Nested Nonparametric
Instrumental Variable Regression:
Long Term, Mediated, and Time Varying Treatment Effects

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Abstract

Several causal parameters in short panel data models are scalar summaries of a function called a nested nonparametric instrumental variable regression (nested NPIV). Examples include long term, mediated, and time varying treatment effects identified using proxy variables. However, it appears that no prior estimators or guarantees for nested NPIV exist, preventing flexible estimation and inference for these causal parameters. A major challenge is compounding ill posedness due to the nested inverse problems. We analyze adversarial estimators of nested NPIV, and provide sufficient conditions for efficient inference on the causal parameter. Our nonasymptotic analysis has three salient features: (i) introducing techniques that limit how ill posedness compounds; (ii) accommodating neural networks, random forests, and reproducing kernel Hilbert spaces; and (iii) extending to causal functions, e.g. long term heterogeneous treatment effects. We measure long term heterogeneous treatment effects of Project STAR and mediated proximal treatment effects of the Job Corps.

Keywords: heterogeneous treatment effect, ill posed inverse problem, proxy variable, semiparametric efficiency, short panel data

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1 Introduction

Long term, mediated, and time varying treatment effects are causal parameters defined in short panel data models. In the presence of unobserved confounding, e.g. latent ability, several recent works have proposed nonparametric identification strategies for these causal parameters using auxiliary variables called proxies that satisfy relevance and exclusion conditions. Across settings, each causal parameter $\theta_0$ turns out to be a scalar summary of a nested nonparametric instrumental variable regression (NPIV) function $h_0$.

A nested NPIV function $h_0$ is a solution to an inverse problem of the form $\mathbb{E}\{h(B)|C\} = \mathbb{E}\{g_0(A)|C\}$, where $g_0$ is itself an NPIV function that solves an inverse problem. For example, $g_0$ is a solution to $\mathbb{E}\{g(A)|C'\} = \mathbb{E}(Y|C')$.\(^1\) It appears that no consistency results for the nested NPIV function $h_0$ are known, preventing semiparametric estimation and inference of the causal parameter $\theta_0$. Analysis of the nested NPIV $h_0$ is more challenging than that of the NPIV $g_0$ because ill posedness of the nested inverse problems may compound, in potentially complex ways.

We study nested NPIV as a new challenge for causal inference. Our research question is how (and when) it is possible to flexibly estimate causal parameters in short panel data models using proxy variables, where nested NPIV arises. An answer requires original estimators and guarantees for this class of estimands. Our main contribution is a theory of nested NPIV that prevents ill posedness from compounding in complex ways, and that is optimistic for causal inference.

We provide a suite of increasingly strong results under increasingly strong assumptions. Our weakest results only require a permissive assumption: the function space $\mathcal{H}$ used in estimation is not too complex, satisfying a critical radius condition that is standard in the adversarial estimation literature and that is satisfied by “simple” neural networks, random forests, and reproducing kernel Hilbert spaces. Our moderately strong

\(^1\)In general, $C \not\subset C'$ and $C' \not\subset C$, departing from the literature on sequential moment restrictions [Chamberlain, 1992, Brown and Newey, 1998, Ai and Chen, 2012].
results further require that the nested NPIV function \( h_0 \) is smooth, satisfying a source condition that is standard in the NPIV literature. Our strongest results additionally require what appears to be a new condition: the nested inverse problems have a well behaved relative measure of ill posedness, which we formalize in Section 3.

**Contributions.** First, we propose and analyze what appear to be the earliest estimators for nested NPIV. Since nested NPIV reduces to NPIV when \( g_0(A) = Y \), we modify known NPIV estimators in a couple ways: (i) a sequential approach replaces \( Y \) with an initial NPIV estimator \( \hat{g}(A) \) to estimate \( \hat{h}(B) \); (ii) a simultaneous approach jointly estimates \( \hat{g}(A) \) and \( \hat{h}(B) \). For sequential estimators, we prove projected mean square rates under a critical radius condition, which we strengthen to mean square rates under a further source condition. For simultaneous estimators, we prove faster projected mean square rates and faster mean square rates under the additional assumption that the nested inverse problems are well posed in a relative sense. The NPIV nuisance \( \hat{g}(A) \) demands new techniques to limit how the ill posedness of \( g_0 \) and \( h_0 \) may interact.

Second, we translate our analysis of nested NPIV into new guarantees for causal inference. Following the principles of targeted and debiased machine learning, we combine \((\hat{h}, \hat{g})\) and their dual analogues into an estimator \( \hat{\theta} \). We show \( \hat{\theta} \) is consistent, asymptotically normal, and semiparametrically efficient with multiple robustness to ill posedness: it tolerates moderate ill posedness of multiple inverse problems, as long as other inverse problems are mildly ill posed. Formally, we prove nonasymptotic Gaussian approximation of \( n^{1/2}\sigma^{-1}(\hat{\theta} - \theta_0) \) under product conditions. Each product condition combines a projected mean square rate with a mean square rate. Our results apply to a broad class of bilinear functionals and corresponding causal functions, including several for which machine learning estimation and inference were not previously known; see Section 2.

