robust identification formula. The results in Theorem 1 and Lemma 1 under our Assumption 1 can be viewed as a corollary of Theorem 3, with  $q_0$  and q restricted to  $P\xi_0$  and  $\{P\xi:\xi\in\mathcal{H}\}$  respectively. As we will show later, this kind of restriction will enable us to construct  $\sqrt{n}$ -consistent and asymptotically normal estimators for the target functional, even when the primary nuisance is weakly identified. See Section 4.3 for more discussions.

#### 4.1.4 Relation to Other Conditions

Theorem 2 shows that our Assumption 1 is equivalent to  $\alpha \in \mathcal{R}(P^*P)$ . This can seen as a so-called "source condition" on the Riesz representer  $\alpha$ , restricting the regularity of  $\alpha$  with respect to the linear operator P [e.g., Carrasco et al., 2007, Florens et al., 2011].

Our Assumption 1 is, however, fundamentally different from imposing source conditions on the primary nuisance function, such as the IV regression itself [e.g., Carrasco et al., 2007, Florens et al., 2011, Babii and Florens, 2017, Darolles et al., 2011, Singh et al., 2019]. For example, Darolles et al. [2011] assumes that the true IV regression  $h^*$  lies in the space  $\mathcal{R}((P^*P)^{\beta/2})$  for some exponent  $\beta > 0$ . This source condition directly restricts the smoothness of the IV regression and the degree of ill-posedness of the IV conditional moment restriction.

Alternatively, some other literature define and bound so-called "ill-posedness measures" of the inverse problem defining  $h^*$  relative to a function class [e.g., Chen and Pouzo, 2012, 2015, Chen and Christensen, 2018, Dikkala et al., 2020, Kallus et al., 2021]. These ill-posedness measures bound the ratio between weak-metric and strong-metric errors, so that bounds on the former yield bounds on the latter, making  $h^*$  itself strongly identified, that is, unique (in the function class) and well-estimable. This would allow us, in particular, to do inference on the functional by bounding the strong-metric error in the second branch of Eq. (21). For inference on the functional, we could alternatively impose similar ill-posedness measures on  $q_0 \in \mathcal{Q}_0$ , so as to instead control the strong-metric error in the first branch [e.g., Kallus et al., 2021]. In either case, we are effectively imposing strong identification of functions. Our Assumption 1 is fundamentally different and complements this literature.

We remark that our Assumption 1 is also deeply connected to several ostensibly different conditions in some previous literature. In Appendix A.1, we equivalently characterize  $\xi_0 \in \Xi_0$  in terms of a certain projection of  $q_0 \in \mathcal{Q}_0$ , thereby showing that our Assumption 1 strengthens a condition in Ichimura and Newey [2022]. Moreover, in Appendix A.2, we show that a key condition in Ai and Chen [2007], when specialized to our setting, actually implies our Assumption 1. In Section 7.1, we show that a condition in Chen [2021] for partially linear IV models also implicitly imposes our Assumption 1. Therefore, our Assumption 1 also provides new and generalized interpretations for the assumptions in these existing work.

#### 4.2 Revisiting the Examples

We now revisit the examples from Section 2 to instantiate the conditions discussed above.

**Example 1, Cont'd** (Functionals of NPIV Regression). Consider the parameter  $\theta^*$  given in Equation (9). Then Equation (20) posits the existence of functions  $q_{0,1}, \ldots, q_{0,d} \in \mathcal{L}_2(Z)$  for  $d = d_X$ , such that  $q_0 = (q_{0,1}, \ldots, q_{0,d})$  solves

$$\mathbb{E}[q(Z) \mid X] = \alpha(X) = X. \tag{23}$$

Assumption 1 further requires the existence of  $\xi_0 = (\xi_{0,1}, \dots, \xi_{0,d})$  such that  $\xi_{0,i} \in \mathcal{L}_2(X)$  and  $q^{\dagger} = (\mathbb{E}[\xi_{0,1}(X) \mid Z], \dots, \mathbb{E}[\xi_{0,d}(X) \mid Z])^{\top}$  satisfies Equation (23). Alternatively, any such  $\xi_0$  is given by

$$\xi_{0,i} \in \underset{\xi_i \in \mathcal{L}_2(X)}{\operatorname{argmin}} \, \mathbb{E}\Big[ (\mathbb{E}[\xi_i(X) \mid Z])^2 \Big] - \mathbb{E}[\alpha_i(X)\xi_i(X)], \tag{24}$$

where  $\alpha_i$  is the *i*th coordinate of  $\alpha$  in Equation (23). According to Theorems 1 and 3, even when the NPIV regression  $h^*$  is unidentifiable, the parameter  $\theta^*$  is still identifiable by any  $h_0$  solving Equation (8), any  $q_0$  solving Equation (23), or any  $\xi_0$  solving Equation (24).

Escanciano and Li [2021] also study the estimation of and inference on the best linear approximation coefficient  $\mathbb{E}[XX^{\top}]^{-1}\theta^*$ , allowing the NPIV regression  $h^*$  to be unidentifiable. The assumption 3 in their paper is equivalent to the existence of a function  $q_0$  that solves Equation (23) (although  $q_0$  is not necessarily in the range space  $\mathcal{R}(P)$ ). They propose a penalized linear sieve estimator that can converge to a particular solution  $q_0$  to Equation (23), and then use it to construct their estimator for  $\theta^*$ . They restrict the ill-posedness of the NPIV regression by imposing a source condition [Escanciano and Li, 2021, assumption A4] and prove that their resulting estimator can achieve desirable asymptotic properties.

In our paper, we will accommodate general flexible hypothesis classes. This permits going beyond sieve estimation and its involved technical assumptions (Assumptions A.2–A.6 in Escanciano and Li, 2021) and allows us to rely instead on high-level conditions for approximation by general hypothesis classes. To enable this, we instead incorporate penalization into the general minimax estimation framework with general hypothesis classes [Dikkala et al., 2020, Kallus et al., 2021] and we employ the doubly robust identification formula in Theorem 1 to cancel out estimation errors in these nuisances so that we do not need strong assumptions to characterize their behavior. This leverages highly flexible machine learning nuisance estimators and the resulting functional estimator still has desirable asymptotic properties. Moreover, under Assumption 1, these can be achieved even without restricting the ill-posedness of the NPIV problem.

**Example 2, Cont'd** (Proximal Causal Inference). For the average treatment effect  $\theta^*$  identified via Equation (11), Equation (20) corresponds to the existence of another nuisance function  $q_0(Z, X, A)$  solving

$$\mathbb{E}[q(Z, X, A) \mid V, X, A] = \alpha(V, X, A) = \frac{A - \mathbb{P}(A = 1 \mid V, X)}{\mathbb{P}(A = 1 \mid V, X)(1 - \mathbb{P}(A = 1 \mid V, X))}.$$
 (25)

We note that the  $q_0$  here corresponds to a treatment bridge function, which is a second type of bridge function in proximal causal inference [Cui et al., 2022, Kallus et al., 2021].

Our Assumption 1 further requires the existence of  $\xi_0 \in \mathcal{L}_2(V, X, A)$  such that  $q^{\dagger}(Z, X, A) = [P\xi_0](Z, X, A) = \mathbb{E}[\xi_0(V, X, A) \mid Z, X, A]$  satisfies Equation (25), *i.e.*, there exists a treatment bridge function in the range space  $\mathcal{R}(P)$ . Any such  $\xi_0$  is also given by

$$\xi_0 \in \operatorname*{argmin}_{\xi \in \mathcal{L}_2(V, X, A)} \mathbb{E}\Big[ (\mathbb{E}[\xi(V, X, A) \mid Z, X])^2 \Big] - \mathbb{E}[\alpha(V, X, A)\xi(V, X, A)]. \tag{26}$$

Then Theorems 1 and 3 imply that  $\theta^*$  can be identified by any  $h_0$  solving Equation (12), any  $q_0$  solving Equation (25), and any  $\xi_0$  solving Equation (26).

Although any solutions to Equations (12), (25) and (26) identify  $\theta^*$ , multiplicity of solutions raises significant challenges for statistical inference. Indeed, even if uniqueness is not assumed for identification, the existing proximal causal inference literature largely assumes uniqueness for statistical inference [e.g., Cui et al., 2022, Kallus et al., 2021, Ghassami et al., 2021, Mastouri et al., 2021, Singh, 2020, Miao and Tchetgen, 2018]. One exception is Imbens et al. [2021], which handles the nonunique nuisances by a penalized generalized method of moment estimator, but their approach only applies in their specific panel-data setting where the nuisance is linearly parameterized. In this paper, we will develop new estimators and inferential procedures that are robust to the nonuniqueness of general nonparametric nuisance functions. Another exception is Deaner [2018], which focuses on the conditional average treatment effect, and establishes identification and well-posedness without requiring identification of the bridge function. Moreover, existing literature on nonparametric proximal causal inference restricts the ill-posedness of the inverse problem in Equation (12) for the primary bridge function, by either assuming source conditions on the bridge

function [Singh, 2020, Mastouri et al., 2021] or relying on ill-posedness measures [Ghassami et al., 2021, Kallus et al., 2021]. Our paper shows that these are not necessary if the linear functional is regular enough in the sense that there exists solutions to Equation (26). Given Theorem 2, this follows if the observable propensity function P(A = 1 | V, X) is sufficiently regular.

**Example 3, Cont'd** (Missing-Not-at-Random Data with Shadow Variables). For the parameter  $\theta^*$  in Equation (13), Assumption 1 requires the existence of  $\xi_0 \in \mathcal{L}(X, V)$  such that

$$\xi_0 \in \underset{\xi \in \mathcal{L}(X,V)}{\operatorname{argmin}} \, \mathbb{E}\Big[ (\mathbb{E}[\xi(X,V) \mid X,Z])^2 \Big] - \mathbb{E}[\alpha(X,V)\xi(X,V)]. \tag{27}$$

Then Theorem 1 implies that  $\theta^*$  can be identified by any  $h_0$  solving Equation (14) or any  $\xi_0$  solving Equation (27). Moreover, Theorem 2 means that any such  $\xi_0$  can be equivalently characterized by

$$\mathbb{E}\left[Aq^{\dagger}(X,Z) \mid X,V\right] = \alpha(X,V) = V,$$
where  $q^{\dagger}(X,Z) = [P\xi_0](X,Z) = \mathbb{E}[\xi_0(X,V) \mid X,Z].$  (28)

Li et al. [2022] also assumes a condition that requires the existence of a  $q_0$  that satisfies Equation (28) (although their  $q_0$  function is not necessarily in the range space  $\mathcal{R}(P)$ ). Then they develop estimation and inferential methods robust to nonunique nuisances. Their method extends that in Santos [2011]: they first use a linear sieve estimator proposed by Chernozhukov et al. [2007] to estimate the *set* of solutions to Equation (28) (namely the set  $\mathcal{Q}_0$  defined in Equation (20)), and then pick a unique element therein that maximizes a certain criterion. In contrast, the methods we will propose can accommodate flexible hypothesis classes, rely on high-level conditions about these classes, and avoid the challenging task of estimating solution sets to conditional moment restrictions.

#### 4.3 Challenges with Ill-posed Nuisance Estimation

In Theorem 3, we show that the doubly robust identification formula satisfies the Neyman orthogonality property. Following the recent literature on debiased machine learning cited above, it can therefore be hoped we can simply plug in any flexible nuisance estimators and use the debiased machine learning inference algorithm.

However, because of the *ill-posedness* of the nuisance estimation problem, statistical inference on the target parameter based on asymptotic normality can be very challenging. To illustrate the challenge, consider some generic nuisance estimators  $\hat{h}, \hat{q}$  for certain  $h_0 \in \mathcal{H}_0, q_0 \in \mathcal{Q}_0$ , and the corresponding doubly robust estimator for the target parameter:

$$\tilde{\theta} = \frac{1}{n} \sum_{i=1}^{n} \psi(W_i; \hat{h}, \hat{q}).$$

The estimation error of this estimator is decomposed as follows: for any  $h_0 \in \mathcal{H}_0, q_0 \in \mathcal{Q}_0$ ,

$$\sqrt{n}(\tilde{\theta} - \theta^*) = \mathbb{G}_n(\psi(W; h_0, q_0) - \theta^*) + \mathbb{G}_n\Big(\psi(W; \hat{h}, \hat{q}) - \psi(W; h_0, q_0)\Big) + \sqrt{n}\mathbb{P}\Big(\psi(W; \hat{h}, \hat{q}) - \psi(W; h_0, q_0)\Big).$$
(29)

While the first term in Equation (29) can be proved to be asymptotically normal by the central limit theorem, the second and third terms depend on the estimation errors of  $\hat{h}, \hat{q}$  and they are particularly challenging to handle because of the ill-posedness of the nuisance estimation. The second

term suffers from issues of non-uniqueness while the third term suffers from issues of discontinuity of inverse problems.

The second term in Equation (29) is a stochastic equicontinuity term. To make this term negligible, we typically need to require that the nuisance estimators  $\hat{h}, \hat{q}$  converge to fixed  $h_0 \in \mathcal{H}_0, q_0 \in \mathcal{Q}_0$ , in terms of strong metrics like the  $L_2$  norm [e.g., Lemma 19.24 in Van der Vaart, 2000]. This remains the case even if we employ cross fitting as described in Definition 1 below [e.g., see discussions below Assumption 3.2 in Chernozhukov et al., 2018a]. In this paper, we study ill-posed inverse problems where nuisances  $h_0, q_0$  can be non-unique. In this case, common nuisance estimators  $\hat{h}, \hat{q}$  typically do not converge to any fixed asymptotic limits. As a result, the stochastic equicontinuity term is generally not negligible, and the resulting functional estimator can easily have an intractable asymptotic distribution (see section 3.1 in Chen, 2021 for a concrete example in the IV setting). To overcome this challenge, we will develop penalized nuisance estimators that converge to fixed asymptotic limits even when the nuisances are non-unique, so that the second term in Equation (29) is negligible.

The third term in Equation (29) quantifies the bias due to the estimation errors of  $\hat{h}$  and  $\hat{q}$ . According to Theorem 3, this term can be bounded in terms of either  $\|\hat{h} - h_0\|_2 \|P^*[\hat{q} - q_0]\|_2$  or  $||P[\hat{h}-h_0]||_2||\hat{q}-q_0||_2$ . If we estimate  $\hat{h}$  and  $\hat{q}$  by directly solving empirical analogues of Equations (2) and (19), then we can establish convergence rates of  $\hat{h}, \hat{q}$  in terms of the weak projected metrics  $||P[\hat{h}-h_0]||_2$  and  $||P^*[\hat{q}-q_0]||_2$  [e.g., Chen and Pouzo, 2012, Dikkala et al., 2020, Kallus et al., 2021]. However, the strong-metric estimation errors,  $\|\hat{h} - h_0\|_2$  or  $\|\hat{q} - q_0\|_2$ , may converge arbitrarily slowly (or even not at all), depending on the degrees of ill-posedness of the inverse problems associated with  $h_0$  and  $q_0$ . Consequently, when these inverse problems are severely ill-posed, the resulting functional estimator may converge slowly and not be asymptotically normal. To overcome this challenge, we impose our Assumption 1, which restricts the inverse problem associated with  $q_0$  (see discussions around Lemma 3). Under this assumption, we can instead estimate  $q^{\dagger} = \operatorname{argmin}_{q \in \mathcal{Q}_0} \|q\|_2$ , which by Lemma 3 is equal to  $P\xi_0$  for any  $\xi_0 \in \Xi_0$ . In the next section, we will propose a minimax estimator for  $q^{\dagger} = P\xi_0$  based on the formulation of  $\xi_0$  in Assumption 1, and provide a strong-metric convergence rate of this estimator that does not involve any additional ill-posedness measure. The intuition behind this strong-metric result for  $q^{\dagger}$  stems from the fact that, under Assumption 1, it essentially corresponds to a weak-metric convergence for  $\xi_0$ , for which we can provide ill-posednessfree rates. With the strong-metric convergence rate for  $\hat{q}$ , we only need a weak-metric convergence rate of  $\hat{h}$  to make the third term in Equation (29) vanish. As a result, our functional estimator can be asymptotically normal even without restricting the ill-posedness of Equation (2) for the primary nuisance function.

## 5 Minimax Estimation of Nuisances

Here we present and analyze our minimax estimators of the primary and debiasing nuisances. In this section we use the notation  $h_0$  to denote an arbitrary element of  $\mathcal{H}_0$ , and  $h^{\dagger}$  to denote the minimum-norm element of  $\mathcal{H}_0$ , to which we will establish consistency. Note again that this element is always unique, since  $\mathcal{H}_0$  is a closed linear subspace. Similarly, we let  $q^{\dagger} = P\xi_0$  for any  $\xi_0 \in \Xi_0$ , which per Lemma 3 is the minimum-norm element of  $\mathcal{Q}_0$ .

### 5.1 Penalized Estimation of the Primary Nuisance Function

We first consider estimation of the minimum-norm primary nuisance function  $h^{\dagger}$ . We will consider estimators of the form

$$\hat{h}_n = \underset{h \in \mathcal{H}_n}{\operatorname{argmin}} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n \left[ \left( g_1(W) h(S) - g_2(W) \right) q(T) - \frac{1}{2} q(T)^2 + \mu_n h(S)^2 \right], \tag{30}$$

where  $\mathcal{H}_n$  and  $\mathcal{Q}_n$  are function classes for empirical minimax estimation, and  $\mu_n$  is a regularization hyperparameter for the penalized estimation.

Before we provide finite-sample bounds for this class of estimators, we must establish some technical conditions. First, we assume  $g_1$ ,  $g_2$  are bounded. (We use 1 as the bound without loss of generality, since they appear linearly in the conditional moment restriction in Eq. (2).)

**Assumption 2.** We have that: (1)  $||g_2||_2 \le 1$ ; and (2)  $||g_1||_{\infty} \le 1$ .

Next, we require that  $\mathcal{H}_n$ ,  $\mathcal{Q}_n$  lie within some well-behaved classes, satisfying some regularity conditions, as follows.

**Assumption 3.** There exist some function classes  $\bar{\mathcal{H}} \subset \mathcal{H}$  and  $\bar{\mathcal{Q}} \subset L_2(T)$ , such that: (1)  $\mathcal{H}_n \subseteq \bar{\mathcal{H}}$  and  $\mathcal{Q}_n \subseteq \bar{\mathcal{Q}}$ ; (2)  $||h||_{\infty}, ||q||_{\infty} \leq 1$  for all  $h \in \bar{\mathcal{H}}$  and  $q \in \bar{\mathcal{Q}}$ ; (3)  $h^{\dagger} \in \bar{\mathcal{H}}$ ; (4)  $\mathbb{E}[g_1(W)h(S) - g_2(W) \mid T = \cdot] = P(h - h^{\dagger}) \in \bar{\mathcal{Q}}$  for all  $h \in \bar{\mathcal{H}}$ ; and (5)  $\bar{\mathcal{H}}$  is compact under the  $L_2$  norm.

Note that  $\mathbb{E}[g_1(W)h^{\dagger}(S) - g_2(W) \mid T] = P(h^{\dagger} - h^{\dagger}) = 0$ , so implicit in above is that  $0 \in \bar{\mathcal{Q}}$ . Next, we require that  $\mathcal{H}_n$ ,  $\mathcal{Q}_n$  approximate  $\bar{\mathcal{H}}$ ,  $\bar{\mathcal{Q}}$ .

**Assumption 4.** There exists some  $\delta_n < \infty$  such that: (1) for every  $h \in \overline{\mathcal{H}}$  there exists  $\Pi_n h \in \mathcal{H}_n$  such that  $||h - \Pi_n h||_2 \le \delta_n$ ; and (2) for every  $q \in \overline{\mathcal{Q}}$  there exists  $\Pi_n q \in \mathcal{Q}_n$  such that  $||q - \Pi_n q||_2 \le \delta_n$ .

This condition is trivial when  $\mathcal{H}_n = \bar{\mathcal{H}}$  and  $\mathcal{Q}_n = \bar{\mathcal{Q}}$ . It also holds when  $\mathcal{H}_n$  and  $\mathcal{Q}_n$  are linear sieves or neural net classes, and  $\bar{\mathcal{H}}$  and  $\bar{\mathcal{Q}}$  are Sobolev balls (see *e.g.* Chen [2007] for linear sieves, or Yarotsky [2017] for neural nets).

Fourth, we require that some particular function classes defined in terms of  $\mathcal{H}_n$  and  $\mathcal{Q}_n$  have well-behaved critical radii.

**Assumption 5.** There exists some  $r_n$  that bounds the critical radii of the star-shaped closures of the function classes  $\mathcal{Q}_n$  and  $\{g_1(W)(h-h^{\dagger})(S)q(T): h \in \mathcal{H}_n, q \in \mathcal{Q}_n\}$ . In addition, we have  $\sup_{h \in \mathcal{H}_n} |(\mathbb{E}_n - \mathbb{E})[h(S)^2]| = o_p(1)$ .

Examples of bounds on critical radii of such functions classes are considered in Dikkala et al. [2020], Kallus et al. [2021] for a variety of choices for  $\mathcal{H}_n$ ,  $\mathcal{Q}_n$ , such as Hölder and Sobolev balls, RKHS balls, linear sieves, neural networks, etc.

Under the above assumptions, we can provide the finite-sample bound for the estimation error of the minimax estimator  $\hat{h}_n$ . The bound is derived from a novel analysis of the minimax estimation problem in Equation (30) that differs substantially from the analysis in the seminal work Dikkala et al. [2020].

**Theorem 4.** Suppose Assumptions 2 to 5 hold. For some universal constant  $c_0, c_1$ , we have that, for  $\zeta \in (0, 1/2)$ , with probability at least  $1 - \zeta$ ,

$$||P(\hat{h}_n - h_0)||_2 \le c_0(r_n + \sqrt{\log(c_1/\zeta)/n} + \delta_n + \mu_n^{1/2})$$

for any  $h_0 \in \mathcal{H}_0$ . Furthermore, as long as  $\mu_n = o(1)$ ,  $\mu_n = \omega(r_n^2)$ , and  $\mu_n = \omega(\delta_n^2)$ , we have

$$\|\hat{h}_n - h^{\dagger}\|_2 = o_p(1)$$
.

### 5.2 Estimation of the Debiasing Nuisance Function

Next, we consider the estimation of the debiasing nuisance function  $q^{\dagger}$ . Here, we will consider estimators of the form

$$\hat{q}_n = \underset{q \in \widetilde{\mathcal{Q}}_n}{\operatorname{argmin}} \, \mathbb{E}_n \left[ \left( g_1(W) \hat{\xi}_n(S) - q(T) \right)^2 \right] = \underset{q \in \widetilde{\mathcal{Q}}_n}{\operatorname{argmax}} \, \mathbb{E}_n \left[ g_1(W) \hat{\xi}_n(S) q(T) - \frac{1}{2} q(T)^2 \right], \tag{31}$$

where 
$$\hat{\xi}_n = \underset{\xi \in \Xi_n}{\operatorname{argmin}} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n \left[ g_1(W)\xi(S)q(T) - \frac{1}{2}q(T)^2 - m(W;\xi) \right].$$
 (32)

Note that in the case that  $\widetilde{Q}_n = Q_n$  we have that  $\widehat{q}_n$  is the corresponding supremum solution in the minimax estimation of  $\widehat{\xi}_n$ , so they could be solved for together. However, we allow for the possibility of separate classes for practical empirical reasons. For example, we may wish to use a kernel estimator where the inner maximization is performed analytically for  $\widehat{\xi}_n$ , then use a different class based on, e.g., neural nets or random forests for the corresponding  $\widehat{q}_n$  estimate.

For this nuisance, we do not need to worry about uniqueness of the estimation, since  $q^{\dagger} = P\xi_0$  is unique for any  $\xi_0 \in \Xi_0$  according to Lemma 3 and we will be able to obtain rates for the estimation of  $q^{\dagger}$  under  $L_2$  norm. However, in order to provide a finite-sample estimation result, we require analogues of Assumptions 3 to 5, as follows.

**Assumption 6.** There exist some function classes  $\bar{\Xi} \subset \mathcal{H}$  and  $\bar{\mathcal{Q}} \subset L_2(T)$ , and function  $\xi^{\dagger} \in \Xi_0$ , such that: (1)  $\Xi_n \subseteq \bar{\Xi}$  and  $\mathcal{Q}_n \subseteq \bar{\mathcal{Q}}$ ; (2)  $\|\xi\|_{\infty}$ ,  $\|q\|_{\infty} \leq 1$  for all  $\xi \in \Xi$  and  $q \in \bar{\mathcal{Q}}$ ; (3)  $\xi^{\dagger} \in \bar{\Xi}$ ; and (4)  $\mathbb{E}[g_1(W)\xi(S) \mid T] = P\xi \in \bar{\mathcal{Q}}$  for all  $\xi \in \bar{\Xi}$ . In addition we have  $\|q\|_{\infty} \leq 1$  for all  $q \in \tilde{\mathcal{Q}}_n$ .

**Assumption 7.** There exists some  $\delta_n < \infty$  such that: (1) for every  $\xi \in \bar{\Xi}$  there exists  $\Pi_n \xi \in \Xi_n$  such that  $\|\xi - \Pi_n \xi\|_2 \leq \delta_n$ ; (2) for every  $q \in \bar{Q}$  there exists  $\Pi_n q \in Q_n$  such that  $\|q - \Pi_n q\|_2 \leq \delta_n$ ; and (3) there exists  $\Pi_n q^{\dagger} \in \tilde{Q}_n$  such that  $\|q^{\dagger} - \Pi_n q^{\dagger}\|_2 \leq \delta_n$ .

**Assumption 8.** There exists some  $r_n$  that bounds the critical radii of the star-shaped closures of the function classes: (1)  $\{q - q^{\dagger} : q \in \widetilde{\mathcal{Q}}_n\}$ ; (2)  $\{q - q^{\dagger} : q \in \mathcal{Q}_n\}$ ; (3)  $\{\xi - \xi^{\dagger} : \xi \in \Xi_n\}$ ; (4)  $\{g_1(W)(\xi - \xi^{\dagger})(S)(q - q^{\dagger})(T) : \xi \in \Xi_n, q \in \widetilde{\mathcal{Q}}_n\}$ ; and (5)  $\{g_1(W)(\xi - \xi^{\dagger})(S)(q - q^{\dagger})(T) : \xi \in \Xi_n, q \in \mathcal{Q}_n\}$ , for some fixed  $\xi^{\dagger} \in \Xi_0 \cap \Xi$ .

We note that the required assumptions on  $\widetilde{\mathcal{Q}}_n$  are significantly stricter than those on  $\mathcal{Q}_n$ . In particular,  $\widetilde{\mathcal{Q}}_n$  only needs to be able to approximate the single function  $q^{\dagger}$ , rather than all functions of the form  $\mathbb{E}[g_1(W)\xi(S)\mid T]$  for  $\xi\in\bar{\Xi}$ . We also note that most parts of Assumptions 6 to 8 are identical to Assumptions 3 to 5 when  $\Xi_n=\mathcal{H}_n$  and  $\bar{\Xi}=\bar{\mathcal{H}}$ . We also note that in the case that  $\widetilde{\mathcal{Q}}_n=\mathcal{Q}_n$  then the first and second function classes in Assumption 8 are identical, as are the fourth and fifth function classes.

We further impose a boundedness assumption on m.

**Assumption 9.** We have that  $||m(W;h)||_2 \le ||h||_2$  for all  $h \in \mathcal{H}$ .

Under the above assumptions, we can provide the following finite-sample bound.

**Theorem 5.** Suppose Assumptions 1, 2 and 6 to 9 hold. For some universal constants  $c_0, c_1, c_2$  and any given  $\zeta \in (0, 1/2)$ , if n is sufficiently large such that  $r_n + c_2\sqrt{\log(c_1/\zeta)} \leq 1$ , then with probability at least  $1 - \zeta$ ,

$$\|\hat{q}_n - q^{\dagger}\|_2 \le c_0 (r_n^{1/2} + (\log(c_1/\zeta)/n))^{1/4} + \delta_n).$$

Compared with Theorem 4, this bound only gives a slow rate in the order of  $\sqrt{r_n} + \delta_n + 1/n^{1/4}$ , rather than the fast rate of order  $r_n + \delta_n + 1/\sqrt{n}$ . However, the rate here is in terms of the strong  $L_2$  norm, rather than a weak projected norm. Note that this result is based on our novel analysis of the estimation problems in Equations (31) and (32). They are different from the canonical forms of minimax problems in Dikkala et al. [2020].

## 6 Debiased Inference on the Linear Functional

Given the finite sample bounds from the previous section, and the discussion in Section 4.3, we can now present our main results on the estimation and inference of  $\theta^*$ . First we define the K-fold cross-fitting estimator, for some fixed K that does not depend on n, as follows.

**Definition 1** (Debiased Machine Learning Estimator). Fix an integer  $K \geq 2$ .

- 1. Randomly split the n observations into K (approximately) even folds, whose index sets are denoted by  $\mathcal{I}_1, \ldots, \mathcal{I}_K$ , respectively.
- 2. For k = 1, ..., K, use all data except that in  $\mathcal{I}_k$  to construct nuisance estimators  $\hat{h}^{(k)}$  and  $\hat{q}^{(k)}$  as described in Equations (30) and (31), respectively.
- 3. Construct the final debiased machine learning estimator:

$$\hat{\theta}_n = \frac{1}{K} \sum_{k=1}^K \frac{1}{|\mathcal{I}_k|} \sum_{i \in \mathcal{I}_k} \psi(W_i; \hat{h}^{(k)}, \hat{q}^{(k)}), \quad \psi(W; h, q) = m(W; h) + q(T)(g_2(W) - g_1(W)h(S)).$$

Then, we can obtain the following result.

**Theorem 6.** Let the estimator  $\hat{\theta}_n$  be defined as in Definition 1, and suppose the full conditions of Theorems 4 and 5 hold. Then, as long as  $r_n = o(n^{-1/3})$ ,  $\delta_n = o(n^{-1/4})$ ,  $\delta_n r_n^{1/2} = o(n^{-1/2})$ ,  $\mu_n r_n = o(n^{-1})$ , and  $\mu_n \delta_n^2 = o(n^{-1})$ , we have  $\|P(\hat{h}_n - h_0)\|_2 \|\hat{q}_n - q^{\dagger}\|_2 = o_p(n^{-1/2})$ , and that as  $n \to \infty$ ,

$$\sqrt{n} \left( \hat{\theta}_n - \theta^* \right) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left( \psi(W_i; h^{\dagger}, q^{\dagger}) - \theta^* \right) + o_p(1) \rightsquigarrow \mathcal{N} \left( 0, \sigma_0^2 \right),$$

where  $\mathcal{N}(0,\sigma_0^2)$  denotes a Gaussian distribution with mean 0 and variance

$$\sigma_0^2 = \mathbb{E}\left[\left(\theta^* - \psi(W; h^\dagger, q^\dagger)\right)^2\right]. \tag{33}$$

We note that for the full conditions of Theorem 4 to hold, the penalization hyperparameter  $\mu_n$  only needs to converge arbitrarily slower than the critical radii bound  $r_n^2$  and the approximation error bound  $\delta_n^2$ , i.e.,  $\mu_n = \omega(\max(r_n^2, \delta_n^2))$ . At the same time, the condition  $\mu_n r_n = o(n^{-1})$  and  $\mu_n \delta_n^2 = o(n^{-1})$  requires  $\mu_n = o(\min(n^{-1}r_n^{-1}, n^{-1}\delta_n^{-2}))$ . Moreover, when  $r_n = o(n^{-1/3})$ , the condition  $\delta_n r_n^{1/2} = o(n^{-1/2})$  automatically holds if further  $\delta_n = o(n^{-1/3})$ . The conditions on the critical radii  $r_n = o(n^{-1/3})$  and and approximation error  $\delta_n = o(n^{-1/3})$  can be justified for many commonly used machine learning function classes with appropriate structure; see for instance the references on existing results for approximation errors and critical radii cited below Assumptions 4 and 5.

Furthermore, we can estimate the asymptotic variance using the cross-fitting nuisance estimators:

$$\hat{\sigma}_n^2 = \frac{1}{K} \sum_{k=1}^K \frac{1}{|\mathcal{I}_k|} \sum_{i \in \mathcal{I}_k} \left( \hat{\theta}_n - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \right)^2$$
(34)

We can further use the variance estimator above to construct a confidence interval:

$$CI = \left[ \hat{\theta}_n - \Phi^{-1} (1 - \alpha/2) \hat{\sigma}_n^2, \ \hat{\theta}_n + \Phi^{-1} (1 - \alpha/2) \hat{\sigma}_n^2 \right], \tag{35}$$

where  $\hat{\theta}_n$  is the debiased machine learning estimator in Definition 1, and  $\Phi^{-1}(1-\alpha/2)$  is the  $1-\alpha/2$  quantile of the standard normal distribution.

In the following theorem, we show that the variance estimator and the confidence interval above are asymptotically valid.

**Theorem 7.** Let  $\sigma_0^2$  be the asymptotic variance in Equation (33),  $\hat{\sigma}_n^2$  be the variance estimator in Equation (34), and CI be the confidence interval in Equation (35). If the conditions of Theorem 6 hold, then as  $n \to \infty$ ,  $\hat{\sigma}_n^2$  converges to  $\sigma_0^2$  in probability, and  $\mathbb{P}(\theta^* \in \text{CI}) \to 1 - \alpha$ .

## 7 Application to Partially Linear Models

In Examples 1 and 2, we consider IV estimation and proximal causal inference with general non-parametric nuisance functions. In this section, we apply our methods to partially linear models in these settings. Partially linear model is a semiparametric model that has been widely used in exogenous regressions because it retains both the flexibility of nonparametric models and the ease of interpretation of linear models [Härdle et al., 2000]. Our analyses in this section extend the existing literature on partially linear IV models, and also broaden the scope of proximal causal inference literature by studying partially linear models for the first time.

## 7.1 Partially Linear IV Estimation

In Example 1, we considered a general NPIV regression model with  $\mathcal{H} = \mathcal{L}_2(X)$ , where X are endogenous variables. Now we consider  $X = (X_a, X_b) \in \mathbb{R}^{d_a} \times \mathbb{R}^{d_b}$ , and focus on a partially linear IV regression model:

$$\mathcal{H} = \mathcal{H}_{\mathrm{PL}} := \left\{ \theta^{\top} X_a + g(X_b) : \theta \in \mathbb{R}^{d_a}, g \in \mathcal{L}_2(X_b) \right\}.$$

With some slight abuse of notation, we will alternatively refer to any element of  $\mathcal{H}_{PL}$  as h or as the corresponding tuple  $(\theta, g)$ . Accordingly, the true IV regression can be denoted as  $h^{\star}(X) = \theta^{*\top} X_a + g^{\star}(X_b) \in \mathcal{H}_{PL}$ , such that

$$[Ph^{\star}](Z) = \mathbb{E}\left[\theta^{*\top}X_a + g^{\star}(X_b) \mid Z\right] = \mathbb{E}[Y \mid Z]. \tag{36}$$

As in the partially linear regression model, we are interested in the coefficient parameter  $\theta^*$  and view  $g^*$  as a nonparametric nuisance function.

Partially linear IV models have already been studied by a few previous works [Florens et al., 2012, Chen, 2021, Chernozhukov et al., 2018a]. Chernozhukov et al. [2018a], Florens et al. [2012] assume that the IV regression  $h^*$  is uniquely identified by the conditional moment equation in Equation (36). While Chernozhukov et al. [2018a] consider a simpler setting where the nuisance  $g^*$  is a function of exogenous random variables (i.e.,  $X_b$  is part of Z), Florens et al. [2012] allow all variables in IV regression (both  $X_a, X_b$ ) to be endogenous and develop a Tikohnov regularized estimator with strong theoretical guarantees under a source condition on the IV regression. Chen [2021] also allows both  $X_a, X_b$  to be potentially endogenous, and additionally allows the nonparameteric nuisance  $g^*$  to be underidentified. This is also the setting we consider in this part. However,

unlike the penalized sieve-based estimators developed in Chen [2021], we will employ our penalized minimax estimator that can leverage more flexible function classes.

We first note that the target parameter  $\theta^*$  can be written as a linear functional:

$$\theta^* = \mathbb{E}[\alpha(X)h^*(X)],$$

where 
$$\alpha(X) = M^{-1}(X_a - \mathbb{E}[X_a \mid X_b]), M = \mathbb{E}\left[(X_a - \mathbb{E}[X_a \mid X_b])(X_a - \mathbb{E}[X_a \mid X_b])^{\top}\right]$$
 (37)

where we assume the matrix M is invertible.

For  $i = 1, ..., d_a$ , and arbitrary  $h = (\theta, g) \in \mathcal{H}_{PL}$ , we define  $m_i(W; h) = \theta_i$ . Then, for each such i, we can define linear functional  $h \mapsto \mathbb{E}[m_i(W; h)] = \mathbb{E}[\alpha_i(X)h(X)]$  where  $\alpha_i(X)$  is the ith coordinate of  $\alpha$  in Equation (37). Moreover, since  $\alpha_i(X) = \theta_{\alpha,i}^{\top} X_a + g_{\alpha,i}(X_b)$  with  $\theta_{\alpha,i} = [M^{-1}]_{i,:}$ ,  $g_{\alpha,i}(X_b) = -\theta_{\alpha,i}^{\top} \mathbb{E}[X_a \mid X_b]$ , it also belongs to  $\mathcal{H}_{PL}$ , so it is the unique Riesz representer for the linear functional  $h \mapsto \mathbb{E}[m_i(W; h)]$ .

In this setting, the condition proposed by Severini and Tripathi [2012] and described in Equation (20) requires the existence of  $q_0 = (q_{0,1}, \ldots, q_{0,d_a})$  such that for  $i = 1, \ldots, d_a$ , we have  $q_{0,i} \in \mathcal{L}_2(Z)$  and

$$\mathbb{E}[(q_{0,i}(Z) - \alpha_i(X))h(X)] = 0, \quad \forall h \in \mathcal{H}.$$
(38)

Any such  $q_0$  can be alternatively characterized by the following proposition.

**Proposition 1.** Let  $q_0 = (q_{0,1}, \ldots, q_{0,d_a})^{\top}$  where  $q_{0,i} \in \mathcal{L}_2(Z)$  for  $i = 1, \ldots, d_a$ . Then  $q_{0,i}$  satisfies Equation (38) for all  $i = 1, \ldots, d_a$  if and only if

$$\mathbb{E}[q_0(Z) \mid X_b] = \mathbf{0}_{d_a}, \quad \mathbb{E}\left[q_0(Z)X_a^{\top}\right] = I_{d_a},\tag{39}$$

where  $\mathbf{0}_{d_a}$  is an all-zero vector of length  $d_a$  and  $I_{d_a}$  is the  $d_a \times d_a$  identity matrix.

According to Theorem 2, our Assumption 1 strengthens the condition in Equation (39), by requiring the existence of  $\xi_{0,i}(A,X) = \theta_{0,i}^{\top} X_a + g_{0,i}(X_b) \in \mathcal{H}$  for  $i = 1, \ldots, d_a$ , such that  $q^{\dagger} = (\mathbb{E}[\xi_{0,1}(X) \mid Z], \ldots, \mathbb{E}[\xi_{0,d_a}(X) \mid Z])^{\top}$  satisfies Equation (39). Such  $\xi_{0,i}$  is given by

$$\xi_{0,i} \in \underset{\xi_i \in \mathcal{H}}{\operatorname{argmin}} \mathbb{E}\left[ \left( \mathbb{E}[\xi_i(X) \mid Z] \right)^2 \right] - 2\mathbb{E}[m_i(W; \xi_i)]. \tag{40}$$

In order to estimate the nuisance functions, we need to first specify partially linear function classes  $\mathcal{H}_n \subseteq \mathcal{H}_{PL}$ ,  $\Xi_n \subseteq \mathcal{H}_{PL}$  as hypothesis classes for IV regression  $h^*$  and a solution  $\xi_{0,i}$  to Equation (40) respectively, a function class  $\mathcal{Q}_n \subseteq \mathcal{L}_2(Z)$  used to form the inner maximization problem in minimax objectives, and a function class  $\widetilde{\mathcal{Q}}_n \subseteq \mathcal{L}_2(Z)$  as the hypothesis class for  $P\xi_{0,i}$ . Note that again we alternatively refer to elements of  $\mathcal{H}_n$  or  $\Xi_n$  by the overall functions h or  $\xi$ , or as tuples  $(\theta, g)$ . Then we can follow Equation (30) to construct an estimator for the partially IV regression:

$$\begin{split} \hat{h}_n(X) &= \tilde{\theta}^\top X_a + \hat{g}_n(X_b), \\ \text{where } (\tilde{\theta}, \hat{g}_n) &= \underset{(\theta, g) \in \mathcal{H}_n}{\operatorname{argmin}} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n \Big[ \Big( \theta^\top X_a + g(X_b) - Y \Big) q(Z) - \frac{1}{2} q(Z)^2 - \mu_n \Big( \theta^\top X_a + g(X_b) \Big)^2 \Big] \,. \end{split}$$

Although the above already gives a coefficient estimator  $\tilde{\theta}$ , the estimator  $\tilde{\theta}$  is generally not  $\sqrt{n}$ -consistent or asymptotically normal because of the estimation bias of  $\hat{g}_n$ , especially when  $\hat{g}_n$  is constructed by black-box machine learning methods.

To debias the initial coefficient estimator  $\tilde{\theta}$ , we further construct the nuisance estimator  $\hat{q}_n = (\hat{q}_{1,n}, \dots, \hat{q}_{d_a,n})^{\top}$ :

$$\hat{q}_{i,n} = \operatorname*{argmax}_{q \in \widetilde{\mathcal{Q}}_n} \mathbb{E}_n \left[ \bar{\xi}_i(X) q(Z) - \frac{1}{2} q(Z)^2 \right],$$

where  $\bar{\xi}_i(X) = \bar{\theta}_i^{\top} X_a + \bar{g}_i(X_b)$  with

$$(\bar{\theta}_i, \bar{g}_i) = \operatorname*{argmin}_{(\theta, g) \in \Xi_n} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n \left[ \left( \theta^\top X_a + g(X_b) \right) q(Z) - \theta_i - \frac{1}{2} q(Z)^2 \right].$$

Finally, we construct the debiased coefficient estimator as follows:

$$\hat{\theta}_n = \tilde{\theta} + \mathbb{E}_n \Big[ \Big( Y - \tilde{\theta}^\top X_a - \hat{g}_n(X_b) \Big) \hat{q}_n(Z) \Big].$$

Here to obtain the final estimator  $\hat{\theta}_n$ , the initial coefficient estimator  $\tilde{\theta}$  is debiased by the second augmented term that involves the additional debiasing nuisance estimator  $\hat{q}_n$ . Above we use the same data to construct nuisance estimators and the final coefficient estimator for simplicity. But we can easily incorporate the cross-fitting described in Definition 1.

### 7.1.1 Connection to Chen [2021]

Chen [2021] also studies the estimation of partially linear IV regression when the nonparametric component is under-identified. A key condition in Chen [2021] is actually closely related to our existence assumption of functions  $\xi_0$ . Chen [2021] implicitly assumes the existence of  $\rho_0(X_b) = (\rho_{0,1}(X_b), \ldots, \rho_{0,d_a}(X_b))$  such that for  $X_a^{(i)}$ , the *i*th component of  $X_a$ , we have

$$\rho_{0,i} \in \underset{\rho \in \mathcal{L}_2(W)}{\operatorname{argmin}} \, \mathbb{E}\left[\left(\mathbb{E}\left[X_a^{(i)} - \rho(X_b) \mid Z\right]\right)^2\right], \quad i = 1, \dots, d_a.$$

$$(41)$$

In addition, he explicitly assumes that the resulting  $\rho_0$  satisfies that

$$\Gamma = \mathbb{E}\left[\mathbb{E}[X_a - \rho_0(X_b) \mid Z](\mathbb{E}[X_a - \rho_0(X_b) \mid Z])^{\top}\right] \text{ is invertible.}$$
(42)

In the following proposition, we show that these assumptions are actually sufficient conditions for the existence of  $\xi_0 = (\xi_{0,1}, \dots, \xi_{0,d_a})$  characterized by Equation (40).

**Proposition 2.** Let  $\rho_0 = (\rho_{0,1}, \dots, \rho_{0,d_a})$  and  $\Gamma$  be given in Equations (41) and (42) respectively, and define  $\tilde{\xi}_0 = \Gamma^{-1}(X_a - \rho_0(X_b))$ . Then for each  $i = 1, \dots, d_a$ , the ith coordinate of  $\tilde{\xi}_0$ , namely  $\tilde{\xi}_{0,i}$ , is a solution to Equation (40).

Proposition 2 provides another perspective to understand the conditions assumed in Chen [2021]. It shows that Chen [2021] also implicitly assume our Assumption 1 for the partially linear IV model. Chen [2021] does not estimate the functions  $\rho_{0,i}$  or  $\Gamma$  defined in Equations (41) and (42), instead they use them to analyze the asymptotic distribution of his penalized linear sieve estimator. In contrast, we use Equation (40) to estimate the nuisance  $\xi_0$  in Equation (40), so that we can leverage the doubly robust identification formula in Theorem 1. This allows us to employ general minimax nuisance estimators beyond linear sieve estimation. We also note that Proposition 2 implies that we could consider a different method for estimating  $q^{\dagger}$ , based on first directly estimating  $\tilde{\xi}_0$  by solving the minimum projected distance problem of Equation (41), and then estimating the projection of this function via least squares. However, we do not theoretically analyze this approach.

### 7.2 Partially Linear Proximal Causal Inference

In Example 2, we introduced proximal causal inference with a binary treatment and a general nonparametric class of bridge functions  $\mathcal{H} = \mathcal{L}_2(V, X, A)$ . When the treatment is more complex (e.g., continuous), we may be interested in restricting bridge functions to some structured classes. In this part, we consider the following class of partially linear bridge functions:

$$\mathcal{H} = \tilde{\mathcal{H}}_{PL} := \left\{ \theta^{\top} A + g(V, X) : \theta \in \mathbb{R}^{d_A}, g \in \mathcal{L}_2(V, X) \right\}.$$

In addition, let us denote the total set of outcome bridge functions as

$$\widetilde{\mathcal{H}}_{OB} := \left\{ h \in L_2(V, X, A) : \mathbb{E}[Y - h(V, X, Z) \mid U, X, A] = 0 \right\}.$$

To the best of our knowledge, this partially linear model has not been applied to proximal causal inference yet. Previous literature on proximal causal inference focus on either parametric estimation or nonparametric estimation of the bridge functions [e.g., Cui et al., 2022, Miao and Tchetgen, 2018, Kallus et al., 2021, Singh, 2020, Ghassami et al., 2021, Mastouri et al., 2021]. In the following proposition, we give an justification for the partially linear bridge function model.

**Proposition 3.** Suppose that  $\mathbb{E}[Y(a) \mid U, X] = \theta^{\star \top} a + \phi^{\star}(U, X)$ , for some vector  $\theta^{\star}$  and function  $\phi^{\star} \in \mathcal{L}_2(U, X)$ , and that  $\tilde{\mathcal{H}}_{OB}$  is non-empty. Then, we have that  $\tilde{\mathcal{H}}_{PL} \cap \tilde{\mathcal{H}}_{OB}$  is non-empty; that is, there exists a partially-linear outcome bridge function.

Furthermore, suppose in addition that  $\Gamma := \mathbb{E}[(A - \mathbb{E}[A \mid V, X])(A - \mathbb{E}[A \mid V, X])^{\top}]$  is invertible, and that for each  $i \in [d_A]$  there exists  $q_{0,i} \in L_2(Z, X, A)$  such that  $\mathbb{E}[q_{0,i}(Z, X, A)(\theta^{\top}A + g(V, X))] = \theta_i$  for all  $(\theta, g) \in \tilde{\mathcal{H}}_{PL}$ . Then, for any partially linear bridge function  $\theta^{\top}A + g(V, X) \in \tilde{\mathcal{H}}_{OB}$ , we have  $\theta = \theta^*$ ; that is, the partially-linear coefficients are unique.

In Proposition 3, we show that if the conditional expectation of potential outcome Y(a) given unobserved confounders U and covariatess X is partially linear in the treatment a, then there exists a partially linear bridge function. In particular, given the additional conditions in the second part of the proposition, the linear coefficients  $\theta^*$  of any such bridge function characterize the treatment effects.

Now, given the conditions of Proposition 3, this implies that estimating  $\theta^*$  is a special case of the partially-linear IV problem considered in Section 7.1, with the variables  $X_a$ ,  $X_b$ , and Z there corresponding to A, (V, X), and (Z, X, A) here respectively. In particular, all of the results from that section immediately follow here, given with these variable substitutions. That is, we can again estimate  $\theta^*$  using the same de-biased estimator, with  $q^{\dagger}$  estimated following either the estimator  $(\hat{q}_{1,n}, \ldots, \hat{q}_{d_a,n})$  proposed in that section, or the alternative approach based on Proposition 2 discussed in Section 7.1.1.

Furthermore, by the definition of the Riesz representer, it is clear that the functions  $q_{0,i}$  in Proposition 3 satisfy

$$\Pi_{\tilde{\mathcal{H}}_{\mathrm{PL}}}[q_{0,i}(Z,X,A) \mid V,X,A] = \alpha_i(V,X,A) \quad \forall i \in [d_A],$$

where  $\alpha_i$  is the Riesz representer for the partially linear IV functional  $m(W;(\theta,g)) = \theta_i$  as in Section 7.1. That is, the extra condition in Proposition 3 used to justify the uniqueness of  $\theta^*$  in partially linear bridge functions is equivalent to the condition  $\alpha \in \mathcal{R}(P^*)$ , which as discussed in Section 4.1 is guaranteed by Assumption 1. Alternatively, the existence of  $q_0 = (q_{0,1}, \ldots, q_{0,d_A})^{\top}$  could be interpreted as the existence of a treatment-style bridge function for the marginal treatment effect of varying the vector-valued A.

<sup>&</sup>lt;sup>1</sup>Technically it is not exactly the same as treatment bridge functions in the standard proximal causal inference

## 8 Generalized Framework

Finally, we briefly discuss a generalized version of the conditional moment restriction framework laid out in Section 1, and provide corresponding results for estimation and inference in this more general setting. Here, we let some Hilbert spaces  $\mathcal{H} \subseteq L_2(S)^{d_h}$  and  $\mathcal{Q} \subseteq L_2(T)^{d_q}$  be given under the standard  $L_2$  inner products, for some positive integers  $d_h$  and  $d_q$ .