Third, we use our estimators to uncover new insights in economic data. We replicate and extend the program evaluation of Project STAR, which randomly assigned

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2By contrast, naive product conditions that combine two mean square rates pay a higher cost of ill posedness.
kindergarten students to small or large class sizes. We document significant heterogeneity in the long term effects of enrollment in a small class, with the strongest long term effects for students at the bottom of their kindergarten class. Empirical evidence of this phenomenon is only possible due to our new theoretical results for long term heterogeneous treatment effects. We also replicate and extend the program evaluation of the US Job Corps, which randomly assigned eligibility for job training. A previous, parametric approach finds a zero or imprecise change in arrests directly due to job training. Using our machine learning nested NPIV approach, we find a small and precise decrease in arrests directly due to job training. These empirical results suggest that our estimator’s flexibility is useful in real data.

Structure. Section 2 situates our contributions within the context of related work. Section 3 shows how several causal parameters are functionals of a nested NPIV function, and formalizes our key assumptions. Section 4 proposes our procedure and demonstrates its performance in simulations. Section 5 theoretically justifies our procedure, and demonstrates how our key assumptions deliver multiple robustness to ill posedness. Section 6 presents real world applications: long term heterogeneous treatment effects of Project STAR, and the direct proximal treatment effect of the US Job Corps. Section 7 concludes. This paper was previously circulated under a different title [Singh, 2021].

2 Related work

Proxy identification in short panel data. This paper is motivated by recent identification results for long term [Imbens et al., 2022, Ghassami et al., 2022a], mediated [Dukes et al., 2023], and time varying [Ying et al., 2023] treatment effects with proxy variables. Prior works in this literature define the nested NPIV, but do not provide an estimator or rate of convergence, in any norm. More generally, we continue the agenda of proxy estimation in short panel data settings [Deaner, 2018, Imbens et al., 2021]. The nested NPIV does not arise in [Deaner, 2018], where Markov restrictions truncate

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This direct effect is the component of the total effect that is not mediated by employment.
dependence. It does not arise in [Imbens et al., 2021], which assumes a linear factor model. Reference therein describe many earlier identifications of long term, mediated, and time varying treatment effects, as well as earlier proxy identification in cross sectional data [Miao et al., 2018, Deaner, 2018].

**Nonparametric instrumental variable regression.** We extend the techniques and assumptions of classical NPIV [Newey and Powell, 2003, Ai and Chen, 2003, Hall and Horowitz, 2005, Blundell et al., 2007, Darolles et al., 2011, Chen and Reiss, 2011, Chen and Pouzo, 2012, Santos, 2012, Severini and Tripathi, 2012] to nested NPIV. We employ Tikhonov regularization while conducting estimation in machine learning function spaces that satisfy a critical radius condition. See e.g. [Darolles et al., 2011, Hall and Horowitz, 2005, Horowitz and Lee, 2005, Carrasco et al., 2007, Chen and Pouzo, 2012, Gagliardini and Scaillet, 2012, Singh et al., 2019], and references therein, for NPIV estimators that employ various types of Tikhonov regularization over various function spaces. In this literature, the source condition controls the bias from Tikhonov regularization in order to provide rates of convergence in projected mean square error and mean square error.

**Adversarial estimation in econometrics.** We directly build on adversarial approaches to NPIV and causal estimation in cross sectional data. For NPIV, several works prove projected mean square error [Dikkala et al., 2020] and mean square error [Liao et al., 2020, Bennett et al., 2023a, Bennett et al., 2023b, Bennett et al., 2023c] rates under critical radius and source conditions.\(^4\) By contrast, we prove such rates for nested NPIV. For causal parameters in cross sectional data, several works prove Gaussian approximation, either under exogeneity [Hirshberg and Wager, 2021, Chernozhukov et al., 2020] or with proxy variables [Kallus et al., 2021, Ghassami et al., 2022b]. By contrast, we prove Gaussian approximation for causal parameters in panel data, under exogeneity or with proxies. [Kaji et al., 2023] propose a parametric adversarial approach to structural estimation. Future work may extend our results to structural estimands.

**Semiparametric inference with machine learning.** We prove new nonasympt-
totic results for bilinear functionals of nested NPIV. In particular, our multiple robust-
ness to ill posedness generalizes the double robustness to ill posedness known for linear
functionals of NPIV [Chernozhukov et al., 2023] such as proximal treatment effects in
cross sectional data [Kallus et al., 2021, Ghassami et al., 2022b]. Multiple robustness
to ill posedness has not been characterized in previous work on generic nonlinear
functionals of machine learning nuisance estimators [Zheng and Van der Laan, 2011,
Chernozhukov et al., 2018, Chernozhukov et al., 2022a].