In this general setting, we are interested in the parameter  $\theta^* = \mathbb{E}[m(W; h^*)]$ , where the primary nuisance function  $h^* \in \mathcal{H}$  solves the following orthogonality condition

$$\mathbb{E}\left[G(W;h,q) - r(W;q)\right] = 0 \qquad \forall q \in \mathcal{Q},$$
(43)

for some given r such that  $q \mapsto \mathbb{E}[r(W;q)]$  is a continuous linear functional, that is, there exists  $\beta \in \mathcal{Q}$  such that

$$\mathbb{E}[r(W;q)] = \mathbb{E}[\beta(T)^{\top}q(T)] \qquad \forall q \in \mathcal{Q},$$

and some given G such that there exists  $k(S,T) \in L_2(S,T)^{d_h \times d_q}$  such that

$$\mathbb{E}[G(W; h, q)] = \mathbb{E}[h(S)^{\top} k(S, T) q(T)] \qquad \forall h \in \mathcal{H}, q \in \mathcal{Q}.$$

That is,  $h, q \mapsto \mathbb{E}[G(W; h, q)]$  is bi-linear functional and satisfies a bi-linear version of the standard Riesz representation formula for continuous linear operators. Again, we allow for *weak identification* of  $h^*$  via the orthogonality condition in Equation (43). That is, Equation (43) can be severely illposed and may admit multiple solutions. As before, we let  $\mathcal{H}_0$  denote the set of all such solutions.

We again focus on m such that  $h \mapsto \mathbb{E}[m(W;h)]$  is a continuous linear functional; that is, there exists a unique  $\alpha \in \mathcal{H}$  such that

$$\mathbb{E}[m(W;h)] = \mathbb{E}[\alpha(S)^{\top}h(S)] \qquad \forall h \in \mathcal{H}.$$

This framework subsumes the simpler framework considered in Section 1. Indeed, we can recover the setup in Section 1 by setting  $d_h = 1$ ,  $d_q = 1$ ,  $Q = L_2(T)$ ,  $G(W, h, q) = g_1(W)h(S)q(T)$ , and  $r(W;q) = g_2(W)q(T)$ , because then the above equations are satisfied with  $k(S,T) = \mathbb{E}[g_1(W) \mid S,T]$ ,  $\beta(T) = \mathbb{E}[g_2(W) \mid T]$ , and

$$\mathbb{E} \Big[ g_1(W) h_0(S) q(T) - g_2(W) q(T) \big] = 0 \quad \forall q \in L_2(T) \iff \mathbb{E} [g_1(W) h_0(S) - g_2(W) \mid T] = 0.$$

However, the framework in this section is much more general. For example, it can encompass multiple conditional moment restrictions with different conditioning variables [Ai and Chen, 2012, 2007], or the treatment bridge function in proximal causal inference as the primary nuisance [Cui et al., 2022].

Now, define the operator  $P: \mathcal{H} \to \mathcal{Q}$  and its adjoint  $P^*: \mathcal{Q} \to \mathcal{H}$  by

$$[Ph](T) = \Pi_{\mathcal{Q}}[k(S,T)^{\top}h(S) \mid T], \quad [P^*q](S) = \Pi_{\mathcal{H}}[k(S,T)q(T) \mid S], \quad \forall h \in \mathcal{H}, q \in \mathcal{Q}.$$
 (44)

These generalize the corresponding operators P and  $P^*$  in Sections 1 and 4. We can then verify that Lemma 2 is still true, namely,  $\theta^*$  is identified by all  $h_0$  satisfying the orthogonality condition in Equation (43) if and only if  $\alpha \in \mathcal{N}(P)^{\perp} = \operatorname{cl}(\mathcal{R}(P^*))$ .

literature as in, e.g., Cui et al. [2022]. There, where  $A \in \{0,1\}$ , the treatment bridge functions (up to multiplication by  $(-1)^{1-a}$ ) are defined according to  $\mathbb{E}[q_0(Z,X,a)\mid V,X,A=a]=(-1)^{1-a}\mathbb{P}(A=a\mid V,X)^{-1}$ , where  $(-1)^{1-a}\mathbb{P}(A=a\mid V,X)^{-1}$  is the Riesz representer of the linear functional  $h\mapsto \mathbb{E}[h(V,X,1)-h(V,X,0)]$ . This is equivalent to requiring that  $\mathbb{E}[q_0(Z,X,A)h(V,X,A)]=\mathbb{E}[h(V,X,1)-h(V,X,0)]$  for all  $h\in L_2(V,X,A)$ . Instead, here we require the analogous condition that  $q_0$  satisfies  $\mathbb{E}[q_0(Z,X,A)(\theta^\top A+g(V,X))]=\theta$  for all  $(\theta,g)\in \tilde{\mathcal{H}}_{\rm PL}$ .

To enable the inference of  $\theta^*$ , we need to strengthen the identification condition. In particular, the condition in Equation (20) can be generalized to

$$\mathcal{Q}_0 \neq \emptyset$$
, where  $\mathcal{Q}_0 = \left\{ q_0 \in \mathcal{Q} : P^*q = \alpha \right\} = \left\{ q_0 \in \mathcal{Q} : \mathbb{E} \left[ G(W; h, q_0) - m(W; h) \right] = 0, \ \forall h \in \mathcal{H} \right\}$ .

We further strengthen this condition by imposing our strong identification condition in Assumption 1. This requires the existence of a solution  $\xi_0 \in \mathcal{H}$  to Equation (3), where the optimization objective now depends on the general operator P given in Equation (44). We can easily prove that Theorem 2 still holds, namely, Assumption 1 restricts the Riesz representer  $\alpha$  to the range space  $\mathcal{R}(P^*P)$ . Moreover, like Lemma 3, the debiasing nuisance  $P\xi_0$  for  $\xi_0 \in \Xi_0$  is the minimum-norm function in  $\mathcal{Q}_0$ .

Next, we define the doubly robust equation

$$\psi(W; h, q) = m(W; h) + r(W; q) - G(W; h, q). \tag{45}$$

Then, it is straightforward to argue that Lemma 1 still hold with this equation. We formally state the results in the following lemma.

**Lemma 4.** Let some arbitrary  $h_0 \in \mathcal{H}_0$  and  $q_0 \in \mathcal{Q}_0$  be given and  $\psi(W; h, q)$  be the doubly robust equation in Equation (45). For every  $h \in \mathcal{H}$  and  $q \in \mathcal{Q}$ , we have

$$\mathbb{E}[\psi(W; h, q)] - \theta^* = \mathbb{E}[G(W; h - h_0, q - q_0)].$$

Consequently, it follows that for any  $h \in \mathcal{H}$  and  $q \in \mathcal{Q}$  we have

$$\left| \mathbb{E}[\psi(W; h, q)] - \theta^* \right| \le \min \left\{ \|P(h - h_0)\|_{2,2} \|q - q_0\|_{2,2}, \|h - h_0\|_{2,2} \|P^*(q - q_0)\|_{2,2} \right\},$$

and

$$\frac{d}{dt}\bigg|_{t=0} \mathbb{E}\Big[\psi(W; h_0 + th, q_0 + tq)\Big] = 0.$$

Then, we can apply a similar debiased inference analysis in this more general setting, as long as we can get similar rates for  $||P(\hat{h}_n - h_0)||_{2,2}$  and  $||q - q_0||_{2,2}$  as we obtained in Section 5. Below, we provide appropriate conditions under which we can obtain such rates by generalizing Theorems 4 and 5.

#### 8.1 Penalized Estimation of the Primary Nuisance Function

Here, we consider estimators for the minimum-norm function  $h^{\dagger}$  in  $\mathcal{H}_0$  as follows:

$$\hat{h}_n = \underset{h \in \mathcal{H}_n}{\operatorname{argmin}} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n \left[ G(W; h, q) - r(W; q) - \frac{1}{2} q(Z)^{\top} q(Z) - \mu_n h(S)^{\top} h(S) \right], \tag{46}$$

where all definitions are analogous to those in Section 5.1. Below we provide natural generalizations for the technical assumptions in Section 5.1.

**Assumption 10.** There exist some function classes  $\bar{\mathcal{H}} \subset \mathcal{H}$  and  $\bar{\mathcal{Q}} \subset \mathcal{Q}$ , such that: (1)  $\mathcal{H}_n \subseteq \bar{\mathcal{H}}$  and  $\mathcal{Q}_n \subseteq \bar{\mathcal{Q}}$ ; (2)  $||h||_{\infty}$ ,  $||q||_{\infty} \leq 1$  for all  $h \in \bar{\mathcal{H}}$  and  $q \in \bar{\mathcal{Q}}$ ; (3)  $h^{\dagger} \in \bar{\mathcal{H}}$ ; (4)  $\Pi_{\mathcal{Q}}[k(S,T)^{\top}h(S) - \beta(T) \mid \cdot] \in \bar{\mathcal{Q}}$  for all  $h \in \bar{\mathcal{H}}$ ; and (5)  $\bar{\mathcal{H}}$  is compact under the  $L_2$  norm.

**Assumption 11.** There exists some  $\delta_n < \infty$  such that: (1) for every  $h \in \bar{\mathcal{H}}$  there exists  $\Pi_n h \in \mathcal{H}_n$  such that  $\|h - \Pi_n h\|_{2,2} \leq \delta_n$ ; and (2) for every  $q \in \bar{\mathcal{Q}}$  there exists  $\Pi_n q \in \mathcal{Q}_n$  such that  $\|q - \Pi_n q\|_{2,2} \leq \delta_n$ .

**Assumption 12.** There exists some  $r_n$  that bounds the critical radii of the star-shaped closures of the function classes  $\mathcal{Q}_n$  and  $\{G(W; h-h^{\dagger}, q) : h \in \mathcal{H}_n, q \in \mathcal{Q}_n\}$ . In addition, we have  $\sup_{h \in \mathcal{H}_n} |(\mathbb{E}_n - \mathbb{E})[h(S)^{\top}h(S)]| = o_p(1)$ .

**Assumption 13.** We have that: (1)  $||G(W; h, q)||_2 \le ||h||_{2,2} ||q||_{2,2}$  for all  $q \in \bar{\mathcal{Q}}$  and  $h \in \bar{\mathcal{H}}$ ; (2)  $||r(W; q)|| \le ||q||_{2,2}$  for every  $q \in \mathcal{Q}$ ; (3)  $||G(W; h, q)||_{\infty} \le 1$  for every  $h \in \bar{\mathcal{H}}$  and  $q \in \bar{\mathcal{Q}}$ ; and (4)  $||P(h - h^{\dagger})||_{2,2} \le ||h - h^{\dagger}||_{2,2}$  for every  $h \in \bar{\mathcal{H}}$ .

It is trivial to verify that these conditions generalize those in Section 5. Then, under these assumptions, we can provide the following generalization of Theorem 4.

**Theorem 8.** Suppose Assumptions 10 to 13 hold. For some universal constant  $c_0$ , we have that, for  $\zeta \in (0, 1/2)$ , with probability at least  $1 - \zeta$ ,

$$||P(\hat{h}_n - h_0)||_{2,2} \le c_0(r_n + \sqrt{\log(1/\zeta)/n} + \delta_n + \mu_n^{1/2})$$

for any  $h_0 \in \mathcal{H}_0$ . Furthermore, as long as  $\mu_n = o(1)$ ,  $\mu_n = \omega(r_n^2)$ , and  $\delta_n = o(\mu_n^{1/2})$ , we have  $\|\hat{h}_n - h^{\dagger}\|_{2,2} = o_p(1)$ .

#### 8.2 Estimation of the Debiasing Nuisance Function

Next, we consider the estimation of the debiasing nuisance function  $q^{\dagger}$  in the general setting. Here, we will consider estimators of the form

$$\hat{q}_n = \underset{q \in \widetilde{\mathcal{Q}}_n}{\operatorname{argmax}} \, \mathbb{E}_n \left[ G(W; \hat{\xi}_n, q) - \frac{1}{2} q(T)^\top q(T) \right], \tag{47}$$

where

$$\hat{\xi}_n = \underset{\xi \in \Xi_n}{\operatorname{argmin}} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n \left[ G(W; \xi, q) - m(W; \xi) - \frac{1}{2} q(T)^{\top} q(T) \right]. \tag{48}$$

Again, all definitions here are analogues to those in Section 5.2. Notably, the minimax objective function in Equation (48) is very close to the minimax objective in Equation (46), except that  $m(W;\xi)$  appears in Equation (48) while r(W;q) appears in Equation (46).

Below, we further generalize our previous technical assumptions in Section 5.2.

**Assumption 14.** There exist some function classes  $\bar{\Xi} \subset \mathcal{H}$  and  $\bar{\mathcal{Q}} \subset L_2(T)$ , and  $\xi^{\dagger} \in \Xi_0$ , such that: (1)  $\Xi_n \subseteq \bar{\mathcal{H}}$  and  $\mathcal{Q}_n \subseteq \bar{\mathcal{Q}}$ ; (2)  $\|\xi\|_{\infty}$ ,  $\|q\|_{\infty} \leq 1$  for all  $\xi \in \Xi$  and  $q \in \bar{\mathcal{Q}}$ ; (3)  $\xi^{\dagger} \in \bar{\Xi}$ ; and (4)  $\mathbb{E}[k(S,T)^{\top}\xi(S) \mid T] \in \bar{\mathcal{Q}}$  for all  $\xi \in \bar{\Xi}$ . In addition we have  $\|q\|_{\infty} \leq 1$  for all  $q \in \tilde{\mathcal{Q}}_n$ .

**Assumption 15.** There exists some  $\delta_n < \infty$  such that: (1) for every  $\xi \in \bar{\Xi}$  there exists  $\Pi_n \xi \in \Xi_n$  such that  $\|\xi - \Pi_n \xi\|_{2,2} \leq \delta_n$ ; (2) for every  $q \in \bar{Q}$  there exists  $\Pi_n q \in Q_n$  such that  $\|q - \Pi_n q\|_{2,2} \leq \delta_n$ ; and (3) there exists  $\Pi_n q^{\dagger} \in \tilde{Q}_n$  such that  $\|q^{\dagger} - \Pi_n q^{\dagger}\|_{2,2} \leq \delta_n$ 

**Assumption 16.** There exists some  $r_n$  that bounds the critical radii of the star-shaped closures of the function classes: (1)  $\{q-q^{\dagger}:q\in\widetilde{\mathcal{Q}}_n\}$ ; (2)  $\{q-q^{\dagger}:q\in\mathcal{Q}_n\}$ ; (3)  $\{\xi-\xi^{\dagger}:\xi\in\Xi_n\}$ ; (4)  $\{G(W;\xi-\xi^{\dagger},q-q^{\dagger}):\xi\in\Xi_n,q\in\widetilde{\mathcal{Q}}_n\}$ ; and (5)  $\{G(W;\xi-\xi^{\dagger},q-q^{\dagger}):\xi\in\Xi_n,q\in\mathcal{Q}_n\}$ , for some fixed  $\xi^{\dagger}\in\Xi_0$ .

**Assumption 17.** We have that  $||m(W;q)||_2 \le ||q||_{2,2}$  for all  $q \in \bar{\mathcal{Q}}$ .

Then, we provide the following generalization of Theorem 5.

**Theorem 9.** Suppose Assumptions 1 and 13 to 17 hold. For some universal constants  $c_0, c_1, c_2$  and any given  $\zeta \in (0, 1/2)$ , if n is sufficiently large such that  $r_n + c_2\sqrt{\log(c_1/\zeta)} \leq 1$ , then with probability at least  $1 - \zeta$ ,

$$\|\hat{q}_n - q^{\dagger}\|_{2,2} \le c_0 (r_n^{1/2} + (\log(1/\zeta)/n))^{1/4} + \delta_n).$$

### 8.3 Asymptotic Normality and Inference

Finally, we provide analogues of the results form Section 6 for the more general setting.

**Theorem 10.** Let the estimator  $\hat{\theta}_n$  be defined following the cross-fitting procedure as in Definition 1, with  $\hat{q}$  and  $\hat{h}$  defined following Equations (46) and (47) respectively, and  $\psi(W; h, q)$  defined according to Equation (45). Suppose that the full conditions of Theorems 8 and 9 hold. Then, as long as  $r_n = o(n^{-1/3})$ ,  $\delta_n = o(n^{-1/4})$ ,  $\delta_n r_n^{1/2} = o(n^{-1/2})$ ,  $\mu_n r_n = o(n^{-1})$  and  $\mu_n \delta_n^2 = o(n^{-1})$ , we have  $\|P(\hat{h}_n - h_0)\|_2 \|\hat{q}_n - q^{\dagger}\|_2 = o_p(n^{-1/2})$ , and that as  $n \to \infty$ ,

$$\sqrt{n} \left( \hat{\theta}_n - \theta^* \right) = \frac{1}{\sqrt{n}} \sum_{i=1}^n \left( \psi(W_i; h^{\dagger}, q^{\dagger}) - \theta^* \right) + o_p(1) \rightsquigarrow \mathcal{N} \left( 0, \sigma_0^2 \right)$$

where  $\mathcal{N}(0,\sigma_0^2)$  denotes a Gaussian distribution with mean 0 and variance

$$\sigma_0^2 = \mathbb{E}\Big[\Big(\theta^* - \psi(W; h^\dagger, q^\dagger)\Big)^2\Big]$$

Similarly, we can construct a variance estimator and confidence interval by following Equations (34) and (35) respectively, and prove that they are asymptotically valid.

**Theorem 11.** Let  $\hat{\sigma}_n^2$  and CI be the variance estimator and confidence interval constructed from Equations (34) and (35), with the  $\psi(W; h, q)$  function defined according to Equation (45). If the conditions of Theorem 10 hold, then as  $n \to \infty$ ,  $\hat{\sigma}_n^2$  converges to  $\sigma_0^2$  in probability, and  $\mathbb{P}(\theta^* \in \text{CI}) \to 1 - \alpha$ .

## 9 Conclusions and Future Directions

In this paper, we study the estimation of and inference on strongly identified linear functionals of weakly identified nuisance functions. This challenge arises in a variety of applications in causal inference and missing data, where the primary nuisance (e.g., NPIV regression) is defined by an ill-posed conditional moment equation. Not only is the primary nuisance usually not uniquely identifiable – even if it were, it still discontinuous in the underlying distributions. Side-stepping conditions that control the learnability of the primary nuisance function(s), we propose a novel assumption for the strong identification of just the functional of it. Mere identification of the functional (i.e., uniqueness) is equivalent to restricting the Riesz representer of the functional to a certain subspace. Our assumption further restricts it to a subspace of that subspace. This additional restrictions can in fact be written as the existence of a solution to an optimization problem, which motivates us to propose new minimax estimators for the unknown nuisances. Via a novel analysis, we show our nuisance estimators can converge to fixed limits in terms of the  $L_2$  norm error even when the nuisances are underidentified. Moreover, our nuisance estimators can accommodate a wide variety of flexible machine learning methods like RKHS methods or neural networks. We then use our estimators to construct debiased estimators for the functionals of interest. Put together, we obtain high-level conditions under which our functional estimator is asymptotically normal and under which our estimated-variance Wald confidence intervals are valid.

There are several interesting future directions of research. Our paper currently focuses on *linear* functionals of nuisance functions defined by *linear* conditional moment equations. It would be interesting to explore more general *nonlinear* functionals and/or *nonlinear* conditional moment equations without requiring point identification of the nuisances. As an example of the former, we may consider inference on consumer surplus and deadweight loss as functionals of a demand

function estimated using an IV for an endogenous price [e.g., Chen and Christensen, 2018]. As an example of the latter, we may consider functionals of NPIV quantile regressions [e.g., Example 3.3 in Ai and Chen, 2009]. One important challenge in this direction is to establish the identifiability of the functionals of interest [Chen et al., 2014]. Moreover, our paper studies point-identified functionals (though the nuisances are not identified). We may relax the identification restriction on the functionals, and instead study partial identification bounds of the functionals [Escanciano and Li, 2013]. In particular, debiased inference on partial identification bounds is an area of growing interest [Dorn et al., 2021, Kallus et al., 2022, Kallus, 2022, Yadlowsky et al., 2018] where our new theory may provide new directions.

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# Appendices

## A More on Connections to Some Previous Literature

In this section, we connect our paper to Ichimura and Newey [2022], Ai and Chen [2007]. These two papers study functionals of some functions defined by conditional moment restrictions. They can handle general nonlinear functionals and nonlinear conditional moment restrictions, but they focus on point-identified conditional moment restrictions. In contrast, our paper focuses on linear functionals and linear conditional moment restrictions but we allow for under-identified conditional moment restrictions. In this section, we specialize the results in Ichimura and Newey [2022], Ai and Chen [2007] to the linear setting studied in our paper, aiming to connect our strong identification condition in Assumption 1 to conditions in these two existing papers.

## A.1 Connection to Ichimura and Newey [2022]

Ichimura and Newey [2022] study the influence function of a two-stage sieve estimator for the parameter  $\theta^* = \mathbb{E}[m(W; h^*)]$  where  $h \mapsto \mathbb{E}[m(W; h)]$  defines a functional of  $h \in \mathcal{H} \subseteq \mathcal{L}_2(S)$ , and  $h^*$  is uniquely identified by the orthogonality condition

$$\mathbb{E}[q(T)\rho(W;h)] = 0, \quad q \in \mathcal{Q} \subseteq \mathcal{L}_2(T), h \in \mathcal{H} \subseteq \mathcal{L}_2(S).$$

for a generalized residual function  $\rho(W;h)$ . Ichimura and Newey [2022] study a general nonlinear residual function and hopes to estimate a general nonlinear functional. In contrast, our paper focuses on a linear residual function and targets a linear functional  $h \mapsto \mathbb{E}[m(W;h)]$ . In particular, the conditional moment formulation in our Section 1 can be viewed as a special example with  $\mathcal{Q} = \mathcal{L}_2(T)$  and  $\rho(W;h) = g_2(W) - g_1(W)h(S)$ . Our general formulation in Section 8 further allows for a general  $\mathcal{Q}$  function class, although the corresponding residual function is still linear.

In this subsection, we relate our Section 8 to Ichimura and Newey [2022]. For simplicity, we focus on the conditional-moment formulation with  $Q = \mathcal{L}_2(T)$ ,  $\rho(W; h) = g_2(W) - g_1(W)h(S)$  and  $h \mapsto \mathbb{E}[m(W; h)]$  being a linear functional. In the notations here, Ichimura and Newey [2022] require the functional  $h \mapsto \mathbb{E}[m(W; h)]$  to be continuous with a Riesz representer  $\alpha \in \mathcal{H}$ . Moreover, they assume the existence of  $g_0$  such that

$$[P^*q_0](S) = \Pi_{\mathcal{H}}[g_1(W)q_0(T) \mid S] = \alpha(S). \tag{49}$$

This is identical to Equation (19). Under these two assumptions, their Proposition 3 derives the influence function of a certain two-stage sieve estimator for  $\theta^*$ :

$$\varphi(W; h^{\star}, q^{\star}) = m(W; h^{\star}) - \theta^{\star} + q^{\star}(T)(q_2(W) - q_1(W)h^{\star}(S)), \tag{50}$$

where  $q^*$  is the least squares projection of the  $q_0$  in Equation (49) onto  $\bar{\mathcal{R}}(P)$ , the mean square closure of the range space  $\mathcal{R}(P)$ , namely,

$$q^* = \underset{q \in \bar{\mathcal{R}}(P)}{\operatorname{argmin}} \mathbb{E}\Big[ (q_0(T) - q(T))^2 \Big]. \tag{51}$$

In the following proposition, we show that the debiasing nuisance derived from our Assumption 1 is closely related to the nuisance defined in Equation (51).

**Proposition 4.** For any  $\xi_0 \in \Xi_0$  defined in Assumption 1, we have

$$q^{\dagger} = P\xi_0 = \underset{q \in \mathcal{R}(P)}{\operatorname{argmin}} \mathbb{E}\Big[ (q_0(T) - q(T))^2 \Big]. \tag{52}$$

Proposition 4 shows that our debiasing nuisance  $q^{\dagger} = P\xi_0$  for  $\xi_0$  given in our Assumption 1 is very similar to the function  $q^{\star}$  in Equation (51). The difference is that the former is a projection onto the range space of P, while the latter is the projection onto the closure of the range space. According to the projection theorem [Luenberger, 1997, Theorem 2, Section 3.3], the nuisance  $q^{\star}$  defined by Ichimura and Newey [2022] in Equation (51) always exists without any extra condition, since  $\bar{\mathcal{R}}(P)$  is a closed subspace of  $\mathcal{L}_2(T)$ . In contrast, the existence of our nuisance in Assumption 1 needs to impose extra restrictions on the Riesz representer, as we discussed in Section 4. We note that when our Assumption 1 indeed holds, the influence function in Equation (50) with  $q^{\star} = P\xi_0$  is actually identical to the influence function of our proposed functional estimator (see Theorem 6).

Although Ichimura and Newey [2022] do not impose restrictions like our Assumption 1, their least squares nuisance  $q^*$  in Equation (51) is not amenable to direct estimation, as it involves another unknown function  $q_0$ . Moreover, Ichimura and Newey [2022] focus on deriving the candidate influence function  $\varphi(W; h^*, q^*)$  in Equation (50), but not on estimation and inference details. For example, they do not provide conditions for when their two-stage sieve estimator is indeed asymptotically linear with  $\varphi(W; h^*, q^*)$  as its actual influence function. Establishing these asymptotic guarantees will need extra conditions. In contrast, our paper aims to propose practical estimation and inference methods for the functionals of interest. In particular, the characterization of our nuisance in Assumption 1 Equation (3) does not involve any unknown function, so it is particularly convenient for estimation. This allows us to establish that our proposed estimator is asymptotically linear with the stated influence function, under generic high-level conditions that can accommodate flexible machine learning nuisance estimators. Importantly, our asymptotic guarantees are robust to the weak identification of the primary nuisance.

## A.2 Connection to Ai and Chen [2007]

Ai and Chen [2007] study the semiparametric estimation and inference of possibly misspecified but point identified conditional moment equations. In this subsection, we specialize their results to linear functionals and linear conditional moment restrictions. In this setting, the sieve minimum distance estimator proposed in Ai and Chen [2007] can be also applied to our problem, and the consistency and asymptotic distribution of this sieve estimator can be established following their theory.

In our notations, the asymptotic distribution analysis of the sieve estimator in Ai and Chen [2007] requires the existence of solution  $\nu^*(S) \in \mathcal{H}$  to the following minimization problem:

$$\nu^{\star} \in \underset{v \in \operatorname{cl}(\mathcal{H} - \{h^{\star}\})}{\operatorname{argmin}} \mathbb{E}\Big[ ([P\nu](T))^2 \Big] + (1 - \mathbb{E}[m(W; \nu)])^2.$$

Since in our setting  $\mathcal{H}$  is a closed linear space, we have  $cl(\mathcal{H} - \{h^*\}) = \mathcal{H}$ , so the problem above can be also written as

$$\nu^* \in \operatorname*{argmin}_{v \in \mathcal{H}} \mathbb{E}\Big[ ([P\nu](T))^2 \Big] + (1 - \mathbb{E}[m(W;\nu)])^2. \tag{53}$$

We denote the minimum objective value in Equation (53) as  $V^*$ , *i.e.*, the objective value attained by  $\nu^*$ .

Then we can follow the theory in Ai and Chen [2007] to show that under suitable technical conditions, the sieve estimator for  $\theta^*$  is asymptotically linear with influence function given below:

$$\varphi(W; h^{\star}, \nu^{\star}) = V^{\star - 1} (1 - \mathbb{E}[m(W; \nu^{\star})]) (m(W; h^{\star}) - \theta^{\star}) + V^{\star - 1} [P\nu^{\star}] (T) (g_2(W) - g_1(W)h^{\star}(S)).$$

In the following proposition, we show that the existence of an optimal solution to Equation (53) is actually a sufficient condition for our Assumption 1. This proposition provides a new perspective for a key assumption in Ai and Chen [2007]: their assumption implicitly restricts the functional of interest like our Assumption 1.

**Proposition 5.** If there exists a solution  $\nu^* \in \mathcal{H}$  to the minimization problem in Equation (53), then  $\alpha = P^*P\xi^* \in \mathcal{R}(P^*P)$  where  $\xi^* = \nu^*/V^*$ . Moreover,

$$\varphi(W; h^*, \nu^*) = (m(W; h^*) - \theta^*) + [P\xi^*](T)(g_2(W) - g_1(W)h^*(S)).$$

Although here  $\nu^*$  and  $V^*$  correspond to our debiasing nuisance function, Ai and Chen [2007] do not estimate them when constructing the estimator of  $\theta^*$  (although they propose to estimate  $\nu^*$  and  $V^*$  when estimating the asymptotic variance of their sieve estimator). In contrast, we propose to directly estimate the debiasing nuisance based on the formulation in Assumption 1 Equation (3), and use it in the estimation of  $\theta^*$ . This allows us to move beyond sieve estimation and leverage flexible machine learning nuisance estimators. Moreover, our paper does not require the nuisance functions to be uniquely idenfied by the conditional moment restrictions.

## B Extension to Convex Classes

In the main text, we focus on a closed linear function class. In this section, we extend the results to convex classes. In this section, we let  $\mathcal{H}$  be a closed convex function class.

**Assumption 18.** There exists  $\xi_0 \in \text{int}(\mathcal{H})$  such that

$$\xi_0 \in \underset{\xi \in \mathcal{H}}{\operatorname{argmin}} \, \mathbb{E}\Big[ ([P\xi](T))^2 \Big] - 2\mathbb{E}[m(W;\xi)] \,. \tag{54}$$

Here Assumption 18 is an analogue of Assumption 1. Indeed, when  $\mathcal{H}$  is a closed and linear space,  $\operatorname{int}(\mathcal{H}) = \mathcal{H}$  so the interior restriction in Assumption 1 is vacuous. Here for a closed and convex class, we additionally restrict  $\xi_0$  to the interior of  $\mathcal{H}$ .

In the following theorem, we show an analogue of Theorem 2 that characterizes interior solution to Equation (54) in trems of the Riesz representer. Note that the projection operator  $\Pi_{\mathcal{H}}$  is also well defined for a closed and convex class  $\mathcal{H}$ .

**Theorem 12.** If there exists  $\xi_0 \in \text{int}(\mathcal{H})$  that solves Equation (54) in Assumption 18, then

$$\Pi_{\mathcal{H}}\mathbb{E}[q_1(W)[P\xi_0](T) \mid S] = \alpha(S). \tag{55}$$

We again consider the doubly robust identification given by  $q^{\dagger} = P\xi_0$ :

$$\theta^{\star} = \mathbb{E}\Big[\psi(W; h_0, q^{\dagger})\Big],$$

where  $h_0$  is any function in  $\mathcal{H}_0$  and  $\xi_0$  is any interior solution to Equation (54). In the lemma below, we show that this doubly robust identification formula still has the bias-product property and Neyman orthogonality property. Therefore, our debiased inference theory in Section 6 still works through.

**Lemma 5.** Suppose Assumption 18 holds. Then for any  $h \in \mathcal{H}, q \in \mathcal{L}_2(T), h_0 \in \mathcal{H}_0$ , any interior solution  $\xi_0$  to Equation (54) and  $q^{\dagger} = P\xi_0$ , we have

$$\left| \mathbb{E}[\psi(W; h, q)] - \theta^{\star} \right| = \left| \langle P(h - h_0), q - q^{\dagger} \rangle \right| \le \|P(h - h_0)\|_2 \|q - q^{\dagger}\|_2. \tag{56}$$

Moreover, we have

$$\frac{\partial}{\partial t} \mathbb{E}\left[\psi(W; h_0 + t(h - h_0), q^{\dagger})\right]\big|_{t=0} = \frac{\partial}{\partial t} \mathbb{E}\left[\psi(W; h_0, q^{\dagger} + t(q - q_0))\right]\big|_{t=0} = 0.$$
 (57)

# C Supporting Lemmas

**Lemma 6.** The following three conditions are equivalent: (i) the function  $h^*$  is identifiable, (ii)  $\mathcal{N}(P) = \{0\}$ , (iii)  $\mathbb{E}[m(W; h^*)]$  is identifiable for every function m such that  $\mathbb{E}[m(W; \cdot)]$  is continuous linear.

**Lemma 7** (Theorem 14.1 in Wainwright [2019]). Given a star-shaped and b-uniformly bounded function class  $\mathcal{G}$ , let  $\eta_n$  be any positive solution of the inequality  $\mathcal{R}_n(\mathcal{G}^{|\eta}) \leq \eta^2/b$ . Then there exist universal positive constants  $c_1, c_2$ , such that for any  $t \geq \eta_n$ , we have

$$\left| \|g\|_n^2 - \|g\|_2^2 \right| \le \frac{1}{2} \|g\|_2^2 + \frac{1}{2} t^2, \quad \forall g \in \mathcal{G},$$

with probability at least  $1 - c_1 \exp\left(-c_2 \frac{nt^2}{b^2}\right)$ .

**Lemma 8** (Lemma 11 in Foster and Syrgkanis [2019]). Let  $\mathcal{F}: \mathcal{X} \to \mathbb{R}^d$  be a 1-uniformly bounded function class, whose t th coordinate projection is denoted as  $\mathcal{F}|_t$ . Let  $\ell: \mathbb{R}^d \times \mathcal{Z} \to \mathbb{R}$  be a loss function Lipschitz in its first argument with a Lipschitz constant L. We receive an i.i.d. sample set  $S = \{Z_1, \ldots, Z_n\}$ . Let  $\mathcal{L}_f$  denote the random variable  $\ell(f(X), Z)$  and let

$$\mathbb{P}\mathcal{L}_f = \mathbb{E}[\ell(f(X), Z)], \quad and \quad \mathbb{P}_n\mathcal{L}_f = \frac{1}{n} \sum_{i=1}^n \ell(f(X_i), Z_i).$$

There exists universal positive constants  $c_1, c_2, c_3$  such that for any  $\delta_n^2 \ge \frac{4d \log(41 \log(2c_1 n))}{c_1 n}$  that solves the inequalities  $\mathcal{R}\left(\operatorname{star}\left(\mathcal{F}|_t - f_t^{\star}\right), \delta\right) \le \delta^2$  for any  $t \in \{1, \ldots, d\}$ , we have

$$\left|\mathbb{P}_{n}\left(\mathcal{L}_{f}-\mathcal{L}_{f^{\star}}\right)-\mathbb{P}\left(\mathcal{L}_{f}-\mathcal{L}_{f^{\star}}\right)\right|\leq18Ld\delta_{n}\left\{\sum_{t=1}^{d}\left\|f_{t}-f_{t}^{\star}\right\|_{2}+\delta_{n}\right\},\quad\forall f\in\mathcal{F},$$

with probability at least  $1 - c_2 \exp(-c_3 n \delta_n^2)$ .

**Lemma 9.** Let some b, c > 0 be given, and suppose that

$$\frac{1}{2}x^2 \le bx + c\,,$$

for some x > 0. Then, we have

$$x \leq 2b + \sqrt{2c}$$

Proof of Lemma 9. Since b, and c are both positive, the quadratic  $\frac{1}{2}x^2 - bx - c$  must have a positive and a negative root. Therefore, this quadratic is negative if and only if x is less than the positive root; that is, we have

$$\frac{1}{2}x^2 - bx - c \le 0$$

$$\iff x \le b + \sqrt{b^2 + 2c}$$

$$\implies x \le 2b + \sqrt{2c},$$

as required.

# D Proofs of Results on Identification, Double Robustness, and Newyman Orthogonality

Here we present the proofs of our theorems relating to the general properties of our influence function  $\psi$ ; *i.e.* those relating to identification, double robustness, and Neyman orthogonality. We present both the results for our simplified setting from Section 4, as well as our generalized setting from Section 8.

#### D.1 Results from Section 4

Proofs for Theorem 1 and Lemma 1. Theorem 1 and Lemma 1 directly follow from Theorem 3 so we defer the details to the proof for Theorem 3.  $\Box$ 

Proof for Lemma 2. First consider  $\alpha \in \mathcal{N}(P)^{\perp}$ . Since any  $h \in \mathcal{H}_0$  can be written as  $h = h^* + h^{\perp}$  for some  $h^{\perp} \in \mathcal{N}(P)$ , we have

$$\mathbb{E}[m(W;h)] = \mathbb{E}[\alpha(S)h(S)] = \mathbb{E}[\alpha(S)h^{\star}(S)] = \mathbb{E}[m(W;h^{\star})], \quad \forall h \in \mathcal{H}_0.$$

This shows that  $\theta^*$  is identifiable when  $\alpha \in \mathcal{N}(P)^{\perp}$ .

On the other hand, when  $\theta^*$  is identifiable, we must have  $\alpha \in \mathcal{N}(P)^{\perp}$ . Suppose the latter is not true, then there exists  $h^{\perp} \in \mathcal{N}(P)$  such that  $\mathbb{E}\left[\alpha(S)h^{\perp}(S)\right] \neq 0$ . Then for  $h = h^* + h^{\perp} \in \mathcal{H}_0$ , we have

$$\mathbb{E}[m(W;h)] = \mathbb{E}[\alpha(S)h(S)] = \mathbb{E}[\alpha(S)h^{\star}(S)] + \mathbb{E}\left[\alpha(S)h^{\perp}(S)\right] \neq \mathbb{E}[\alpha(S)h^{\star}(S)] = \mathbb{E}[m(W;h^{\star})].$$

This contradicts the identifiability of  $\theta^*$ . Thus if  $\theta^*$  is identifiable, then  $\alpha \in \mathcal{N}(P)^{\perp}$ .

Proof for Theorem 2. According to the definition of  $\Xi_0$  in Assumption 1,  $\xi_0 \in \Xi_0$  if and only if it satisfies the first order condition of the optimization problem in Equation (3):

$$\mathbb{E}[[P\xi_0](T)[Ph](T)] - \mathbb{E}[\alpha(S)h(S)] = 0, \quad \forall h \in \mathcal{H},$$

This is equivalent to

$$\mathbb{E}[\alpha(S)h(S)] = \mathbb{E}[h(S)g_1(W)[P\xi_0](T)], \quad \forall h \in \mathcal{H}.$$

Therefore,

$$\Pi_{\mathcal{H}}[g_1(W)[P\xi_0](T) \mid S] = [P^*P\xi_0](S) = \alpha(S).$$

The steps above can be all reversed, which proves the asserted conclusion.

Proof for Lemma 3. According to the definition of  $\xi_0$  in Assumption 1, we immediately have  $P\xi_0 \in \mathcal{Q}_0$ . Moreover,  $P\xi_0 \in \mathcal{R}(P)$ . Note the function class  $\mathcal{Q}_0$  in Equation (20) can be written as  $q_0 + \mathcal{N}(P^*) = q_0 + \mathcal{R}(P)^{\perp}$  for any  $q_0 \in \mathcal{Q}_0$ . So  $P\xi_0$  is exactly the minimum-norm element in  $\mathcal{Q}_0$ .

Proof for Theorem 3. According to Lemma 2, we have  $\theta^* = \mathbb{E}[m(W; h_0)]$  for any  $h_0 \in \mathcal{H}$ . Moreover, any  $q_0 \in \mathcal{Q}_0$  satisfies that

$$\mathbb{E}[q_1(W)q_0(T)h(S)] = \mathbb{E}[\alpha(S)h(S)] = \mathbb{E}[m(W;h)], \text{ for any } h \in \mathcal{H}.$$

In particular, the above holds for  $h = h_0 \in \mathcal{H}$ , namely,

$$\mathbb{E}[m(W; h_0)] = \mathbb{E}[g_1(W)q_0(T)h_0(S)].$$

It follows that

$$\theta^* = \mathbb{E}[q_0(T)g_1(W)h_0(S)] = \mathbb{E}[q_0(T)\mathbb{E}[g_1(W)h_0(S) \mid T]] = \mathbb{E}[q_0(T)\mathbb{E}[g_2(W) \mid T]] = \mathbb{E}[q_0(T)g_2(W)].$$

Finally,

$$\mathbb{E}[m(W; h_0) + q_0(T)(g_2(W) - g_1(W)h_0(S))]$$

$$= \mathbb{E}[q_0(T)g_2(W)] + \mathbb{E}[m(W; h_0) - q_0(T)g_1(W)h_0(S)]$$

$$= \mathbb{E}[q_0(T)g_2(W)] = \theta^*.$$

The above also holds for  $q_0 = P\xi_0$  with  $\xi_0 \in \Xi_0$  since such  $q_0$  is also in  $Q_0$ . This recovers the conclusion in Theorem 1.

We next prove Equation (21). Note that for any  $h \in \mathcal{L}_2(S)$ ,  $q \in \mathcal{L}_2(T)$  and  $h_0 \in \mathcal{H}_0$ ,  $q_0 \in \mathcal{Q}_0$ ,

$$\mathbb{E}[\psi(W; h, q)] - \theta^* = \mathbb{E}[\psi(W; h, q)] - \mathbb{E}[\psi(W; h_0, q_0)]$$

$$= \mathbb{E}[m(W; h - h_0)] + \mathbb{E}[q(T)(g_2(W) - g_1(W)h(S))]$$

$$= \mathbb{E}[\alpha(S)(h(S) - h_0(S))] + \mathbb{E}[q(T)(\mathbb{E}[g_2(W) \mid T] - g_1(W)h(S))]$$

$$= \mathbb{E}[g_1(W)q_0(T)(h(S) - h_0(S))] + \mathbb{E}[g_1(W)q(T)(h_0(S) - h(S))]$$

$$= \mathbb{E}[q_1(W)(q(T) - q_0(T))(h(S) - h_0(S))].$$

This means that

$$\mathbb{E}[\psi(W; h, q)] - \theta^* = \mathbb{E}[\mathbb{E}[g_1(W)(h(S) - h_0(S)) \mid T](q(T) - q_0(T))]$$
  
=  $\mathbb{E}[(P[h(S) - h_0(S)])(q(T) - q_0(T))] = \langle P(h - h_0), q - q_0 \rangle.$ 

and

$$\mathbb{E}[\psi(W; h, q)] - \theta^* = \mathbb{E}[(h(S) - h_0(S))\mathbb{E}[g_1(W)(q(T) - q_0(T)) \mid S]]$$
  
=  $\mathbb{E}[(h(S) - h_0(S))(P^*[q(T) - q_0(T)])] = \langle h - h_0, P^*(q - q_0) \rangle.$ 

Then Equation (21) follows from Cauchy-Schwartz inequality. In particular, for  $q \in \{P\xi : \xi \in \mathcal{H}\}$  and  $q_0 = P\xi_0$  for  $\xi_0 \in \Xi_0$ , the above implies

$$\mathbb{E}[\psi(W; h, q)] - \theta^* = \langle P(h - h_0), P(\xi - \xi_0) \rangle.$$

This proves the conclusion in Lemma 1 Equation (16).

We finally prove Equation (22). Note that

$$\frac{\partial}{\partial t} \mathbb{E}[\psi(W; h_0 + th, q_0)]\big|_{t=0} = \mathbb{E}[\alpha(S)h(S)] - \mathbb{E}[g_1(W)q_0(T)h(S)].$$

It is equal to 0 for any  $h \in \mathcal{H}$  if and only  $\Pi_{\mathcal{H}}[g_1(W)q_0(T) \mid S] = \alpha(S)$ , namely,  $q_0 \in \mathcal{Q}_0$ . Moreover,

$$\frac{\partial}{\partial t} \mathbb{E}[\psi(W; h_0, q_0 + tq)]\big|_{t=0} = \mathbb{E}[q(T)(g_2(W) - g_1(S)h_0(S))].$$

It is equal to 0 for any  $q \in \mathcal{L}_2(T)$  if and only if  $\mathbb{E}[g_2(W) - g_1(S)h_0(S) \mid T] = 0$ , namely,  $h_0 \in \mathcal{H}_0$ . Restricting the above to  $q_0 = P\xi_0$  for  $\xi_0 \in \Xi_0$  and  $q \in \{P\xi : \xi \in \mathcal{H}\}$  proves the conclusion in Lemma 1 Equation (17).

## D.2 Results from Section 8

Proof of Lemma 4. First, we have

$$\begin{split} \mathbb{E}\Big[\psi(W;h,q)\Big] &= \mathbb{E}\Big[m(W;h) + r(W;q) - G(W;h,q)\Big] \\ &= \mathbb{E}[m(W;h_0)] + \mathbb{E}\Big[m(W;h-h_0) + r(W;q) - G(W;h,q)\Big] \\ &= \theta^{\star} + \mathbb{E}\Big[m(W;h-h_0) - G(W;h-h_0,q) + r(W;q) - G(W;h_0,q)\Big] \\ &= \theta^{\star} + \mathbb{E}\Big[m(W;h-h_0) - G(W;h-h_0,q)\Big] \\ &= \theta^{\star} + \mathbb{E}\Big[m(W;h-h_0) - G(W;h-h_0,q_0) - G(W;h-h_0,q-q_0)\Big] \\ &= \theta^{\star} - \mathbb{E}\Big[G(W;h-h_0,q-q_0)\Big] \,, \end{split}$$

where above we apply the fact that  $\theta^* = \mathbb{E}[m(W; h_0)]$ , as well as the definitions of  $\mathcal{Q}_0$  and  $\mathcal{H}_0$ . For the second part of the lemma, applying the previous equality gives us

$$\frac{d}{dt}\Big|_{t=0} \mathbb{E}\Big[\psi(W; h_0 + th, q_0 + tq)\Big] = -\frac{d}{dt}\Big|_{t=0} \mathbb{E}\Big[G(W; th, tq)\Big]$$

$$= -\mathbb{E}\Big[G(W; h, q)\Big] \frac{d}{dt}\Big|_{t=0} t^2$$

$$= 0$$

Finally, for the third part of the lemma, applying the previous equality again, along with our continuous bi-linear assumption on G, gives us

$$\left| \mathbb{E}[\psi(W; h, q)] - \theta^* \right| = \left| \mathbb{E}[G(W; h - h_0, q - q_0)] \right|$$
$$= \left| \mathbb{E}[(h - h_0)(S)k(S, T)(q - q_0)(T)] \right|.$$

Then, since  $q - q_0 \in \mathcal{Q}$ , and applying the definition of P, we can further simply the above by

$$\begin{split} \left| \mathbb{E} \Big[ (h - h_0)(S) k(S, T) (q - q_0)(T) \Big] \right| &= \left| \mathbb{E} \Big[ \Pi_{\mathcal{Q}} \Big[ k(S, T)^\top (h - h_0)(S) \mid T \Big]^\top (q - q_0)(T) \Big] \right| \\ &= \left| \mathbb{E} \Big[ (P(h - h_0))(T)^\top (q - q_0)(T) \Big] \right| \\ &\leq \| P(h - h_0) \|_{2,2} \| q - q_0 \|_{2,2} \,, \end{split}$$

where in the final step we apply Cauchy Schwartz. Alternatively, if we instead project on to  $\mathcal{H}$ , symmetrical reasoning gives us

$$\begin{split} \left| \mathbb{E} \Big[ (h - h_0)(S) k(S, T) (q - q_0)(T) \Big] \right| &= \left| \mathbb{E} \Big[ \Pi_{\mathcal{H}} \Big[ k(S, T) (q - q_0)(T) \mid S \Big]^{\top} (h - h_0)(S) \Big] \right| \\ &= \left| \mathbb{E} \Big[ (P^* (q - q_0))(S)^{\top} (h - h_0)(S) \Big] \right| \\ &\leq \| P^* (q - q_0) \|_{2,2} \| h - h_0 \|_{2,2} \,. \end{split}$$

Then, taking the minimum of these two bounds gives us our final required result.

# E Proofs for Minimax Estimation Theory

Here we consider the proof of our minimax estimation theory, specifically Theorems 4 and 5, and their generalizations Theorems 8 and 9. Since the former two theorems are just special cases of the latter, we will only present explicit proofs below for the latter, and then the former immediately follow.

#### E.1 Proof of Theorem 8

Let us define

$$\phi(h,q) = G(W; h,q) - r(W;q) - q(T)^{\top} q(T)$$
.

Then, the estimator we are studying is given by

$$\hat{h}_n = \underset{h \in \mathcal{H}_n}{\operatorname{argmin}} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\phi(h, q) - \mu_n h(S)^2],$$

First, note that the population version of the minimax objective trivially satisfies

$$\begin{split} \sup_{q \in \mathcal{Q}} \mathbb{E}[\phi(h,q)] &= \sup_{q \in \mathcal{Q}} \mathbb{E}\Big[\Big(k(S,T)^\top h(S) - \beta(T)\Big)^\top q(T) - \frac{1}{2}q(T)^\top q(T)\Big] \\ &= \frac{1}{2} \Big\| \Pi_{\mathcal{Q}}\Big[k(S,T)^\top h(S) - \beta(T) \mid T\Big] \Big\|_{2,2}^2 \,, \end{split}$$

for any  $h \in \mathcal{H}$ . Motivated by this, let us define the population projected loss objective

$$J(h) = \frac{1}{2} \left\| \Pi_{\mathcal{Q}} \left[ k(S, T)^{\top} h(S) - \beta(T) \mid T \right] \right\|_{2,2}^{2} = \sup_{q \in \mathcal{Q}} \mathbb{E}[\phi(h, q)].$$

In addition, we define the weak norm of interest

$$||h - h'||_{w} = ||\Pi_{\mathcal{Q}}[k(S, T)^{\top}(h - h')(S) | T]||_{2,2}$$
$$= ||P(h - h')||_{2,2},$$

for any  $h, h' \in \mathcal{H}$ . Note that according to these definitions we trivially have  $J(h_0) = 0$  for all  $h \in h_0$ , and  $||h - h_0||_w = ||h - h'_0||_w$  for any  $h \in \mathcal{H}$  and  $h_0, h'_0 \in \mathcal{H}_0$ . That is, without loss of generality we can prove the required bound for  $h_0 = h^{\dagger}$ .

Then our goal is to provide a high-probability bound on  $\|\hat{h}_n - h^{\dagger}\|_w$ . We will provide a high-level overview of the proof in terms of some intermediate lemmas below, and then relegate the proof of these intermediate lemmas to the end of the subsection.

### Bounding Weak Norm by Population Objective Sub-optimality

First, we can provide the following lemma which follows by strong convexity.

**Lemma 10.** For any  $h \in \mathcal{H}$  we have

$$\frac{1}{2} \|h - h^{\dagger}\|_{w}^{2} \le J(h) - J(h^{\dagger})$$

This lemma is the first step for proving fast rates, since it allows us to bound

$$\frac{1}{2}\|\hat{h}_n - h^{\dagger}\|_w^2 \le \sup_{q \in \mathcal{Q}} \mathbb{E}[\phi(\hat{h}_n, q)] - \sup_{q \in \mathcal{Q}} \mathbb{E}[\phi(h^{\dagger}, q)].$$

This is powerful, since  $\hat{h}_n$  minimizes the empirical version of the RHS, which allows us to apply a empirical risk minimization analysis to this minimax loss.

### **High-Probability Bound**

Next, we establish an important high-probability event, which will be applied in various lemmas in the rest of the proof sketch. Specifically, we ensure the following.

**Lemma 11.** Let  $\epsilon_n = r_n + c_2 \sqrt{\log(c_1/\zeta)}$ , where the constants  $c_1$  and  $c_2$  are defined analogously as in Foster and Syrgkanis [2019, Lemma 11], and let

$$\Phi_n(q) = G(W; h^{\dagger}, q) - r(W; q) - \frac{1}{2}q(T)^{\top}q(T),$$

for any  $q \in \mathcal{Q}_n$ . Then, with probability at least  $1 - 2\zeta$ , we have

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ \Phi_n(q) \right] \right| \le 54\epsilon_n \|q\|_{2,2} + 54\epsilon_n^2,$$

for every  $q \in \mathcal{Q}_n$ , as well as

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ G(W; h - h^{\dagger}, q) \right] \right| \le 18\epsilon_n \|h - h^{\dagger}\|_{2,2} \|q\|_{2,2} + 36\epsilon_n^2,$$

for every  $h \in \mathcal{H}_n$  and  $q \in \mathcal{Q}_n$ .