We provide new nonasymptotic results for causal functions in panel data, e.g. long
term heterogeneous treatment effects. Previous nonasymptotic inference results focus on
cross sectional causal functions [Chernozhukov et al., 2022b, Chernozhukov et al., 2023,
Agarwal and Singh, 2021].

Setting aside proxies and causal functions, we provide some modest contributions
even in the basic set up of exogeneity and causal scalars. Our initial draft [Singh, 2021]
included new debiased machine learning theory for the long term treatment effect
of [Athey et al., 2019], using the efficient score of [Chen and Ritzwoller, 2021]. A
subsequent draft [Chen and Ritzwoller, 2022] provides asymptotic debiased machine
learning theory for the special case of exogeneity and causal scalars. Our results
strengthen and unify asymptotic debiased machine learning results for mediation analy-
sis [Farbmacher et al., 2022] and time varying treatment effects [Bodory et al., 2022].

3 Model overview

Concrete examples. For readability, we maintain two running examples throughout
the main text before implementing them on real data: (i) long term heterogeneous
treatment effects under exogeneity [Athey et al., 2019]; and (ii) the direct effect identi-
fied with proxy variables [Dukes et al., 2023]. Appendix D considers a general class of
non- and semiparametric estimands. The class includes long term, mediated, and time
varying causal functions and parameters, with or without proxies.

In (i), the goal is to combine data from a short term experimental group ($G = 0$)
and a long term observational group \((G = 1)\) to evaluate the long term effects of an intervention. In the experimental group, the economist sees baseline covariates \((V, X)\), the binary treatment \(D\), and a short term surrogate outcome \(M\), but not the long term outcome \(Y\) because experiments are expensive. In the observational group, the economist sees \((V, X, M, Y)\) but not the treatment \(D\) because there was no experiment. Let \(Y^{(d)}\) be the potential outcome under intervention \(D = d\). We study heterogeneity of long term effects, with respect to an interpretable subcovariate \(V \in \mathbb{R}\), as the causal function \(\text{LONG}(v) = \mathbb{E}\{Y^{(d)}|V = v\}\).

Concretely, we may wish to extrapolate long term effects of kindergarten class size \(D\) on middle school test scores \(Y\). The experimental group \(G = 0\) are students in Project STAR, for whom we see elementary school test scores \(M\) rather than middle school test scores \(Y\). The observational group \(G = 1\) are students in New York City public schools, for whom we see elementary and middle school test scores but not kindergarten class size. We ask whether there are significantly different long term effects of kindergarten class size for students who had different levels of aptitude \(V\) while entering kindergarten.

**Example 1** (Long term heterogeneous treatment effects). Let \(h_0(V, X, M, G) = \mathbb{E}(Y|V, X, M, G)\) be the outcome mechanism, and let \(P(M|V, X, D, G)\) be the surrogate mechanism. Under the exogeneity assumptions of [Athey et al., 2019], the long term heterogeneous treatment effects are \(\text{LONG}(v) = \lim_{\nu \to 0} \mathbb{E}\{\int \ell_{\nu}(V) h_0(V, X, m, 1) d(m|V, X, d, 0)\}\).

Here, \(\ell_{\nu}(V)\) is a local weighting around the value \(v\) with bandwidth \(\nu\), i.e. \(\ell_{\nu}(V) = \omega^{-1} K\{(V - v)/\nu\}\) where \(\omega = \mathbb{E}[K\{(V - v)/\nu\}]\) is its normalization.\(^5\)

In (ii), the goal is to discern how much of the total effect of the treatment \(D\) on the outcome \(Y\) is direct, as opposed to being mediated by the mechanism \(M\). The economist sees baseline covariates \(X\) but is concerned about unobserved confounding \(U\). The economist therefore uses auxiliary variables called proxies \((Z, W)\) satisfying certain exclusion and relevance conditions: \(Z\) does not directly cause \((M, Y)\), \(W\) is not directly caused by \((D, M)\), and \((Z, W)\) are relevant to \(U\). Let \(M^{(d)}\) be the potential

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\(^5\)Formally, \(K\) is a bounded and symmetric kernel that integrates to one.
mediator and \( Y^{(d,m)} \) be the potential outcome. We study the pure direct effect as the scalar \( \text{DIRECT} = E[Y^{(1,M(0))}] \).\(^6\)

Concretely, we may wish to measure the direct effect of US Job Corps job training \( D \) on subsequent arrests \( Y \) that is not mediated by employment \( M \). Unobserved motivation \( U \) may confound employment and arrests. Researchers have used the time spent with a Job Corps recruiter as an auxiliary variable \( Z \) that reflects motivation yet does not directly cause employment or arrests. Researchers have used pre-training expectations as an auxiliary variable \( W \) that reflects motivation yet cannot be caused by training or employment. We replicate and extend this empirical strategy, relaxing previous parametric assumptions.