#### Reduction to Stochastic Equicontinuity Problem

Now, let us define

$$q_n(h) = \operatorname*{argmax}_{q \in \mathcal{Q}_n} \mathbb{E}_n[\phi(h, q)]$$
$$q_0(h) = \operatorname*{argmax}_{q \in \mathcal{Q}} \mathbb{E}[\phi(h, q)],$$

for any  $h \in \mathcal{H}$ , with tie-breaking performed arbitrarily. Note that it is trivial to verify that  $q_0(h)(T) = \Pi_{\mathcal{Q}}[k(S,T)^{\top}h(S) - \beta(T) \mid T]$ . Given these notations, and applying Lemma 11, we can establish the following lemma.

**Lemma 12.** Under the high-probability event of Lemma 11, we have

$$J(\hat{h}_n) - J(h^{\dagger}) \leq (\mathbb{E} - \mathbb{E}_n) \Big[ \phi(\hat{h}_n, \Pi_n q_0(\hat{h}_n)) - \phi(h^{\dagger}, q_n(h^{\dagger})) \Big]$$

$$+ 2\delta_n \|\hat{h}_n - h^{\dagger}\|_w + \frac{1}{2}\delta_n^2 + (1 + 18\epsilon_n)\delta_n \|q_n(\Pi_n h^{\dagger})\|_{2,2} + 36\epsilon_n^2$$

$$+ \mu_n \mathbb{E}_n [(\Pi_n h^{\dagger})(S)^2 - \hat{h}_n(S)^2].$$

### Bounding the Stochastic Equicontinuity Term using Localization

Next, we focus on the "stochastic equicontinuity"-style term in bound from the previous lemma. By some simple algebra, we can see that

$$\begin{split} &\phi(\hat{h}_{n},\Pi_{n}q_{0}(\hat{h}_{n})) - \phi(h^{\dagger},q_{n}(h^{\dagger})) \\ &= G(W;\hat{h}_{n} - h^{\dagger},q_{0}(h^{\dagger})) + G(W;\hat{h}_{n} - h^{\dagger},\Pi_{n}q_{0}(\hat{h}_{n}) - q_{0}(h^{\dagger})) \\ &+ G(W;h^{\dagger},\Pi_{n}q_{0}(\hat{h}_{n}) - q_{0}(h^{\dagger})) - G(W;h^{\dagger},q_{n}(h^{\dagger}) - q_{0}(h^{\dagger})) \\ &- r(W;\Pi_{n}q_{0}(\hat{h}_{n}) - q_{0}(h^{\dagger})) + r(W;q_{n}(h^{\dagger}) - q_{0}(h^{\dagger})) \\ &- \frac{1}{2} \Big(\Pi_{n}q_{0}(\hat{h}_{n}) - q_{0}(h^{\dagger})\Big)(T)^{\top} \Big(\Pi_{n}q_{0}(\hat{h}_{n}) - q_{0}(h^{\dagger})\Big)(T) \\ &+ \frac{1}{2} \Big(q_{n}(h^{\dagger}) - q_{0}(h^{\dagger})\Big)(T)^{\top} \Big(q_{n}(h^{\dagger}) - q_{0}(h^{\dagger})\Big)(T) \\ &- q_{0}(h^{\dagger})(T)^{\top} \Big(\Pi_{n}q_{0}(\hat{h}_{n}) - q_{0}(h^{\dagger})\Big)(T) + q_{0}(h^{\dagger})(T)^{\top} \Big(q_{n}(h^{\dagger}) - q_{0}(h^{\dagger})\Big)(T) \,. \end{split}$$

Furthermore, since  $q_0(h^{\dagger}) = 0$  by construction, the first and last two terms vanish. Instantiating this reasoning, and applying Lemma 11, we can easily derive the following lemma.

Lemma 13. Under the high-probability event of Lemma 11, we have

$$\begin{split} & \left| (\mathbb{E}_n - \mathbb{E}) \left[ \phi(\hat{h}_n, \Pi_n q_0(\hat{h}_n)) - \phi(h^{\dagger}, q_n(h^{\dagger})) \right] \right| \\ & \leq 90\epsilon_n \|\hat{h}_n - h_0\|_w + 54\epsilon_n \|q_n(h^{\dagger})\|_{2,2} + 144\epsilon_n^2 + 90\delta_n \epsilon_n \,. \end{split}$$

#### Bounding the Saddle-Point Estimate

Given the results so far, it remains to bound  $||q_n(\Pi_n h^{\dagger})||_{2,2}$  and  $||q_n(h^{\dagger})||_{2,2}$ . Now, these are empirical saddle-point solution, whose (approximate) population analogues satisfy  $||q_0(h)||_{2,2} = ||h - h^{\dagger}||_w$ . This suggests that we can bound these terms by applying a localization analysis to the interior optimization problem. Following reasoning along those lines gives the following lemma.

**Lemma 14.** Under the same high-probability event of Lemma 11, we have

$$||q_n(h)||_2 \le 246\epsilon_n + 9\delta_n + 9||h - h^{\dagger}||_w$$

for every  $h \in \mathcal{H}$ .

#### Final Projected Norm Bound

Putting together the results of the above intermediate lemmas, we get

$$\frac{1}{2} \|\hat{h}_n - h_0\|_w^2 \le (90\epsilon_n + 2\delta_n) \|\hat{h}_n - h_0\|_w + \left(36 + 144 + 54 \times 246\right) \epsilon_n^2 
+ \left(246(1 + 18\epsilon_n) + 90 + 54 \times 9\right) \delta_n \epsilon_n + \left(9(1 + 18\epsilon_n) + \frac{1}{2}\right) \delta_n^2 
+ 9(1 + 18\epsilon_n) \|\Pi_n h^{\dagger} - h^{\dagger}\|_w \delta_n + \mu_n \mathbb{E}_n [(\Pi_n h^{\dagger})(S)^2 - \hat{h}_n(S)^2],$$

with probability at least  $1-2\zeta$ .

Then, applying Lemma 9 to the above inequality, along with Assumption 13, that  $\delta_n \leq 2$  without loss of generality, and that  $\|\Pi_n h^{\dagger} - h^{\dagger}\|_w \leq \delta_n$  by Assumption 11, we get

$$\|\hat{h}_n - h_0\|_w \le 180\epsilon_n + 4\delta_n + \sqrt{44640\epsilon_n^2 + 2940\delta_n\epsilon_n + 37\delta_n^2 + 4\mu_n}$$

$$\le 180\epsilon_n + 4\delta_n + \sqrt{46110\epsilon_n^2 + 1507\delta_n^2 + 4\mu_n}$$

$$\le 395\epsilon_n + 43\delta_n + 2\mu_n^{1/2},$$

where in the second inequality we apply AM-GM, and in the third we apply the fact that  $\sqrt{x+y} \le \sqrt{x} + \sqrt{y}$  for non-negative x and y. Then, the bound in the statement of Theorem 8 trivially follows by plugging in the definition of  $\epsilon_n$  from Lemma 11.

#### Strong Norm Consistency

Finally, we will argue that  $\hat{h}_n$  not only converges to  $h_0$  under weak norm (for any  $h_0 \in \mathcal{H}_0$ ), but converges to  $h^{\dagger}$  in strong norm.

Let  $\zeta_n$  be any arbitrary sequence such that  $\zeta_n = o(1)$  and  $\sqrt{\log(c_1/\zeta_n)/n} = o(\mu_n)$ , and define  $\tilde{\epsilon}_n = r_n + c_2 \sqrt{\log(c_1/\zeta_n)/n}$ . Now, from the above bounds, we have

$$\mu_n \mathbb{E}_n[(\Pi_n h^{\dagger})(S)^2 - \hat{h}_n(S)^2] \leq (\tilde{\epsilon}_n + \delta_n) ||\hat{h}_n - h^{\dagger}||_w + \tilde{\epsilon}_n^2 + \delta_n \tilde{\epsilon}_n + \delta_n^2$$
  
$$\leq \tilde{\epsilon}_n + \delta_n,$$

with probability at least  $1-\zeta_n$ . Now, since by assumption we have that  $r_n=o(\mu_n)$  and  $\delta_n=o(\mu_n)$ , the above gives us

$$\mathbb{E}_n[\hat{h}_n(S)^2] \leq \mathbb{E}_n[(\Pi_n h^{\dagger})(S)^2] + o(1),$$

with probability at least  $1 - \zeta_n$ . Therefore, since the left hand side of the above inequality is uniformly bounded, this implies that

$$\mathbb{E}_n[\hat{h}_n(S)^2] \leq \mathbb{E}_n[(\Pi_n h^{\dagger})(S)^2] + o_p(1).$$

That is, intuitively,  $\hat{h}_n$  cannot converge to any element in  $\mathcal{H}_0$  other than the minimum  $L_2$ -norm solution. Concretely, we can instantiate the above intuition to derive the following.

**Lemma 15.** Suppose  $r_n = o(\mu_n)$  and  $\delta_n = o(\mu_n)$ . Then, we have

$$\|\hat{h}_n - h^{\dagger}\|_2 \to 0,$$

in probability.

#### **Proofs of Intermediate Lemmas**

Finally, we list the proofs of the above intermediate lemmas

Proof of Lemma 10. Consider some arbitrary  $h \in \mathcal{H}$ , and define

$$L(t) = J(h^{\dagger} + t(h - h^{\dagger})).$$

Then, the first two derivatives of L are given by

$$L'(t) = \mathbb{E}\left[\Pi_{\mathcal{Q}}\left[k(S,T)^{\top}(h-h^{\dagger})(S) \mid T\right]^{\top}\Pi_{\mathcal{Q}}\left[k(S,T)^{\top}\left(h^{\dagger}+t(h-h^{\dagger})\right)(S)-\beta(T) \mid T\right]\right]$$

and

$$L''(t) = \left\| \Pi_{\mathcal{Q}} \left[ k(S, T)(h - h^{\dagger})(S) \mid T \right] \right\|_{2,2}^{2} = \|h - h^{\dagger}\|_{w}^{2}.$$

Note that the first derivative follows since projections onto Hilbert spaces are linear. Furthermore, we have  $L(0) = J(h^{\dagger})$ , and L(1) = J(h). Also, since  $h^{\dagger} \in \mathcal{H}_0$ , we have

$$L'(0) = \mathbb{E}\Big[\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}(h-h^{\dagger})(S) \mid T\Big]\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}h^{\dagger}(S) - \beta(T) \mid T\Big]\Big]$$

$$= \mathbb{E}\Big[\Big(k(S,T)^{\top}h^{\dagger}(S) - \beta(T)\Big)\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}(h-h^{\dagger})(S) \mid T\Big]\Big]$$

$$= \mathbb{E}[G(W;h^{\dagger},q') - r(W;q')]$$

$$= 0.$$

where  $q' = \Pi_{\mathcal{Q}}[k(S,T)^{\top}(h-h^{\dagger})(S) \mid T]$ , and the final two equalities follow since  $q' \in \mathcal{Q}$  by construction. Therefore, noting that L''(t) does not depend on t, strong convexity gives us

$$L(1) \ge L(0) + L'(0) + \frac{1}{2} \inf_{t \in [0,1]} L''(t)$$

$$\iff \frac{1}{2} ||h - h^{\dagger}||_{w}^{2} \le J(h) - J(h^{\dagger}),$$

as required.

Proof of Lemma 11. First, note that by Assumption 13 we have that  $\Phi_n(q)$  is 3-Lipschitz in q under  $L_2$  norm. Therefore, given Assumption 12 and applying Foster and Syrgkanis [2019, Lemma 11], we have

 $\left| (\mathbb{E}_n - \mathbb{E}) \left[ \Phi_n(q) \right] \right| \le 54\epsilon_n \|q\|_{2,2} + 54\epsilon_n^2,$ 

for all  $q \in \mathcal{Q}_n$ , which holds with probability at least  $1 - \zeta$ .

Second, applying Assumption 12 and Foster and Syrgkanis [2019, Lemma 11] again, and noting that by Assumption 13 we have  $||G(W; h - h^{\dagger}, q)||_{\infty} \leq 2$ , we have

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ \frac{1}{2} G(W; h - h^{\dagger}, q) \right] \right| \le 18\epsilon_n \left\| \frac{1}{2} G(W; h - h^{\dagger}, q) \right\|_{2,2} + 18\epsilon_n^2,$$

for all  $h \in \mathcal{H}_n$  and  $q \in \mathcal{Q}_n$ , which also holds with probability at least  $1 - \zeta$ . Then, applying the Lipschitz assumption from Assumption 13 and re-arranging, we get

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ G(W; h - h^{\dagger}, q) \right] \right| \le 18\epsilon_n \|h - h^{\dagger}\|_{2,2} \|q\|_{2,2} + 36\epsilon_n^2,$$

for all  $h \in \mathcal{H}_n$  and  $q \in \mathcal{Q}_n$  under the same high probability event.

Finally, taking a union bound over the above two high-probability events gives us our required result.

Proof of Lemma 12. First, note that by Assumption 10 we know that  $q_0(h) \in \bar{\mathcal{Q}}$  for every  $h \in \bar{\mathcal{H}}$ ,

and also that  $\hat{h}_n, h^{\dagger} \in \bar{\mathcal{H}}$ . Therefore, we have

$$\begin{split} J(\hat{h}_n) - J(h^\dagger) &= \sup_{q \in \mathcal{Q}} \mathbb{E}[\phi(\hat{h}_n, q)] - \sup_{q \in \mathcal{Q}} \mathbb{E}[\phi(h^\dagger, q)] \\ &= \sup_{q \in \bar{\mathcal{Q}}} \mathbb{E}[\phi(\hat{h}_n, q)] - \sup_{q \in \bar{\mathcal{Q}}} \mathbb{E}[\phi(h^\dagger, q)] \\ &\leq \mathbb{E}[\phi(\hat{h}_n, q_0(\hat{h}_n))] - \mathbb{E}[\phi(h^\dagger, q_n(h^\dagger))] \\ &\leq \mathbb{E}[\phi(\hat{h}_n, q_0(\hat{h}_n))] - \mathbb{E}[\phi(h^\dagger, q_n(h^\dagger))] - \sup_{q \in \mathcal{Q}_n} \left( \mathbb{E}_n[\phi(\hat{h}_n, q)] + \mu_n \mathbb{E}_n[\hat{h}_n(S)^2] \right) \\ &+ \sup_{q \in \mathcal{Q}_n} \left( \mathbb{E}_n[\phi(\Pi_n h^\dagger, q)] + \mu_n \mathbb{E}_n[(\Pi_n h^\dagger)(S)^2] \right) \\ &= \mathbb{E}[\phi(\hat{h}_n, \Pi_n q_0(\hat{h}_n))] - \mathbb{E}[\phi(h^\dagger, q_n(h^\dagger))] - \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\phi(\hat{h}_n, q)] + \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\phi(h^\dagger, q)] \\ &+ \mu_n \mathbb{E}_n[(\Pi_n h^\dagger)(S)^2 - \hat{h}(S)^2] + \mathcal{E}_1 + \mathcal{E}_2 \\ &\leq (\mathbb{E} - \mathbb{E}_n) \left[ \phi(\hat{h}_n, \Pi_n q_0(\hat{h}_n)) - \phi(h^\dagger, q_n(h^\dagger)) \right] + \mu_n \mathbb{E}_n[(\Pi_n h^\dagger)(S)^2 - \hat{h}(S)^2] + \mathcal{E}_1 + \mathcal{E}_2 \right. \end{split}$$

where the first and third inequalities follow by relaxing the supremum in the negative terms, and the second inequality follows by the optimality of  $\hat{h}_n$  for the empirical minimax objective, and where

$$\mathcal{E}_{1} = \mathbb{E}\Big[\phi(\hat{h}_{n}, q_{0}(\hat{h}_{n})) - \phi(\hat{h}_{n}, \Pi_{n}q_{0}(\hat{h}_{n}))\Big]$$
  
$$\mathcal{E}_{2} = \sup_{q \in \mathcal{Q}_{n}} \mathbb{E}_{n}[\phi(\Pi_{n}h^{\dagger}, q)] - \sup_{q \in \mathcal{Q}_{n}} \mathbb{E}_{n}[\phi(h^{\dagger}, q)].$$

Now, let us bound the error terms  $\mathcal{E}_1$  and  $\mathcal{E}_2$ . For the first, using the shorthand  $\Delta = q_0(\hat{h}_n) - \Pi_n q_0(\hat{h}_n)$ , we have

$$\mathcal{E}_{1} = \mathbb{E}\Big[G(W; \hat{h}_{n}, \Delta) - r(W; \Delta) - \frac{1}{2}q_{0}(\hat{h}_{n})(T)^{\top}q_{0}(\hat{h}_{n})(T) + \frac{1}{2}\Pi_{n}q_{0}(\hat{h}_{n})(T)^{\top}\Pi_{n}q_{0}(\hat{h}_{n})(T)\Big]$$

$$= \mathbb{E}\Big[G(W; \hat{h}_{n} - h^{\dagger}, \Delta) - \frac{1}{2}q_{0}(\hat{h}_{n})(T)^{\top}q_{0}(\hat{h}_{n})(T) + \frac{1}{2}\Pi_{n}q_{0}(\hat{h}_{n})(T)^{\top}\Pi_{n}q_{0}(\hat{h}_{n})(T)\Big]$$

$$= \mathbb{E}\Big[(\hat{h}_{n} - h^{\dagger})(S)^{\top}k(S, T)\Delta(T) + \frac{1}{2}\Delta(T)^{\top}\Delta(T) - q_{0}(\hat{h}_{n})^{\top}\Delta(T)\Big]$$

$$\leq 2\|\hat{h}_{n} - h^{\dagger}\|_{w}\delta_{n} + \frac{1}{2}\delta_{n}^{2},$$

where above we apply the fact that  $||q_0(\hat{h}_n)||_2 = ||\Pi_{\mathcal{Q}}(\hat{h}_n - h^{\dagger})(S)^{\top}k(S,T)||_2 = ||\hat{h}_n - h^{\dagger}||_w$ , and the fact that  $||\Delta||_2 \leq \delta_n$  by Assumption 11, along with Cauchy Schwartz.

Next, for the second term above, we can bound

$$\mathcal{E}_{2} \leq \mathbb{E}_{n} \Big[ \phi(\Pi_{n} h^{\dagger}, q_{n}(\Pi_{n} h^{\dagger}) - \phi(h^{\dagger}, q_{n}(\Pi_{n} h^{\dagger})) \Big]$$

$$= \mathbb{E}_{n} \Big[ G(W; \Pi_{n} h^{\dagger} - h^{\dagger}, q_{n}(\Pi_{n} h^{\dagger})) \Big]$$

$$= (\mathbb{E}_{n} - \mathbb{E}) \Big[ G(W; \Pi_{n} h^{\dagger} - h^{\dagger}, q_{n}(\Pi_{n} h^{\dagger})) \Big] + \mathbb{E} \Big[ G(W; \Pi_{n} h^{\dagger} - h^{\dagger}, q_{n}(\Pi_{n} h^{\dagger})) \Big]$$

$$\leq 18\epsilon_{n} \|\Pi_{n} h^{\dagger} - h^{\dagger}\|_{2,2} \|q_{n}(\Pi_{n} h^{\dagger})\|_{2,2} + 36\epsilon_{n}^{2} + \mathbb{E} \Big[ G(W; \Pi_{n} h^{\dagger} - h^{\dagger}, q_{n}(\Pi_{n} h^{\dagger})) \Big]$$

$$\leq (1 + 18\epsilon_{n}) \delta_{n} \|q_{n}(\Pi_{n} h^{\dagger})\|_{2,2} + 36\epsilon_{n}^{2} ,$$

where the first inequality follows by relaxing the sup in the negative term, the second inequality follows from the assumed high-probability event of Lemma 11, and the final inequality follows from our Lipschitz assumptions on G along with our universal approximation assumption.

Finally, putting all of the above together, we get our final required result of

$$J(\hat{h}_n) - J(h^{\dagger}) \leq (\mathbb{E} - \mathbb{E}_n) \Big[ \phi(\hat{h}_n, \Pi_n q_0(\hat{h}_n)) - \phi(h^{\dagger}, q_n(h^{\dagger})) \Big]$$

$$+ 2\delta_n \|\hat{h}_n - h^{\dagger}\|_w + \frac{1}{2}\delta_n^2 + (1 + 18\epsilon_n)\delta_n \|q_n(\Pi_n h^{\dagger})\|_{2,2} + 36\epsilon_n^2$$

$$+ \mu_n \mathbb{E}_n [(\Pi_n h^{\dagger})(S)^2 - \hat{h}(S)^2].$$

Proof of Lemma 13. First, as argued in the proof overview, and plugging in  $q_0(h^{\dagger}) = 0$ , we have

$$\phi(\hat{h}_n,\Pi_nq_0(\hat{h}_n)) - \phi(h^\dagger,q_n(h^\dagger) = \Phi_n\Big(\Pi_nq_0(\hat{h}_n)\Big) - \Phi_n\Big(q_n(h^\dagger)\Big) + G\Big(W;\hat{h}_n - h^\dagger,\Pi_nq_0(\hat{h}_n)\Big),$$

where  $\Phi_n$  is defined as in the statement of Lemma 11. Then, applying Lemma 11, under its high probability event we have

$$\begin{split} & \left| (\mathbb{E}_{n} - \mathbb{E}) \left[ \phi(\hat{h}_{n}, \Pi_{n} q_{0}(\hat{h}_{n})) - \phi(h^{\dagger}, q_{n}(h^{\dagger}) \right] \right| \\ & \leq 54 \epsilon_{n} \left( \|\Pi_{n} q_{0}(\hat{h}_{n})\|_{2,2} + \|q_{n}(h^{\dagger})\|_{2,2} \right) + 18 \epsilon_{n} \|\hat{h}_{n} - h^{\dagger}\|_{2,2} \|\Pi_{n} q_{0}(\hat{h}_{n})\|_{2,2} + 144 \epsilon_{n}^{2} \\ & \leq 90 \epsilon_{n} \|\Pi_{n} q_{0}(\hat{h}_{n})\|_{2,2} + 54 \epsilon_{n} \|q_{n}(h^{\dagger})\|_{2,2} + 144 \epsilon_{n}^{2} \end{split}$$

Next, by Assumption 11, we have

$$\left\| \Pi_n q_0(\hat{h}_n) \right\|_{2,2} \le \|q_0(\hat{h}_n)\|_{2,2} + \left\| \Pi_n q_0(\hat{h}_n) - q_0(\hat{h}_n) \right\|_{2,2}$$

$$\le \|q_0(\hat{h}_n)\|_{2,2} + \delta_n.$$

Furthermore, we have

$$||q_0(\hat{h}_n)||_{2,2} = ||q_0(\hat{h}_n) - q_0(h^{\dagger})||_{2,2} = ||\hat{h}_n - h^{\dagger}||_w$$

Therefore, plugging these into the above bound, under the above high probability event, which occurs with probability at least  $1-2\zeta$ , we have

$$\begin{split} \left| (\mathbb{E}_n - \mathbb{E}) \left[ \phi(\hat{h}_n, \Pi_n q_0(\hat{h}_n)) - \phi(h^{\dagger}, q_n(h^{\dagger})) \right] \right| \\ &\leq 90\epsilon_n \|\hat{h}_n - h^{\dagger}\|_w + 54\epsilon_n \|q_n(h^{\dagger})\|_{2,2} + 144\epsilon_n^2 + 90\delta_n \epsilon_n \,, \end{split}$$

which is our promised bound.

Proof of Lemma 14. First, we can bound

$$\frac{1}{2} \|q_n(h) - q_0(h)\|_{2,2}^2 - \frac{1}{2} \|\Pi_n q_0(h) - q_0(h)\|_{2,2}^2 
= \mathbb{E} \left[ \left( q_0(h)(T)^\top \Pi_n q_0(h)(T) - \frac{1}{2} \Pi_n q_0(h)(T)^\top \Pi_n q_0(h)(T) \right) - \left( q_0(h)(T)^\top q_n(h)(T) - \frac{1}{2} q_n(h)(T)^\top q_n(h)(T) \right) \right] 
= \mathbb{E} \left[ \phi(h, \Pi_n q_0(h)) - \phi(h, q_n(h)) \right],$$

where in the above we apply the fact that for any  $q \in \mathcal{Q}$  and  $h \in \mathcal{H}$  we have

$$\mathbb{E}\left[q(T)^{\top}q_{0}(h)(T) - \frac{1}{2}q(T)^{\top}q(T)\right] = \mathbb{E}\left[q(T)^{\top}\Pi_{\mathcal{Q}}[k(S,T)^{\top}h(S) - \beta(T) \mid T] - \frac{1}{2}q(T)^{\top}q(T)\right]$$

$$= \mathbb{E}\left[[h(S)^{\top}k(S,T)q(T) - \beta(T)^{\top}q(T) - \frac{1}{2}q(T)^{\top}q(T)\right]$$

$$= \mathbb{E}\left[G(W;h,q) - r(W;q) - \frac{1}{2}q(T)^{\top}q(T)\right]$$

$$= \mathbb{E}\left[\phi(h,q)\right].$$

Furthermore, by the optimality of  $q_n(h)$  for the empirical interior supremum problem at h = h, we can further bound the above by

$$\frac{1}{2} \|q_n(h) - q_0(h)\|_{2,2}^2 - \frac{1}{2} \|\Pi_n q_0(h) - q_0(h)\|_{2,2}^2 \\
\leq (\mathbb{E}_n - \mathbb{E}) \Big[ \phi(h, q_n(h)) - \phi(h, \Pi_n q_0(h)) \Big] \\
\leq (\mathbb{E}_n - \mathbb{E}) \Big[ \Phi_n(q_n(h)) - \Phi_n(\Pi_n q_0(h)) \Big] \\
\leq 54\epsilon_n \|q_n(h)\|_{2,2} + 54\epsilon_n \|\Pi_n q_0(h)\|_{2,2} + 108\epsilon_n^2,$$

where  $\Phi_n$  is defined as in the statement of Lemma 11, and the above holds under that lemma's high probability event.

Next, applying the triangle inequality and the fact that  $(a+b)^2 \le 2a^2 + 2b^2$  for  $a, b \ge 0$ , under the above high-probability event we have

$$\frac{1}{2} \|q_n(h)\|_{2,2}^2 \le \|q_n(h) - q_0(\Pi_n(h_0)\|_{2,2}^2 + \|q_0(\Pi_n(h_0)) - q_0(h_0)\|_{2,2}^2 
\le 2 \left(\frac{1}{2} \|q_n(h) - q_0(\Pi_n(h_0)\|_{2,2}^2 - \frac{1}{2} \|\Pi_n q_0(h) - q_0(h)\|_{2,2}^2\right) 
+ \|\Pi_n q_0(h) - q_0(h)\|_{2,2}^2 + \|q_0(h) - q_0(h_0)\|_{2,2}^2 
\le 108\epsilon_n \|q_n(h)\|_{2,2} + 108\epsilon_n \|\Pi_n q_0(h)\|_{2,2} + 216\epsilon_n^2 
+ \|\Pi_n q_0(h) - q_0(h)\|_{2,2}^2 + \|q_0(h) - q_0(h_0)\|_{2,2}^2.$$

Furthermore, applying Assumptions 11 and 13 gives

$$\|\Pi_n q_0(h) - q_0(h)\|_{2,2}^2 \le \delta_n^2$$

$$\|q_0(h) - q_0(h_0)\|_{2,2}^2 = \|h - h^{\dagger}\|_w^2$$

$$\|\Pi_n q_0(h)\|_{2,2} \le \delta_n + \|q_0(h)\|_{2,2}$$

$$= \delta_n + \|q_0(h) - q_0(h_0)\|_{2,2}$$

$$= \delta_n + \|h - h^{\dagger}\|_w.$$

Therefore, plugging these bounds into the above, and applying Lemma 9, we get

$$||q_n(h)||_{2,2} \le 216\epsilon_n + \sqrt{216\epsilon_n(\delta_n + ||h - h^{\dagger}||_w) + 216\epsilon_n^2 + 2\delta_n^2 + 2||h - h^{\dagger}||_w^2}$$

$$\le 231\epsilon_n + \sqrt{2}(\delta_n + ||h - h^{\dagger}||_w) + 15\sqrt{\epsilon_n\delta_n} + 15\sqrt{\epsilon_n||h - h^{\dagger}||_w}$$

$$\le 246\epsilon_n + 9\delta_n + 9||h - h^{\dagger}||_w,$$

where we apply the fact that  $\sqrt{x+y} \le \sqrt{x} + \sqrt{y}$  for positive x, y, as well as the AM-GM inequality. This is our final required bound, so we conclude.

*Proof of Lemma 15.* First, as argued in the proof overview, under our assumptions on  $r_n$  and  $\delta_n$  we have

$$\mathbb{E}_n[\hat{h}_n(S)^2] \le \mathbb{E}_n[(\Pi_n h^{\dagger})(S)^2] + o_p(1).$$

Then, given Assumptions 11 and 12, this implies that

$$\|\hat{h}_n\|_2^2 \le \|h^{\dagger}\|_2^2 + o_p(1)$$
.

Next, let

$$D(h) = \inf_{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}} \|h - h_0\|_2.$$

Then, for any given  $\eta > 0$ , we have

$$\mathbb{P}\Big(D(\hat{h}_n) \ge \eta\Big) \le \mathbb{P}\Big(\|\hat{h}_n - h_0\|_w \ge M(\eta)\Big),\,$$

where

$$M(\eta) = \inf_{h \in \bar{\mathcal{H}}: D(h) > \eta} \|h - h_0\|_w.$$

Now, clearly  $\{h \in \bar{\mathcal{H}} : D(h) \ge \eta\}$  is closed under  $\|\cdot\|_2$ . To see this, suppose  $h'_n$  is a convergent sequence in this set, with limit h'. Then, we have

$$\inf_{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}} \|h' - h_0\|_2 \ge \inf_{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}} \|h_0 - h_n\|_2 - \|h' - h_n\|_2$$

$$= \inf_{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}} \|h_0 - h_n\|_2 - o(1)$$

$$\ge \eta - o(1).$$

But the left hand side does not depend on n, so therefore  $D(h') \geq \eta$ . Furthermore, by assumption the  $\|\cdot\|_2$  norm dominates the  $\|\cdot\|_w$  norm, so therefore  $\|h-h_0\|_w$  is continuous with respect to  $\|\cdot\|_2$ . Also, by assumption  $\bar{\mathcal{H}}$  is compact under  $\|\cdot\|_2$ , and therefore  $\{h \in \bar{\mathcal{H}} : D(h) \geq \eta\}$  is totally bounded. Thus, by the extreme value theorem, for every  $\eta > 0$ , there exists some  $h_{\eta} \in \{h \in \bar{\mathcal{H}} : D(h) \geq \eta\}$  such that  $M(\eta) = \|h_{\eta} - h_0\|_w$ . However, by definition  $h_{\eta} \notin \mathcal{H}_0 \cap \bar{\mathcal{H}}$ , so therefore  $M(\eta) > 0$  for every  $\eta > 0$ . Therefore, since under our assumptions  $\|\hat{h}_n - h_0\|_w \to 0$  in probability, it must be the case that

$$\mathbb{P}\Big(D(\hat{h}_n) \ge \eta\Big) \to 0$$

for every  $\eta > 0$ . That is,

$$\inf_{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}} \|\hat{h}_n - h_0\|_2 \to 0,$$

in probability.

Next, for any given  $h \in \bar{\mathcal{H}}$ , define

$$\Pi_0 h \in \underset{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}}{\operatorname{argmin}} \|h - h_0\|_2.$$

It is trivial by the definition of  $\mathcal{H}_0$  that it is closed under  $\|\cdot\|_w$  norm, so therefore it must also be closed under  $\|\cdot\|_2$  norm as it is stronger. Furthermore, by assumption  $\bar{\mathcal{H}}$  is compact under  $\|\cdot\|_2$ ,

so therefore given the closedness of  $\mathcal{H}_0$  we have that  $\bar{\mathcal{H}} \cap \mathcal{H}_0$  is compact. Therefore, by the extreme value theorem,  $\Pi_0 h$  always exists for any  $h \in \bar{\mathcal{H}}$ .

Now, we can bound

$$\begin{split} \|\hat{h}_n - h^{\dagger}\|_2 &\leq \|\hat{h}_n - \Pi_0 \hat{h}_n\|_2 + \|h^{\dagger} - \Pi_0 \hat{h}_n\|_2 \\ &= \inf_{h_0 \in \mathcal{H}_0} \|\hat{h}_n - h_0\|_2 + \|h^{\dagger} - \Pi_0 \hat{h}_n\|_2 \\ &= \|h^{\dagger} - \Pi_0 \hat{h}_n\|_2 + o_p(1) \,. \end{split}$$

Furthermore, for any given  $\eta > 0$ , analogous to the above, we have

$$\mathbb{P}\Big(\|h^{\dagger} - \Pi_0 \hat{h}_n\|_2 \ge \eta\Big) \le \mathbb{P}\Big(\|\Pi_0 \hat{h}_n\|_2 - \|h^{\dagger}\|_2 \ge \widetilde{M}(\eta)\Big),$$

where

$$\widetilde{M}(\eta) = \inf_{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}: \|h_0 - h^{\dagger}\|_2 > \eta} \|h_0\|_2 - \|h^{\dagger}\|_2.$$

Now, as argued above,  $\mathcal{H}_0 \cap \bar{\mathcal{H}}$  is compact under  $\|\cdot\|_2$ , so therefore so is  $\{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}} : \|h_0 - h^{\dagger}\|_2 \ge \eta\}$ . Therefore the extreme value applies, so we have  $\widetilde{M}(\eta) = \|h_{\eta}\|_2 - \|h^{\dagger}\|_2$  for some  $h_{\eta} \in \bar{\mathcal{H}} \cap \mathcal{H}_0$  such that  $\|h_{\eta} - h^{\dagger}\|_2 \ge \eta$ . Therefore, since by assumption  $h^{\dagger}$  is the unique minimizer of  $\|\cdot\|_2$  in  $\mathcal{H}_0 \cap \bar{\mathcal{H}}$ , we have that  $\widetilde{M}(\eta) > 0$  for every  $\eta$ . Furthermore, we have

$$\|\Pi_0 \hat{h}_n\|_2 - \|h^{\dagger}\|_2 \le \|\Pi_0 \hat{h}_n - \hat{h}_n\|_2 + \|\hat{h}_n\|_2 - \|h^{\dagger}\|_2$$

$$\le \inf_{h_0 \in \mathcal{H}_0 \cap \bar{\mathcal{H}}} \|h_0 - \hat{h}_n\|_2 + \|\hat{h}_n\|_2 - \|h^{\dagger}\|_2$$

$$\le o_p(1),$$

where for the final inequality we plug in our two main bounds we derived above. That is, we have that  $\|\Pi_0\hat{h}_n\|_2 - \|h^{\dagger}\|_2$  converges to zero in probability, so therefore since  $\widetilde{M}(\eta) > 0$  for every  $\eta$  we have that  $\|h^{\dagger} - \Pi_0\hat{h}_n\|_2 \to 0$  in probability also. Therefore, plugging this into the above, we have

$$\|\hat{h}_n - h^{\dagger}\|_2 \to 0,$$

in probability, as required.

## E.2 Proof of Theorem 9

Here, we consider the dual estimator for  $q_0$ , given by

$$\hat{q}_n = \underset{q \in \widetilde{\mathcal{Q}}_n}{\operatorname{argmax}} \mathbb{E}_n[\psi(\hat{\xi}_n, q)],$$

where

$$\hat{\xi}_n = \underset{\xi \in \Xi_n}{\operatorname{argmin}} \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\psi(\xi, q)],$$

and

$$\psi(\xi, q) = G(W; \xi, q) - m(W; \xi) - \frac{1}{2} q(T)^{\top} q(T).$$

That is,  $\hat{\xi}_n$  is the corresponding saddle-point solution for an empirical minimax problem. The proof that follows is very similar to that for Theorem 8, with some important differences that we will

emphasize below. Again, we provide a high-level overview of the proof first, and relegate proofs of intermediate lemmas to the end.

Before we proceed, we will define some simple notation. First, analogous to the proof of Theorem 8, for any  $\xi \in \mathcal{H}$  we define

$$q_0(\xi) = \underset{q \in \mathcal{Q}}{\operatorname{argmax}} \mathbb{E}[\psi(\xi, q)]$$

$$q_n(\xi) = \underset{q \in \mathcal{Q}_n}{\operatorname{argmax}} \mathbb{E}_n[\psi(\xi, q)]$$

$$\tilde{q}_n(\xi) = \underset{q \in \tilde{\mathcal{Q}}_n}{\operatorname{argmax}} \mathbb{E}_n[\psi(\xi, q)].$$

Note that in this case we have separate definitions  $q_n$  and  $\tilde{q}_n$  based on Q and  $\tilde{Q}_n$  respectively. Then, by some simple algebra/calculus it is easy to verify that

$$q_0(\xi) = \Pi_{\mathcal{Q}}[k(S,T)^{\top}\xi(S) \mid T].$$

In addition, in the theory below we will let  $\xi^{\dagger}$  be defined as in the main text.

## Feasibility of Population Saddle Point Solution

First, we provide a lemma that justifies that under Assumption 1, the population saddle-point solution will be equal to the particular  $q^{\dagger} \in \mathcal{Q}_0$  defined above.

Lemma 16. Let Assumption 1 be given. Then, we have

$$\Xi_0 = \operatorname*{argmin}_{h \in \mathcal{H}} \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(h, q)].$$

Furthermore, for any given  $\xi_0 \in \Xi_0$ , we have that  $\operatorname{argmax}_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi_0, q)] = \{q^{\dagger}\}.$ 

This implies that, given Assumption 1, any overall saddle-point solution to the population minimax problem recovers  $q^{\dagger}$ .

#### **High-Probability Bound**

Next, similar to the proof of Theorem 8, we will provide some high-probability bounds, which will be used extensively to prove the remaining sub-lemmas.

**Lemma 17.** Let  $\epsilon_n$  be defined again as in Lemma 11, and let

$$\Psi_{n}(q - q^{\dagger}) = G(W; \xi^{\dagger}, q - q^{\dagger}) - \frac{1}{2}(q - q^{\dagger})(T)^{\top}(q - q^{\dagger})(T) - q^{\dagger}(T)^{\top}(q - q^{\dagger})(T)$$

$$\widetilde{\Psi}_{n}(\xi - \xi^{\dagger}) = G(W; \xi - \xi^{\dagger}, q^{\dagger}) - m(W; \xi - \xi^{\dagger}),$$

for any  $q \in \mathcal{Q}_n$  and  $\xi \in \Xi_n$ . Then, with probability at least  $1 - 3\zeta$ , we have

$$\begin{split} \left| (\mathbb{E}_n - \mathbb{E}) \left[ \Psi_n(q - q^{\dagger}) \right] \right| &\leq 54 \epsilon_n \|q - q^{\dagger}\|_{2,2} + 54 \epsilon_n^2 \\ \left| (\mathbb{E}_n - \mathbb{E}) \left[ \widetilde{\Psi}_n(\xi - \xi^{\dagger}) \right] \right| &\leq 36 \epsilon_n \|\xi - \xi^{\dagger}\|_{2,2} + 36 \epsilon_n^2 \,, \end{split}$$

for every  $q \in \mathcal{Q}_n$  and  $\xi \in \Xi_n$ , as well as

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ G(W; \xi - \xi^{\dagger}, q - q^{\dagger}) \right] \right| \le 18\epsilon_n \|\xi - \xi^{\dagger}\|_{2,2} \|q - q^{\dagger}\|_{2,2} + 72\epsilon_n^2,$$

for every  $\xi \in \Xi_n$  and  $q \in \mathcal{Q}_n$ .

### Convergence Lemma for Empirical Saddle Point Solution

In terms of our above notation, our estimator  $\hat{q}_n$  is given by  $\tilde{q}_n(\hat{\xi}_n)$ . Here we provide a lemma for the convergence of this estimator in terms of the projected-norm behavior of  $\hat{\xi}_n$ . This will then provide the basis of our slow-rates theory below.

**Lemma 18.** Let the conditions of Theorem 9 be given. Then, under the high-probability event of Lemma 17, we have

$$||q_n(\xi) - q^{\dagger}||_{2,2}, ||\tilde{q}_n(\xi) - q^{\dagger}||_{2,2} \le 395\epsilon_n + 14\delta_n + 3||\xi - \xi^{\dagger}||_w,$$

for every  $\xi \in \Xi_n$ , where the weak norm  $\|\cdot\|_w$  is defined as in the proof of Theorem 8.

This lemma implies that we can bound the  $L_2$  error of  $\hat{q}_n$  in terms of the projected error of the minimax estimate  $\hat{\xi}_n$ , since instantiating this result for our estimator gives

$$\|\hat{q}_n - q^{\dagger}\|_{2,2} \le 395\epsilon_n + 14\delta_n + 3\|\hat{\xi}_n - \xi^{\dagger}\|_w$$
.

Unfortunately, the minimax problem is not well-specified for  $\xi^{\dagger}$  so we cannot easily obtain fast rates for  $\|\hat{\xi}_n - \xi^{\dagger}\|_w$ . However, we will establish conditions for obtaining slow rates below. The reasoning that follows is very similar as in the fast-rates analysis, except that we need to deal with some additional nuisance terms since here  $q_0(\xi^{\dagger}) \neq 0$ .

#### Bounding Weak Norm by Population Objective Sub-optimality

Here, we provide an analogue of Lemma 10 for the dual problem.

**Lemma 19.** Under Assumption 1, for every  $\xi \in \mathcal{H}$ , we have

$$\frac{1}{2} \|\xi - \xi^{\dagger}\|_{w}^{2} \leq \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi, q)] - \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi^{\dagger}, q)].$$

#### Reduction to Stochastic Equicontinuity Problem

Next, given our boundedness and universal approximation assumptions, we can provide the following analogue of Lemma 12.

Lemma 20. We have

$$\sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\hat{\xi}_n, q)] - \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi^{\dagger}, q)] \leq (\mathbb{E} - \mathbb{E}_n) \Big[ \psi(\hat{\xi}_n, \Pi_n q_0(\hat{\xi}_n)) - \psi(\xi^{\dagger}, q_n(\xi^{\dagger})) \Big] + 14544\epsilon_n^2 + 234\delta_n^2.$$

Therefore, again we have reduced our analysis to bounding a stochastic equicontinuity term, along with a term of the kind  $||q_n(\xi) - q^{\dagger}||_{2,2}$ .

### Bounding the Stochastic Equicontinuity Term using Localization

Similar as for the estimator of  $h^{\dagger}$ , we can decompose

$$\begin{split} &\psi(\hat{\xi}_{n},\Pi_{n}q_{0}(\hat{\xi}_{n})) - \psi(\xi^{\dagger},q_{n}(\xi^{\dagger})) \\ &= G(W;\hat{\xi}_{n} - \xi^{\dagger},q^{\dagger}) + G(W;\hat{\xi}_{n} - \xi^{\dagger},\Pi_{n}q_{0}(\hat{\xi}_{n}) - q^{\dagger}) \\ &+ G(W;\xi^{\dagger},\Pi_{n}q_{0}(\hat{\xi}_{n}) - q^{\dagger}) - G(W;\xi^{\dagger},q_{n}(\xi^{\dagger}) - q^{\dagger}) \\ &- m(W;\hat{\xi}_{n} - \xi^{\dagger}) \\ &- \frac{1}{2} \Big(\Pi_{n}q_{0}(\hat{\xi}_{n}) - q^{\dagger}\Big)(T)^{\top} \Big(\Pi_{n}q_{0}(\hat{\xi}_{n}) - q^{\dagger}\Big)(T) \\ &+ \frac{1}{2} \Big(q_{n}(\xi^{\dagger}) - q^{\dagger}\Big)(T)^{\top} \Big(q_{n}(\xi^{\dagger}) - q^{\dagger}\Big)(T) \\ &- q^{\dagger}(T)^{\top} \Big(\Pi_{n}q_{0}(\hat{\xi}_{n}) - q^{\dagger}\Big)(T) + q^{\dagger}(T)^{\top} \Big(q_{n}(\xi^{\dagger}) - q^{\dagger}\Big)(T) \;. \end{split}$$

Unfortunately, unlike for Theorem 8, here we have  $q^{\dagger} = q_0(\xi^{\dagger}) \neq 0$  in general, so we cannot eliminate any terms in this decomposition. This will lead to a term proportional to  $\epsilon_n \|\hat{\xi}_n - \xi^{\dagger}\|_{2,2}$  in the localized stochastic equicontinuity bound, which will prevent us from obtaining fast rates in general, given ill-posedness. However, we can still follow a localization analysis and derive an analogue of Lemma 13, which will allow us to obtain slow rates.

**Lemma 21.** Let the assumptions of Theorem 9 be given. Under an event that occurs with probability at least  $1-3\zeta$ , and subsumes the high-probability event of Lemma 18, we have

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ \psi(\hat{\xi}_n, \Pi_n q_0(\hat{\xi}_n)) - \psi(\Pi_n \xi^{\dagger}, \Pi_n q_n(\xi^{\dagger})) \right] \right| \le 576 \epsilon_n$$

Note that since we are only obtaining slow rates, we do not include terms such as  $||q_n(\Pi_n\xi^{\dagger}) - \Pi_n q_0(\Pi_n\xi^{\dagger})||_{2,2}$  or  $||\hat{\xi}_n - \xi^{\dagger}||_w$  in the bound, and instead give a simplified bound proportional to  $\epsilon_n$ . Including those terms could allow us to obtain slightly smaller constants, at the expense of a much more complicated analysis.

#### Putting Together the Final Bound

Combining together the results of Lemmas 19 to 21, we have

$$\|\hat{\xi}_n - \xi_0\|_w^2 \le 1152\epsilon_n + 14544\epsilon_n^2 + 234\delta_n^2$$
  
$$\le 15696\epsilon_n + 234\delta_n^2$$

which occurs with probability at least  $1 - 3\zeta$ . Then, combining this with Lemma 18, under the same high-probability event we have

$$\|\hat{q}_n - q^{\dagger}\|_{2,2} \le 395\epsilon_n + 14\delta_n + 3\sqrt{15696\epsilon_n + 234\delta_n^2}$$
  
$$\le 771\epsilon_n^{1/2} + 30\delta_n,$$

where we apply our assumption that  $\epsilon_n \leq 1$ . Therefore, we have slow rates for  $\hat{q}_n$  in  $L_2$  norm (as long as  $\delta_n$  converges sufficiently fast). Then, plugging in the definition of  $\epsilon_n$  gives us our required bound.

### **Proofs of Intermediate Lemmas**

*Proof of Lemma 16.* First, let some arbitrary  $h \in \mathcal{H}$  be given, and define

$$J(h) = \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(h, q)]$$
$$g(t) = J(\xi^{\dagger} + t(h - \xi^{\dagger})),$$

Now, we have

$$J(h) = \sup_{q \in \mathcal{Q}} \mathbb{E} \left[ G(W; h, q) - m(W; h) - \frac{1}{2} q(T)^{\top} q(T) \right]$$

$$= \sup_{q \in \mathcal{Q}} \mathbb{E} \left[ h(S)^{\top} k(S, T) q(T) - m(W; h) - \frac{1}{2} q(T)^{\top} q(T) \right]$$

$$= \mathbb{E} \left[ \frac{1}{2} \Pi_{\mathcal{Q}} \left[ k(S, T)^{\top} h(S) \mid T \right]^{\top} \Pi_{\mathcal{Q}} \left[ k(S, T)^{\top} h(S) \mid T \right] - m(W; h) \right].$$

Therefore, by the linearity of the projection operator, it easily follows that

$$g'(t) = \mathbb{E}\Big[\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}(h-\xi^{\dagger})(S)\mid T\Big]^{\top}\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}\xi^{\dagger}(S) + t(h-\xi^{\dagger})(S)\mid T\Big] - m(W;h-\xi^{\dagger})\Big]$$

$$= \mathbb{E}\Big[\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}(h-\xi^{\dagger})(S)\mid T\Big]^{\top}q^{\dagger}(T) - m(W;h-\xi^{\dagger})\Big]$$

$$+ t\mathbb{E}\Big[\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}(h-\xi^{\dagger})(S)\mid T\Big]^{\top}\Pi_{\mathcal{Q}}\Big[(h-\xi^{\dagger})(S)\mid T\Big],$$

where in the second equality we apply Assumption 1. Also, we have

$$g''(t) = \left\| \Pi_{\mathcal{Q}} \left[ k(S, T)^{\top} (h - \xi^{\dagger})(S) \mid T \right] \right\|_{2.2}^{2}.$$

That is,  $g''(t) \geq 0$  for all t, so it is convex. Furthermore, since  $q^{\dagger} \in \mathcal{Q}_0$ , we have

$$g'(0) = \mathbb{E}\left[\Pi_{\mathcal{Q}}\left[k(S,T)^{\top}(h-\xi^{\dagger})(S) \mid T\right]^{\top}q^{\dagger}(T) - m(W;h-\xi^{\dagger})\right]$$

$$= \mathbb{E}\left[(h-\xi^{\dagger})(S)^{\top}k(S,T)q^{\dagger}(T) - m(W;h-\xi^{\dagger})\right]$$

$$= \mathbb{E}\left[G(W;h-\xi^{\dagger},q^{\dagger}) - m(W;h-\xi^{\dagger})\right]$$

$$= 0$$

Therefore, putting the above together g(t) is minimized at t = 0. Then, given that the above reasoning holds for arbitrary  $h \in \mathcal{H}$ , it follows that J(h) is minimized at  $h = \xi^{\dagger}$ , which proves the first part of the lemma.

Now, for the second part of the lemma, let  $\xi_0$  be an arbitrary minimzer of J(h), which may or may not be equal to  $\xi^{\dagger}$ . Then, by first-order optimality conditions (which must hold since  $\mathcal{H}$  is linear), we have we have  $\frac{d}{dt}|_{t=0} J(\xi_0 + th) = 0$  for all  $h \in \mathcal{H}$ . That is, applying similar logic to above, we have

$$\mathbb{E}\left[\Pi_{\mathcal{Q}}\left[k(S,T)^{\top}h(S)\mid T\right]^{\top}q_{0}(\xi_{0})(T)-m(W;h)\right]=0 \qquad \forall h\in\mathcal{H},$$

where  $q_0(\xi_0) \in \operatorname{argmax}_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi_0, q)] = \Pi_{\mathcal{Q}}[k(S, T)^{\top} \xi_0(S) \mid T]$ . But then, following analogous reasoning as above, this is equivalent to  $\mathbb{E}[G(W; h, q_0(\xi_0)) - m(W; h)] = 0$  for all  $h \in \mathcal{H}$ , so  $q_0(\xi_0) \in \mathcal{Q}_0$ . Then, since  $q_0(\xi_0)(T) = T^{\dagger} \xi_0$ , and as reasoned previously there is a unique  $q^{\dagger} \in \operatorname{range}(T^{\dagger})$  such that  $q^{\dagger} \in \mathcal{Q}_0$ , it must be the case that  $q_0(\xi_0) = q^{\dagger}$ .

Proof of Lemma 17. First, by Assumption 13, we have  $\|\Psi_n(q-q^{\dagger})\|_2 \leq 3\|q-q^{\dagger}\|_{2,2}$  for every  $q \in \mathcal{Q}_n$ . Therefore, it follows from Assumption 16 that

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ \Psi_n(q - q^{\dagger}) \right] \right| \le 54\epsilon_n \|q - q^{\dagger}\|_{2,2} + 54\epsilon_n^2,$$

for all  $q \in \mathcal{Q}_n$ , which holds with probability at least  $1-\zeta$ . Similar reasoning gives us  $\|\widetilde{\Psi}_n(\xi-\xi^{\dagger})\|_2 \le 2\|\xi-\xi^{\dagger}\|_{2,2}$  for all  $\xi \in \Xi_n$ , and therefore

$$\left| (\mathbb{E}_n - \mathbb{E}) \left| \widetilde{\Psi}_n(\xi - \xi^{\dagger}) \right| \right| \le 36\epsilon_n \|\xi - \xi^{\dagger}\|_{2,2} + 36\epsilon_n^2,$$

for all  $\xi \in \Xi_n$ , which also holds with probability at least  $1 - \zeta$ .

Furthermore, given Assumption 13, we have that  $||G(W; \xi - \xi^{\dagger}, q - q^{\dagger})||_{\infty} \le 4$ . Therefore, similar reasoning to above gives us

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ \frac{1}{4} G(W; h - h^{\dagger}, q - q^{\dagger}) \right] \right| \le 18\epsilon_n \left\| \frac{1}{4} G(W; h - h^{\dagger}, q - q^{\dagger}) \right\|_2 + 18\epsilon_n^2,$$

and re-arranging and applying the Lipschitz assumptions of Assumption 13 consequently gives us

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ G(W; h - h^{\dagger}, q - q^{\dagger}) \right] \right| \le 18\epsilon_n \|h - h^{\dagger}\|_{2,2} \|q - q^{\dagger}\|_{2,2} + 72\epsilon_n^2,$$

which holds for all  $q \in \mathcal{Q}_n$  and  $\xi \in \Xi_n$  with probability at least  $1 - \zeta$ .

Finally, combining the above three bounds with a union bound gives us our desired result.

Proof of Lemma 18. The proof here is very similar to that of Lemma 14. We will prove it below for any arbitrary  $\xi \in \Xi_n$  for the  $||q_n(\xi) - q^{\dagger}||$  bound. Note that the  $||q_n(\xi) - q^{\dagger}||$  also follows by identical reasoning.

First, note that

$$\begin{split} &\frac{1}{2} \|q_{n}(\xi) - q_{0}(\xi)\|_{2,2}^{2} - \frac{1}{2} \|q_{0}(\xi) - q^{\dagger}\|_{2,2}^{2} \\ &= \frac{1}{2} \mathbb{E} \Big[ \Big( q_{n}(\xi)(T) - \Pi_{\mathcal{Q}}[k(S,T)^{\top}\xi(S) \mid T] \Big)^{\top} \Big( q_{n}(\xi)(T) - \Pi_{\mathcal{Q}}[k(S,T)^{\top}\xi(S) \mid T] \Big) \\ &- \Big( q^{\dagger}(T) - \Pi_{\mathcal{Q}}[k(S,T)^{\top}\xi(S) \mid T] \Big)^{\top} \Big( q^{\dagger}(T) - \Pi_{\mathcal{Q}}[k(S,T)^{\top}\xi(S) \mid T] \Big) \Big] \\ &= \mathbb{E} \Big[ \Big( \xi(S)^{\top}k(S,T)q^{\dagger}(T) - \frac{1}{2}q^{\dagger}(T)^{\top}q^{\dagger}(T) \Big) \\ &- \Big( \xi(S)^{\top}k(S,T)q_{n}(\xi)(T) - \frac{1}{2}q_{n}(\xi)(T)^{\top}q_{n}(\xi)(T) \Big) \Big] \\ &= \mathbb{E} \Big[ \psi(\xi,q^{\dagger}) - \psi(\xi,q_{n}(\xi)) \Big] \,. \end{split}$$

Furthermore, by the optimality of  $q_n(\xi)$  for the empirical minimax problem at  $h = \xi$ , we can further bound the above by

$$\frac{1}{2} \|q_{n}(\xi) - q_{0}(\xi)\|_{2,2}^{2} - \frac{1}{2} \|q_{0}(\xi) - q^{\dagger}\|_{2,2}^{2} \\
\leq (\mathbb{E}_{n} - \mathbb{E}) \left[ \psi(\xi, q_{n}(\xi)) - \psi(\xi, q^{\dagger}) \right] + \mathbb{E}_{n} \left[ \psi(\xi, q^{\dagger}) - \psi(\xi, \Pi_{n} q^{\dagger}) \right] \\
= (\mathbb{E}_{n} - \mathbb{E}) \left[ G \left( W; \xi - \xi^{\dagger}, q_{n}(\xi) - q^{\dagger} \right) - G \left( W; \xi - \xi^{\dagger}, \Pi_{n} q^{\dagger} - q^{\dagger} \right) \right] \\
+ \Psi_{n} \left( q_{n}(\xi) - q^{\dagger} \right) - \Psi_{n} \left( \Pi_{n} q^{\dagger} - q^{\dagger} \right) \right] + \mathcal{E}_{1},$$

where  $\Psi_n$  is defined as in the statement of Lemma 17, and

$$\mathcal{E}_{1} = \mathbb{E}\left[\psi(\xi, q^{\dagger}) - \psi(\xi, \Pi_{n}q^{\dagger})\right]$$

$$= \mathbb{E}\left[-G(\hat{\xi}_{n}, \Pi_{n}q^{\dagger} - q^{\dagger}) + \frac{1}{2}(\Pi_{n}q^{\dagger} - q^{\dagger})(T)^{\top}(\Pi_{n}q^{\dagger} - q^{\dagger})(T) + q^{\dagger}(T)^{\top}(\Pi_{n}q^{\dagger} - q^{\dagger})(T)\right]$$

$$\leq \mathbb{E}\left[\left(q^{\dagger}(T) - k(S, T)^{\top}\xi^{\dagger}(S)\right)^{\top}(\Pi_{n}q^{\dagger} - q^{\dagger})(T)\right] - \mathbb{E}\left[G(W; \xi - \xi^{\dagger}, \Pi_{n}q^{\dagger} - q^{\dagger})\right] + \frac{1}{2}\delta_{n}^{2}$$

$$= -\mathbb{E}\left[G(W; \xi - \xi^{\dagger}, \Pi_{n}q^{\dagger} - q^{\dagger})\right] + \frac{1}{2}\delta_{n}^{2}$$

$$\leq \|\xi - \xi^{\dagger}\|_{w}\delta_{n} + \frac{1}{2}\delta_{n}^{2}$$

$$\leq \frac{1}{2}\|\xi - \xi^{\dagger}\|_{w}^{2} + \delta_{n}^{2},$$

where in the above we apply the fact that  $q^{\dagger}(T) = q_0(\xi^{\dagger})(T) = \Pi_{\mathcal{Q}}[k(S,T)^{\top}\xi^{\dagger}(S) \mid T]$ , along with Assumption 15, and the AM-GM inequality.

Now, putting the previous bounds together and plugging in the bounds from the high-probability event of Lemma 17, we get

$$\begin{split} &\frac{1}{2}\|q_n(\xi)-q_0(\xi)\|_{2,2}^2 - \frac{1}{2}\|q_0(\xi)-\Pi_n q^\dagger\|_{2,2}^2 \\ &\leq \Big(54+18\|\xi-\xi^\dagger\|_{2,2}\Big)\Big(\|q_n(\xi)-q^\dagger\|_{2,2} + \|\Pi_n q^\dagger-q^\dagger\|_{2,2}\Big)\epsilon_n + 252\epsilon_n^2 + \frac{1}{2}\|\xi-\xi^\dagger\|_w^2 + \delta_n^2 \\ &\leq 90\epsilon_n\|q_n(\xi)-q^\dagger\|_{2,2} + 90\epsilon_n\delta_n + 252\epsilon_n^2 + \frac{1}{2}\|\xi-\xi^\dagger\|_w^2 + \delta_n^2 \,. \end{split}$$

Next, applying the above bound, we have

$$\frac{1}{2} \|q_n(\xi) - q^{\dagger}\|_{2,2}^2 \le \|q_n(\xi) - q_0(\hat{\xi}_n)\|_{2,2}^2 + \|q_0(\hat{\xi}_n) - q^{\dagger}\|_{2,2}^2 
\le 2 \left(\frac{1}{2} \|q_n(\xi) - q_0(\hat{\xi}_n)\|_{2,2}^2 - \frac{1}{2} \|q_0(\hat{\xi}_n) - q^{\dagger}\|_{2,2}^2\right) + 2 \|q_0(\hat{\xi}_n) - q^{\dagger}\|_{2,2}^2 
\le 180\epsilon_n \|q_n(\xi) - q^{\dagger}\|_{2,2} + 180\epsilon_n \delta_n + 504\epsilon_n^2 + 2\delta_n^2 + 3 \|\xi - \xi^{\dagger}\|_w^2 
\le 180\epsilon_n \|q_n(\xi) - q^{\dagger}\|_{2,2} + 594\epsilon_n^2 + 92\delta_n^2 + 3 \|\xi - \xi^{\dagger}\|_w^2,$$

where in the second last inequality we apply the fact that  $q^{\dagger} = q_0(\xi^{\dagger})$ , so therefore  $||q_0(\xi) - q^{\dagger}||_{2,2} = ||\xi - \xi^{\dagger}||_w$ , and for the final step we apply the AM-GM inequality. Then, applying Lemma 9 to the above, we get the final bound of

$$||q_n(\xi) - q^{\dagger}||_{2,2} \le 360\epsilon_n + \sqrt{1188\epsilon_n^2 + 184\delta_n^2 + 6||\xi - \xi^{\dagger}||_w^2}$$
  
$$\le 395\epsilon_n + 14\delta_n + 3||\xi - \xi^{\dagger}||_w,$$

where above we apply the fact  $\sqrt{x+y} \leq \sqrt{x} + \sqrt{y}$  for non-negative x and y.

Proof of Lemma 19. Define  $J(h) = \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(h,q)]$ . As argued in the proof of Lemma 16, we have

$$J(h) = \mathbb{E}\Big[\frac{1}{2}\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}h(S)\mid T\Big]^{\top}\Pi_{\mathcal{Q}}\Big[k(S,T)^{\top}h(S)\mid T\Big] - m(W;h)\Big].$$

Now, let some arbitrary  $\xi \in \mathcal{H}$  be given, and define

$$g(t) = J(\xi^{\dagger} + t(\xi - \xi^{\dagger})).$$

Then, as argued in the proof of Lemma 16, we have g'(0) = 0, and  $g''(t) = \|\Pi_{\mathcal{Q}}[k(S,T)^{\top}(\xi-\xi^{\dagger})(S) \|$  $T]\|_{2,2}^2 = \|\xi - \xi^{\dagger}\|_w^2$  for all t. Therefore, by strong convexity we have

$$\begin{split} g(1) - g(0) &\geq \frac{1}{2} \|\xi - \xi^{\dagger}\|_{w}^{2} \\ &\iff \frac{1}{2} \|\xi - \xi^{\dagger}\|_{w}^{2} \leq \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi, q)] - \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi^{\dagger}, q)] \,, \end{split}$$

where the second equality follows by noting that  $g(0) = J(\xi^{\dagger})$ ,  $g(1) = J(\xi)$ , and by plugging in the definition of J. Since this holds for arbitrary  $\xi \in \mathcal{H}$ , we are done.

Proof of Lemma 20. The proof here is very similar to that of Lemma 12. First, we have

$$\begin{split} &\sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\hat{\xi}_n,q)] - \sup_{q \in \mathcal{Q}} \mathbb{E}[\psi(\xi^\dagger,q)] \\ &= \sup_{q \in \bar{\mathcal{Q}}} \mathbb{E}[\psi(\hat{\xi}_n,q)] - \sup_{q \in \bar{\mathcal{Q}}} \mathbb{E}[\psi(\xi^\dagger,q)] \\ &\leq \mathbb{E}[\psi(\hat{\xi}_n,q_0(\hat{\xi}_n))] - \mathbb{E}[\psi(\xi^\dagger,q_n(\xi^\dagger))] \\ &\leq \mathbb{E}[\psi(\hat{\xi}_n,q_0(\hat{\xi}_n))] - \mathbb{E}[\psi(\xi^\dagger,q_n(\xi^\dagger))] - \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\psi(\hat{\xi}_n,q)] + \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\psi(\Pi_n\xi^\dagger,q)] \\ &= \mathbb{E}[\psi(\hat{\xi}_n,\Pi_nq_0(\hat{\xi}_n))] - \mathbb{E}[\psi(\xi^\dagger,q_n(\xi^\dagger))] - \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\psi(\hat{\xi}_n,q)] + \sup_{q \in \mathcal{Q}_n} \mathbb{E}_n[\psi(\xi^\dagger,q)] + \mathcal{E}_1 + \mathcal{E}_2 \\ &\leq (\mathbb{E} - \mathbb{E}_n) \left[ \psi(\hat{\xi}_n,\Pi_nq_0(\hat{\xi}_n)) - \psi(\xi^\dagger,q_n(\xi^\dagger)) \right] + \mathcal{E}_1 + \mathcal{E}_2 \,, \end{split}$$

where the first and third inequalities follow by relaxing the supremum in the negative terms, and the second inequality follows by the optimality of  $\hat{\xi}_n$  for the empirical minimax objective, and where

$$\mathcal{E}_{1} = \mathbb{E}\left[\psi(\hat{\xi}_{n}, q_{0}(\hat{\xi}_{n})) - \psi(\hat{\xi}_{n}, \Pi_{n}q_{0}(\hat{\xi}_{n}))\right]$$

$$\mathcal{E}_{2} = \sup_{q \in \mathcal{Q}_{n}} \mathbb{E}_{n}[\psi(\Pi_{n}\xi^{\dagger}, q)] - \sup_{q \in \mathcal{Q}_{n}} \mathbb{E}_{n}[\psi(\xi^{\dagger}, q)].$$

Now, let us bound the error terms  $\mathcal{E}_1$  and  $\mathcal{E}_2$ . For the first, using the shorthand  $\Delta = q_0(\hat{h}_n) - \Pi_n q_0(\hat{h}_n)$ , we have

$$\mathcal{E}_{1} = \mathbb{E}\Big[G(W; \hat{\xi}_{n}, \Delta) - \frac{1}{2}q_{0}(\hat{\xi}_{n})(T)^{\top}q_{0}(\hat{\xi}_{n})(T) + \frac{1}{2}\Pi_{n}q_{0}(\hat{\xi}_{n})(T)^{\top}\Pi_{n}q_{0}(\hat{\xi}_{n})(T)\Big]$$

$$= \mathbb{E}\Big[G(W; \hat{\xi}_{n}, \Delta) - q_{0}(\hat{\xi}_{n})(T)^{\top}\Delta(T) + \frac{1}{2}\Delta(T)^{\top}\Delta(T)\Big]$$

$$= \mathbb{E}\Big[\frac{1}{2}\Delta(T)^{\top}\Delta(T)\Big]$$

$$\leq \frac{1}{2}\delta_{n}^{2},$$

where the second last step follows since  $\mathbb{E}[G(W;\xi,\Delta)] = \mathbb{E}[q_0(\xi)(T)^{\top}\Delta(T)]$  for any  $\xi$ , and the final inequality follows by Assumption 15.

Next, for the second term above, we can bound

$$\mathcal{E}_{2} \leq \mathbb{E}_{n} \left[ \psi(\Pi_{n}\xi^{\dagger}, q_{n}(\Pi_{n}\xi^{\dagger}) - \psi(\xi^{\dagger}, q_{n}(\Pi_{n}\xi^{\dagger})) \right]$$

$$= \mathbb{E}_{n} \left[ G(W; \Pi_{n}\xi^{\dagger} - \xi^{\dagger}, q_{n}(\Pi_{n}\xi^{\dagger}) - q^{\dagger}) + \widetilde{\psi}_{n}(\Pi_{n}\xi^{\dagger} - \xi^{\dagger}) \right]$$

$$= (\mathbb{E}_{n} - \mathbb{E}) \left[ G(W; \Pi_{n}\xi^{\dagger} - \xi^{\dagger}, q_{n}(\Pi_{n}\xi^{\dagger}) - q^{\dagger}) + \widetilde{\psi}_{n}(\Pi_{n}\xi^{\dagger} - \xi^{\dagger}) \right]$$

$$+ \mathbb{E} \left[ G(W; \Pi_{n}\xi^{\dagger} - \xi^{\dagger}; q_{n}(\Pi_{n}\xi^{\dagger})) - m(W; \Pi_{n}\xi^{\dagger} - \xi^{\dagger}) \right]$$

$$= (\mathbb{E}_{n} - \mathbb{E}) \left[ G(W; \Pi_{n}\xi^{\dagger} - \xi^{\dagger}, q_{n}(\Pi_{n}\xi^{\dagger}) - q^{\dagger}) + \widetilde{\psi}_{n}(\Pi_{n}\xi^{\dagger} - \xi^{\dagger}) \right]$$

$$+ \mathbb{E} \left[ G(W; \Pi_{n}\xi^{\dagger} - \xi^{\dagger}; q_{n}(\Pi_{n}\xi^{\dagger}) - q^{\dagger}) \right]$$

$$\leq 18\epsilon_{n}\delta_{n} \|q_{n}(\Pi_{n}\xi^{\dagger}) - q^{\dagger}\|_{2,2} + 36\epsilon_{n}\delta_{n} + 108\epsilon_{n}^{2} + \delta_{n} \|q_{n}(\Pi_{n}\xi^{\dagger}) - q^{\dagger}\|_{2,2}$$

$$\leq (1 + 18\epsilon_{n})\delta_{n} \left( 395\epsilon_{n} + 14\delta_{n} + 3 \|\Pi_{n}\xi^{\dagger} - \xi^{\dagger}\|_{w} \right) + 36\epsilon_{n}\delta_{n} + 108\epsilon_{n}^{2}$$

$$\leq 431\epsilon_{n}\delta_{n} + 17\delta_{n}^{2} + 108\epsilon_{n}^{2} + 7110\delta_{n}\epsilon_{n}^{2}$$

$$\leq 14544\epsilon_{n}^{2} + 233\delta_{n}^{2}$$

where the first inequality follows by relaxing the sup in the negative term, the second inequality follows from the assumed high-probability event of Lemma 17, along with Assumption 15, the third inequality follows by Lemma 18, and the subsequent inequalities follow by applying AM-GM, Assumption 15, and the fact that  $\delta_n \leq 2$ .

Finally, putting all of the above together, we get our final required result of

$$\sup_{q\in\mathcal{Q}} \mathbb{E}[\psi(\hat{\xi}_n,q)] - \sup_{q\in\mathcal{Q}} \mathbb{E}[\psi(\xi^\dagger,q)] \leq (\mathbb{E} - \mathbb{E}_n) \Big[ \psi(\hat{\xi}_n,\Pi_n q_0(\hat{\xi}_n)) - \psi(\xi^\dagger,q_n(\xi^\dagger)) \Big] + 14544\epsilon_n^2 + 234\delta_n^2.$$

Proof of Lemma 21. First, given the decomposition from the proof overview, we have

$$\psi(\hat{\xi}_n, \Pi_n q_0(\hat{\xi}_n)) - \psi(\xi^{\dagger}, q_n(\xi^{\dagger}))$$

$$= \Psi_n \Big( \Pi_n q_0(\hat{\xi}_n) - q^{\dagger} \Big) - \Psi_n \Big( q_n(\xi^{\dagger}) - q^{\dagger} \Big)$$

$$+ \widetilde{\Psi}_n(\hat{\xi}_n - \xi^{\dagger}) + G \Big( W; \hat{\xi}_n - \xi^{\dagger}, \Pi_n q_0(\hat{\xi}_n) - q^{\dagger} \Big).$$

where  $\Psi_n$  and  $\widetilde{\Psi}_n$  are defined as in the proof of Lemma 17.

Now, applying the bounds of Lemma 17 to the above, under its high-probability event we get

$$\begin{split} & \left| (\mathbb{E}_n - \mathbb{E}) \left[ \psi(\hat{\xi}_n, \Pi_n q_0(\hat{\xi}_n)) - \psi(\Pi_n \xi^{\dagger}, q_n(\Pi_n \xi^{\dagger})) \right] \right| \\ & \leq 54 \|\Pi_n q_0(\hat{\xi}_n) - q^{\dagger}\|_{2,2} + 54 \|q_n(\xi^{\dagger}) - q^{\dagger}\|_{2,2} + 36 \|\hat{\xi}_n - \xi^{\dagger}\|_{2,2} \\ & + 18 \|\hat{\xi}_n - \xi^{\dagger}\| \|\Pi_n q_0(\hat{\xi}_n) - q^{\dagger}\|_{2,2} + 216 \epsilon_n^2 \,. \end{split}$$

Finally, given uniform boundedness of all elements of  $\bar{Q}$  and  $\bar{\Xi}$ , and the fact that we have assumed that  $\epsilon_n \leq 1$  (and so  $\epsilon_n^2 \leq \epsilon_n$ ), the above bound can be simplified to

$$\left| (\mathbb{E}_n - \mathbb{E}) \left[ \psi(\hat{\xi}_n, \Pi_n q_0(\hat{\xi}_n)) - \psi(\Pi_n \xi^{\dagger}, q_n(\Pi_n \xi^{\dagger})) \right] \right| \le 576 \epsilon_n ,$$

as required.

# F Proofs for Debiased Inference Results

Here, we provide proofs for our debiased inference results. Specifically, we provide proofs for Theorem 6 and Theorem 7, along with thier general analogues Theorem 10 and Theorem 11. As with the proofs of the minimax estimation results, since the former are special cases of the latter, we only provide explicit proofs of the latter.

Proof of Theorem 10. For any function f(W), denote  $\mathbb{P}f = \int f(w)p(w) \, dw$ , and  $\mathbb{P}_{n,k}f = \sum_{i \in \mathcal{I}_k} f(W_i)/|\mathcal{I}_k|$ . Also denote

$$\hat{\theta}_k = \frac{1}{|\mathcal{I}_k|} \sum_{i \in \mathcal{I}_k} \psi(W_i; \hat{h}^{(k)}, \hat{q}^{(k)}).$$

It is easy to verify that we have

$$\hat{\theta}_k - \theta^* = \mathbb{P}_{n,k} \Big[ \psi(W; h^{\dagger}, q^{\dagger}) - \theta^* \Big]$$

$$+ (\mathbb{P}_{n,k} - \mathbb{P}) \Big[ \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h^{\dagger}, q^{\dagger}) \Big] + \mathbb{P} \Big[ \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h^{\dagger}, q^{\dagger}) \Big].$$

By simple algebra, we can show that there exists a universal constant c such that

$$\mathbb{P}\left[\left(\psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h_R, q_R)\right)^2\right] \le c\|\hat{h}^{(k)} - h_R\|_2^2 + c\|\hat{q} - q\|_2^2 = o_p(1)$$

since  $\|\hat{h}^{(k)} - h_R\|_2^2 = o_p(1)$  and  $\|\hat{q}^{(k)} - q_R\|_2^2 = o_p(1)$  according to Theorems 8 and 9. Thus by Markov inequality, we have

$$\left| (\mathbb{P}_{n,k} - \mathbb{P}) \left[ \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h_R, q_R) \right] \right| = o_p \left( \frac{1}{\sqrt{|\mathcal{I}_k|}} \right) = o_p \left( \frac{1}{\sqrt{n}} \right).$$

Moreover, according to Lemma 4,

$$\left| \mathbb{P} \left[ \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h^{\dagger}, q^{\dagger}) \right] \right| \le \|P[\hat{h}^{(k)} - h_R]\|_2 \|\hat{q}^{(k)} - q_R\|_2.$$

According to Theorems 8 and 9, we have

$$||P(\hat{h}_n - h_0)||_{2,2} \le 395\epsilon_n + 43\delta_n + 2\mu_n^{1/2},$$
  
$$||\hat{q}_n - q^{\dagger}||_2 \le 771\epsilon_n^{1/2} + 30\delta_n,$$

where  $\epsilon_n = r_n + c_2 \sqrt{\log(c_1/\zeta)/n}$ .

It follows that

$$\left| \mathbb{P} \left[ \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h^{\dagger}, q^{\dagger}) \right] \right| = O_p \left( \epsilon_n^{3/2} + \delta_n \epsilon_n^{1/2} + \delta_n \epsilon_n + \delta_n^2 + \delta_n \mu_n^{1/2} + \epsilon_n^{1/2} \mu_n^{1/2} \right).$$

Therefore, when  $r_n = o(n^{-1/3})$ ,  $\delta_n = o(n^{-1/4})$ ,  $\delta_n r_n^{1/2} = o(n^{-1/2})$ ,  $\mu_n r_n = o(n^{-1})$  and  $\mu_n \delta_n^2 = o(n^{-1})$ , we have

$$\left| \mathbb{P} \left[ \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h^{\dagger}, q^{\dagger}) \right] \right| = o_p(n^{-1/2}), \text{ for } k = 1, \dots, K.$$

Therefore,

$$\hat{\theta}_k - \theta^* = \mathbb{P}_{n,k} \left[ \psi(W; h^{\dagger}, q^{\dagger}) - \theta^* \right] + o_p(n^{-1/2}).$$

This implies that

$$\sqrt{n}(\hat{\theta}_n - \theta^*) = \frac{1}{\sqrt{n}} \sum_{i=1}^n (\psi(W_i; h^{\dagger}, q^{\dagger}) - \theta^*) + o_p(1).$$

By Central Limit Theorem, we have that when  $n \to \infty$ ,

$$\sqrt{n}(\hat{\theta}_n - \theta^*) \rightsquigarrow \mathcal{N}(0, \sigma_0^2),$$

where

$$\sigma_0^2 = \mathbb{E}\left[\left(\psi(W; h^{\dagger}, q^{\dagger}) - \theta^{\star}\right)^2\right].$$

Proof of Theorem 11. Let arbitrary fold  $k \in [K]$  be given, and let  $n_k$  denot the size of the fold. Define

$$\hat{\sigma}_{n,k}^2 = \mathbb{E}_{n,k} \left[ \left( \hat{\theta}_n - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \right)^2 \right],$$

where  $\mathbb{E}_{n,k}$  denotes the empirical expectation operator over the data in the k'th fold. Since  $\hat{\sigma}_n^2$  is given by the weighted average of  $\hat{\sigma}_{n,k}^2$  for all  $k \in [K]$ , it is sufficient to argue that  $\hat{\sigma}_{n,k}^2 \to \sigma_0^2$  in probability for arbitrary k.

Now, we have

$$\hat{\sigma}_{n,k}^{2} - \sigma_{0}^{2} = (\mathbb{E}_{n,k} - \mathbb{E}) \left[ \left( \theta_{0} - \psi(W; h_{0}, q_{0}) \right)^{2} \right] + \mathbb{E}_{n,k} \left[ \left( \hat{\theta}_{n} - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \right)^{2} - \left( \theta_{0} - \psi(W; h_{0}, q_{0}) \right)^{2} \right]$$

The former of these terms converges to zero in probability by the law of large numbers, so we can focus on the second of these terms, which we can re-arrange as

$$\mathbb{E}_{n,k} \Big[ \Big( \hat{\theta}_n - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \Big)^2 - \Big( \theta_0 - \psi(W; h_0, q_0) \Big)^2 \Big] \\
= \mathbb{E}_{n,k} \Big[ (\hat{\theta}_n - \theta_0) \Big( \hat{\theta}_n + \theta_0 - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h_0, q_0) \Big) \Big] \\
- \mathbb{E}_{n,k} \Big[ \Big( \psi(W; h_0, q_0) - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \Big) \Big( \hat{\theta}_n + \theta_0 - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h_0, q_0) \Big) \Big]$$

Furthermore, by Assumptions 10, 13 and 14, it easily follows that  $|\theta_0| \le 1$ ,  $|\hat{\theta}_n| \le 3$ ,  $||\psi(W; \hat{h}^{(k)}, \hat{q}^{(k)})||_{\infty} \le 3$ , and  $||\psi(W; h_0, q_0)||_{\infty} \le 3$ . Therefore, we have

$$\left\| \hat{\theta}_n + \theta_0 - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) - \psi(W; h_0, q_0) \right\|_{\infty} \le 10,$$

and so

$$\left| \mathbb{E}_{n,k} \left[ \left( \hat{\theta}_n - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \right)^2 - \left( \theta_0 - \psi(W; h_0, q_0) \right)^2 \right] \right| \\
\leq 10 |\hat{\theta}_n - \theta_0| + 10 \mathbb{E}_{n,k} \left[ \left| \psi(W; h_0, q_0) - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \right| \right]$$

Now, by Theorem 10 we know that  $\hat{\theta}_n - \theta_0 \to 0$  in probability. Furthermore, by Theorems 8 and 9, along with the continuity of  $\psi$  in h and q by Assumption 13, we know that  $\|\psi(W; h_0, q_0) - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)})\|_1 \to 0$  in probability. Therefore, we have

$$\begin{split} & \left| \mathbb{E}_{n,k} \left[ \left( \hat{\theta}_n - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)}) \right)^2 - \left( \theta_0 - \psi(W; h_0, q_0) \right)^2 \right] \right| \\ & \leq 10 (\mathbb{E}_{n,k} - \mathbb{E}) [\Delta_n] + o_p(1) \,, \end{split}$$

where  $\Delta_n = |\psi(W; h_0, q_0) - \psi(W; \hat{h}^{(k)}, \hat{q}^{(k)})|$ . Now, since the randomness of  $(\hat{h}^{(k)}, \hat{q}^{(k)})$  is independent of that of the k'th fold (by cross fitting), we can apply e.g. Höffding's inequality to the above for any given realization of  $(\hat{h}^{(k)}, \hat{q}^{(k)})$ , to get a high-probability bound on  $(\mathbb{E}_{n,k} - \mathbb{E})[\Delta_n]$  over the independent sample of data given by  $\mathbb{E}_{n,k}$ . That is, given any fixed  $\epsilon > 0$ , regardless of the realization of  $(\hat{h}^{(k)}, \hat{q}^{(k)})$  we can define some sequence  $\delta_n \to 0$  such that  $|(\mathbb{E}_{n,k} - \mathbb{E})[\Delta_n]| \le \epsilon$  with probability at least  $1 - \delta_n$  over the randomness of the k'th fold. That is, we have  $(\mathbb{E}_{n,k} - \mathbb{E})[\Delta_n] = o_p(1)$ , so we can conclude that  $\hat{\sigma}_n^2 \to \sigma_0^2$  in probability.

Moreover, the Slutsky's theorem implies that

$$\frac{\sqrt{n}(\hat{\theta}_n - \theta^*)}{\hat{\sigma}_n^2} \rightsquigarrow \mathcal{N}(0, 1).$$

It follows that as  $n \to \infty$ ,

$$\mathbb{P}\left(\theta^{\star} \in \mathrm{CI}\right) \to 1 - \alpha.$$

# G Proofs for Partially Linear Model Estimation

Proof for Proposition 1. According to Equation (38), we have

$$\mathbb{E}[q_0(Z)h(X)] = \mathbb{E}[\alpha(X)h(X)], \quad \forall h \in \mathcal{H}.$$

Since any partially linear  $h \in \mathcal{H}$  can be written as  $h(X) = X_a^{\top} \theta + g(X_b)$ , we have

$$\mathbb{E}\Big[q_0(Z)\Big(X_a^\top \theta + g(X_b)\Big)\Big] = \theta, \ \forall \theta \in \mathbb{R}^{d_a}, g \in \mathcal{L}_2(X_b).$$

This is apparently equivalent to Equation (39).

Proof for Proposition 2. Obviously,  $\xi_{0,i}$  is partially linear in X so it belongs to the partially linear class  $\mathcal{H}$ . According to Theorem 2,  $\xi_{0,i} \in \mathcal{H}$  is a solution to Equation (40) if and only if  $q_{0,i} = P\xi_{0,i}$  satisfies Equation (38), so we can prove the desired conclusion once we prove that  $q_{0,i} = P\xi_{0,i}$  satisfies Equation (38) for all  $i = 1, \ldots, d_a$ . According to Proposition 1, we only need to verify that  $q_0 = (P\xi_{0,1}, \ldots, \xi_{0,d_a})$  satisfy Equation (39).

Since  $\rho_{0,i}$  solves the minimization problem in Equation (41), it satisfies the first order condition that

$$\mathbb{E}\Big[\mathbb{E}\Big[X_a^{(i)} - \rho_{0,i}(X_b) \mid Z\Big] \mathbb{E}[\rho(X_b) \mid Z]\Big] = \mathbb{E}\Big[\mathbb{E}\Big[X_a^{(i)} - \rho_{0,i}(X_b) \mid Z\Big]\rho(X_b)\Big] = 0, \quad \forall \rho \in \mathcal{L}_2(X_b).$$

This implies that

$$\mathbb{E}[[P\xi_{0,i}](Z) \mid X_b] = \mathbb{E}\Big[\Gamma^{-1}\mathbb{E}\Big[X_a^{(i)} - \rho_{0,i}(X_b) \mid Z\Big] \mid X_b\Big] = \Gamma^{-1}\mathbb{E}\Big[\mathbb{E}\Big[X_a^{(i)} - \rho_{0,i}(X_b) \mid Z\Big] \mid X_b\Big] = 0.$$

It follows that  $\mathbb{E}[q_0(Z) \mid X_b] = \mathbf{0}_{d_a}$ . This further implies that

$$\mathbb{E}[q_0(Z)\rho_0(X_b)] = 0.$$

Therefore,

$$\begin{split} \mathbb{E}\Big[q_0(Z)X_a^\top\Big] &= \mathbb{E}\Big[q_0(Z)(X_a - \rho_0(X_b))^\top\Big] = \mathbb{E}\Big[q_0(Z)X_a^\top\Big] \\ &= \mathbb{E}\Big[q_0(Z)(\mathbb{E}[X_a - \rho_0(X_b) \mid Z])^\top\Big] = \Gamma^{-1}\mathbb{E}\Big[(X_a - \rho_0(X_b) \mid Z)(\mathbb{E}[X_a - \rho_0(X_b) \mid Z])^\top\Big] \\ &= I_{d_a}. \end{split}$$

This verifies that  $q_0 = (P\xi_{0,1}, \dots, \xi_{0,d_a})$  satisfies Equation (39), which concludes the proof.

The proof above shows the conclusion of Proposition 2 indirectly through Proposition 1. Below we provide an alternative proof that verifies the conclusion directly.

According to the first order condition for Equation (40), function  $\xi_{0,i}(X) = \theta_{0,i}^{\top} X_a + g_{0,i}(X_b)$  is the optimal solution to Equation (40) if and only if

$$\mathbb{E}\left[\mathbb{E}\left[\theta_{0,i}^{\top}X_a + g_{0,i}(X_b) \mid Z\right]X_a^{\top}\right] = \ell_i,$$

$$\mathbb{E}\left[\mathbb{E}\left[\theta_{0,i}^{\top}X_a + g_{0,i}(X_b) \mid Z\right] \mid X_b\right] = 0,$$

where  $\ell_i \in \mathbb{R}^{d_a}$  is a vector whose ith element is 1 and all other elements are 0.

If we let  $\Theta_0$  be a  $d_a \times d_a$  matrix whose *i*th row is  $\theta_{0,i}^{\top}$ , then we have

$$\mathbb{E}\left[\left(\Theta_0 \mathbb{E}[X_a \mid Z] + \mathbb{E}[g_0(X_b) \mid Z]\right) X_a^{\top}\right] = I_{d_a \times d_a},$$

$$\mathbb{E}[\mathbb{E}[\Theta_0 X_a + g_0(X_b) \mid Z] \mid X_b] = \mathbf{0}_{d_a}.$$

Let's consider solutions in the column space of  $\Theta_0$ , namely, consider  $g_0(X_b) = \Theta_0 g'_0(X_b)$ . Then we have

$$\Theta_0 \mathbb{E} \Big[ \mathbb{E} \big[ X_a - g_0'(X_b) \mid Z \big] X_a^{\top} \Big] = I_{d_a \times d_a}.$$

This in turn implies that

$$\Theta_0 \mathbb{E} \Big[ \mathbb{E} \big[ X_a - g_0'(X_b) \mid Z \big] \big( \mathbb{E} \big[ X_a - g_0'(X_b) \mid Z \big] \big)^\top \Big] \\
= \Theta_0 \mathbb{E} \Big[ \mathbb{E} \big[ X_a - g_0'(X_b) \mid Z \big] \big( X_a - g_0'(X_b) \big)^\top \Big] \\
= \Theta_0 \mathbb{E} \Big[ \mathbb{E} \big[ X_a - g_0'(X_b) \mid Z \big] X_a^\top \Big] = I_{d_a \times d_a},$$

where the second equality follows from the fact that  $\Theta_0 \mathbb{E}[\mathbb{E}[X_a - g_0'(X_b) \mid Z] \mid X_b] = \mathbf{0}_{d_a}$ .

This means that  $\Theta_0$  and  $\mathbb{E}\left[\mathbb{E}[X_a - g_0'(X_b) \mid Z](\mathbb{E}[X_a - g_0'(X_b) \mid Z])^\top\right]$  have to be invertible, and

$$\Theta_0 = \left\{ \mathbb{E} \Big[ \mathbb{E} \big[ X_a - g_0'(X_b) \mid Z \big] \big( \mathbb{E} \big[ X_a - g_0'(X_b) \mid Z \big] \big)^\top \Big] \right\}^{-1}.$$

Moreover,

$$\mathbf{0}_{d_a} = \mathbb{E}[\mathbb{E}[\Theta_0 X_a + g_0(X_b) \mid Z] \mid X_b] = \Theta_0 \mathbb{E}\left[\mathbb{E}\left[X_a - g_0'(X_b) \mid Z\right] \mid X_b\right] \implies \mathbb{E}\left[\mathbb{E}\left[X_a - g_0'(X_b) \mid Z\right] \mid X_b\right] = \mathbf{0}_{d_a}.$$

In other words,

$$\mathbb{E}\Big[\mathbb{E}\Big[X_a^{(i)} - g'_{0,i}(X_b) \mid Z\Big]\rho(X_b)\Big] = 0, \quad \forall \rho \in \mathcal{L}_2(X_b).$$

This is exactly the first order condition for the minimization problem in Equation (41). These show that the solutions to Equation (41) correspond to solutions to Equation (40) with full rank coefficient matrix  $\Theta_0$ .

Proof of Proposition 3. Let some arbitrary  $h \in \mathcal{H}_{OB}$  be given. In addition, define  $\xi(v, x, a) = h(v, x, a) - \theta^{\star \top} a$ . Now, for any given action a, we have

$$\begin{split} \mathbb{E}[\theta^{\star\top}A + \xi(V,X,0) \mid U,X,A = a] &= \theta^{\star\top}a + \mathbb{E}[\xi(V,X,0) \mid U,X,A = a] \\ &= \theta^{\star\top}a + \mathbb{E}[\xi(V,X,0) \mid U,X,A = 0] \\ &= \theta^{\star\top}a + \mathbb{E}[\xi(V,X,A) \mid U,X,A = 0] \\ &= \theta^{\star\top}a + \mathbb{E}[h(V,X,A) - \theta^{\star\top}A \mid U,X,A = 0] \\ &= \theta^{\star\top}a + \mathbb{E}[Y - \theta^{\star\top}A \mid U,X,A = 0] \,. \end{split}$$

where in the second equality we apply the fact that  $V \perp A \mid U, X$ . Next, by assumption, we have  $\mathbb{E}[Y(a) \mid U, X] = \theta^{\star \top} a + \phi^{\star}(U, X)$ , for each a. Furthermore, since  $Y(a) \perp A \mid U, X$  for each a, we have

$$\mathbb{E}[Y \mid U, X, A = a] = \mathbb{E}[Y(a) \mid U, X, A = a]$$

$$= \mathbb{E}[Y(a) \mid U, X]$$

$$= \theta^{\star \top} a + \phi^{\star}(U, X)$$

$$= \mathbb{E}[\theta^{\star \top} A + \phi^{\star}(U, X) \mid U, X, A = a].$$

Therefore, we can further derive

$$\theta^{\star\top} a + \mathbb{E}[Y - \theta^{\star\top} A \mid U, X, A = 0] = \theta^{\star\top} a + \mathbb{E}[\phi^{\star}(U, X) \mid U, X, A = 0]$$
$$= \theta^{\star\top} a + \mathbb{E}[\phi^{\star}(U, X) \mid U, X, A = a]$$
$$= \mathbb{E}[\theta^{\star\top} A + \phi^{\star}(U, X) \mid U, X, A = a]$$
$$= \mathbb{E}[Y \mid U, X, A = a],$$

where in the second equality we again apply the fact that  $V \perp A \mid U, X$ , and in the final equality we again apply the fact that  $Y = \theta^{\star \top} A + \phi^{\star}(U, X)$ . Therefore, putting the above together, we have

$$\mathbb{E}[Y - \theta^{\star \top} A - \xi(V, X, 0) \mid U, X, A = a] = 0 \quad \forall a,$$

so  $\theta^{\star \top} A + \xi(V, X, 0) \in \tilde{\mathcal{H}}_{OB}$ , which proves the first part of the proposition.

For the second part of the proposition, let  $q_0 = (q_{0,1}, \dots, q_{0,d_A})^{\top}$  be defined as in the proposition statement, and let  $\tilde{q}(U, X, A) = \mathbb{E}[q_0(Z, X, A) \mid U, X, A]$ . Then, we have

$$\begin{split} \mathbb{E}[\tilde{q}(U,X,A) \mid V,X,A] &= \mathbb{E}[\mathbb{E}[q_0(Z,X,A) \mid U,X,A] \mid V,X,A] \\ &= \mathbb{E}[\mathbb{E}[q_0(Z,X,A) \mid U,V,X,A] \mid V,X,A] \\ &= \mathbb{E}[q_0(Z,X,A) \mid V,X,A] \,, \end{split}$$

where the second equality follows by the proximal causal inference condition independence assumption  $V \perp \!\!\! \perp Z \mid U, X$ .

Now, suppose that  $h_1(V, A, X) = \theta_1^{\top} A + g_1(V, X)$  and  $h_2(V, A, X) = \theta_2^{\top} A + g_2(V, X)$  are both bridge functions. We know that

$$\mathbb{E}[(\theta_1 - \theta_2)^{\top} A + (g_1 - g_2)(V, A) \mid U, A, X] = 0,$$

and therefore by the prior equation we have

$$0 = \mathbb{E}\Big[\tilde{q}(U, X, A)\Big((\theta_1 - \theta_2)(m(X))^{\top}\phi(A, X) + (g_1 - g_2)(V, X)\Big)\Big]$$
  
=  $\mathbb{E}\Big[q_0(Z, X, A)\Big((\theta_1 - \theta_2)(m(X))^{\top}\phi(A, X) + (g_1 - g_2)(V, X)\Big)\Big]$   
=  $\theta_1 - \theta_2$ .

That is, we have  $\theta_1 = \theta_2$ . Since this applies for any arbitrary partially linear bridge functions, and we know that  $\theta^{\star \top} A + \xi(V, X, 0) \in \tilde{\mathcal{H}}_{OB}$ , it follows that the partially linear parameters  $\theta^{\star}$  are unique.

# H Proofs for Results in Appendices

## H.1 Proofs for Appendix A

Proof for Proposition 4. The optimization problem in Equation (52) can be equivalently written as

$$\min_{\xi \in \mathcal{H}} \mathbb{E} \Big[ (q_0(T) - [P\xi](T))^2 \Big].$$

A function  $\xi_0$  solves the optimization problem above if and only if

$$0 = \mathbb{E}[(q_0(T) - [P\xi_0](T))[P\xi](T)] = \mathbb{E}[(q_0(T) - [P\xi_0](T))g_1(W)\xi(S)], \quad \forall \xi \in \mathcal{H}.$$

According to the definition of  $q_0$  in Equation (49), we have  $\mathbb{E}[g_1(W)q_0(T)\xi(S)] = \mathbb{E}[\alpha(S)\xi(S)]$  for any  $\xi \in \mathcal{H}$ . So any solution  $\xi_0$  can be equivalently characterized by

$$\mathbb{E}[[P\xi_0](T)g_1(W)\xi(S)] = \mathbb{E}[\alpha(S)\xi(S)].$$

This exactly means that

$$[P^*\xi_0](S) = \alpha(S),$$

namely,  $\xi_0 \in \Xi_0$  defined in Assumption 1.

Proof for Proposition 5. Since  $\nu^*$  solves Equation (53), by the first order condition, we have

$$\mathbb{E}[[P\nu^{\star}](T)[Ph](T)] - (1 - \mathbb{E}[m(W;\nu^{\star})])\mathbb{E}[m(W;h)] = 0, \quad \forall h \in \mathcal{H}.$$

It follows that

$$\begin{split} V^{\star} &= \mathbb{E}[[P\nu^{\star}](T)[P\nu^{\star}](T)] + (1 - \mathbb{E}[m(W;\nu^{\star})])^{2} \\ &= (1 - \mathbb{E}[m(W;\nu^{\star})])\mathbb{E}[m(W;\nu^{\star})] + (1 - \mathbb{E}[m(W;\nu^{\star})])^{2} \\ &= 1 - \mathbb{E}[m(W;\nu^{\star})], \end{split}$$

where the second equality uses the first order condition with  $h = \nu^*$ . Dividing the left hand and right hand sides of the first order condition by  $V^*$ , we have

$$\mathbb{E}[[P\xi^{\star}](T)[Ph](T)] = \mathbb{E}[m(W;h)], \quad \forall h \in \mathcal{H}.$$

This implies that

$$\mathbb{E}[h(S)[P^{\star}P\xi^{\star}](S)] = \mathbb{E}[h(S)\alpha(S)], \quad \forall h \in \mathcal{H}.$$

It follows that  $\alpha = P^{\star}P\xi^{\star}$ . The expression for  $\varphi(W; h^{\star}, \nu^{\star})$  follows immediately from  $V^{\star} = 1 - \mathbb{E}[m(W; \nu^{\star})]$  and the definition of  $\xi^{\star}$ .

## H.2 Proofs for Appendix B

Proof for Theorem 12. Equation (54) holds for  $\xi_0 \in \text{int}(\mathcal{H})$  if and only if the first order condition holds: for any  $\xi \in \mathcal{H}$ ,

$$\frac{\partial}{\partial t} \frac{1}{2} \mathbb{E} \Big[ ([P(\xi_0 + t(\xi - \xi_0))](T))^2 \Big] - \mathbb{E} [m(W; \xi_0 + t(\xi - \xi_0))]|_{t=0}$$

$$= \mathbb{E} [[P\xi_0](T)[P(\xi - \xi_0)](T)] - \mathbb{E} [\alpha(S)(\xi - \xi_0)(S)] = 0,$$

or equivalently,

$$\mathbb{E}[[P\xi_0](T)g_1(W)(\xi(S) - \xi_0(S))] = \mathbb{E}[\alpha(S)(\xi(S) - \xi_0(S))]. \tag{58}$$

We can take  $\xi = h \in \mathcal{H}$  and  $\xi = \alpha \in \mathcal{H}$  in Equation (58). This leads to

$$\mathbb{E}[(g_1(W)[P\xi_0](T) - \alpha(S))(h(S) - \xi_0(S))] = 0$$

$$\mathbb{E}[(g_1(W)[P\xi_0](T) - \alpha(S))(\alpha(S) - \xi_0(S))] = 0.$$

Taking a difference of the two equations above gives

$$\mathbb{E}[(g_1(W)[P\xi_0](T) - \alpha(S))(h(S) - \alpha(S))] = 0, \quad \forall h \in \mathcal{H}.$$

$$(59)$$

This proves the conclusion in Equation (55).

*Proof for Lemma 5.* We first prove Equation (56). Note that Equation (58) implies for any  $\xi \in \mathcal{H}$ ,

$$\mathbb{E}[q_0(T)g_1(W)(\xi(S) - \xi_0(S))] = \mathbb{E}[\alpha(S)(\xi(S) - \xi_0(S))], \text{ where } q_0 = P\xi_0.$$

In particular, the above holds for  $\xi = h \in \mathcal{H}$  and  $\xi = h_0 \in \mathcal{H}_0 \subseteq \mathcal{H}$  respectively:

$$\mathbb{E}[q_0(T)g_1(W)(h(S) - \xi_0(S))] = \mathbb{E}[\alpha(S)(h(S) - \xi_0(S))],$$
  
$$\mathbb{E}[q_0(T)g_1(W)(h_0(S) - \xi_0(S))] = \mathbb{E}[\alpha(S)(h_0(S) - \xi_0(S))].$$

Taking a difference of the two equations above gives

$$\mathbb{E}[q_0(T)g_1(W)(h(S) - h_0(S))] = \mathbb{E}[\alpha(S)(h(S) - h_0(S))], \quad \forall h \in \mathcal{H}.$$
(60)

Then for any  $h \in \mathcal{L}_2(S)$ ,  $q \in \mathcal{L}_2(T)$ ,  $h_0 \in \mathcal{H}_0$  and  $q_0 = P\xi_0$  where  $\xi_0$  is an interior solution to Equation (54), we have

$$\mathbb{E}[\psi(W; h, q)] - \theta^* = \mathbb{E}[\psi(W; h, q)] - \mathbb{E}[\psi(W; h_0, q_0)]$$

$$= \mathbb{E}[m(W; h - h_0)] + \mathbb{E}[q(T)(g_2(W) - g_1(W)h(S))]$$

$$= \mathbb{E}[\alpha(S)(h(S) - h_0(S))] + \mathbb{E}[q(T)(\mathbb{E}[g_2(W) \mid T] - g_1(W)h(S))]$$

$$= \mathbb{E}[g_1(W)q_0(T)(h(S) - h_0(S))] + \mathbb{E}[g_1(W)q(T)(h_0(S) - h(S))]$$

$$= \mathbb{E}[g_1(W)(q(T) - q_0(T))(h(S) - h_0(S))].$$

Here the fourth equality follows from Equation (60) and the definition of  $\mathcal{H}_0$ . The rest of the proof can follow from the proof for Theorem 3.

WE next prove Equation (57). Note that

$$\frac{\partial}{\partial t} \mathbb{E}[\psi(W; h_0 + t(h - h_0), q_0)]\Big|_{t=0} = \mathbb{E}[\alpha(S)(h(S) - h_0(S))] - \mathbb{E}[g_1(W)q_0(T)(h(S) - h_0(S))].$$

This is equal to 0 according to Equation (60).

Moreover,

$$\frac{\partial}{\partial t} \mathbb{E}[\psi(W; h_0, q_0 + t(q - q_0))]\big|_{t=0} = \mathbb{E}[(q(T) - q_0(T))(g_2(W) - g_1(S)h_0(S))].$$

This is equal to 0 for any  $q \in \mathcal{L}_2(T)$  because  $\mathbb{E}[g_2(W) - g_1(S)h_0(S) \mid T] = 0$ .