**Example 2** (Direct effect with proxies). Let \( h_0 \) be an outcome confounding bridge that solves the inverse problem \( E\{h(X, D, W)|X, Z, D = 0\} = E\{g_0(X, 1, M, W)|X, Z, D = 0\} \), where \( g_0 \) solves the inverse problem \( E\{g(X, D, M, W)|X, Z, D = 1, M\} = E\{Y|X, Z, D = 1, M\} \). Under the proxy variable assumptions of [Dukes et al., 2023], the direct effect is \( \text{DIRECT} = E\{\int h_0(X, 0, w) dP(w|X)\} \).

**A new, recurring problem: Nested NPIV.** Clearly, the outcome confounding bridge \( h_0 \) in Example 2 is a nested NPIV that solves \( E\{h(B)|C\} = E\{g_0(A)|C\} \), where \( g_0 \) is an NPIV. So is the outcome mechanism in Example 1 taking \( g_0(A) = Y \) and \( B = C \). More generally, the nested NPIV problem includes NPIV and regression as special cases. The nested NPIV is a solution to an inverse problem that involves another inverse problem, and it has been previously defined in identification theory. We provide what appears to be the first nonparametric estimation theory for nested NPIV in its full definition.

Examples 1 and 2 are bilinear functionals with a common structure. In particular, they are of the form \( \theta_0 = E[\int m(B, h_0) dQ(b_2|B_{(1)})] \), where \( h \mapsto m(B, h) \) is linear, \( B = \{B_{(1)}, B_{(2)}\} \) is a partition, and \( Q \) is a conditional distribution.\(^7\) They are bilinear in

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\( ^6 \)This definition follows [Robins and Greenland, 1992]. See e.g. [Richardson and Robins, 2013] for alternatives.

\( ^7 \)Temporarily, we ignore the limit in Example 2.
the sense that they involve two linear operations before taking the final expectation: $h \mapsto m(B, h)$, then $Q \mapsto \int m(B, h) dQ\{b(2)|B(1)\}$. As such, $h \mapsto \mathbb{E}[\int m(B, h) dQ\{b(2)|B(1)\}]$ and $Q \mapsto \mathbb{E}[\int m(B, h) dQ\{b(2)|B(1)\}]$ are linear. Bilinear functionals are a structured subset of nonlinear functionals, and they include long term, mediated, and time varying treatment effects. Therefore we study bilinear functionals of nested NPIV as well as their limits.

**Permissive assumption: Critical radius.** For our weakest results, we only assume that our estimator $\hat{h}$ is not too complex in a familiar sense. We define the critical radius of a generic function space $\mathcal{F}$ abstractly, then instantiate it in different ways for our proposed estimators. For simplicity, we impose that $\mathcal{F}$ contains functions $f : \mathcal{E} \to \mathbb{R}$ that are uniformly and absolutely bounded by one.\(^\text{8}\)

Denote the localized Rademacher complexity $R_n(\mathcal{F}, \delta) = 2^{-n}\sum_{\epsilon \in \{-1, 1\}}^n \mathbb{E}\{\sup_{f \in \mathcal{F}} \|f\| \leq \delta \frac{1}{n} \sum_{i=1}^n \epsilon_i f(E_i)\}$. Denote the star hull of $\mathcal{F}$ by $\text{STAR}(\mathcal{F})\(^\text{9}\)$. The critical radius $\delta_n$ is the smallest possible solution to the inequality $R_n\{\text{STAR}(\mathcal{F}), \delta\} \leq \delta^2$, and it may be thought of as a sequence indexed by $n$.

**Assumption 1 (Critical radius condition).** $\delta_n = \tilde{O}(n^{-\alpha})$ for some $\alpha \in (0, 1/2]\(^\text{10}\). \hfill 9$

We use the critical radius condition to quantify the complexity of our nested NPIV estimator $\hat{h}$. Analytically, we use it to bound the variance from ridge regularization. See e.g. \cite{Wainwright2019} for an equivalent entropy integral condition. See \cite{Chernozhukov2020} for a detailed comparison to the Donsker condition. See e.g. \cite{Foster2023} for the critical radii of simple neural networks, random forests, and reproducing kernel Hilbert spaces, demonstrating that the condition is quite permissive.

**Key assumption: Source condition.** For mean square error results, we assume that the nested NPIV $h_0$ is smooth in a familiar sense. We define the source condition abstractly, then interpret it. Denote the conditional expectation operator $T : h \mapsto \mathbb{E}\{h(B)|C = \cdot\}$.\(^\text{8}\)This can be relaxed to functions that have some finite bound by a rescaling argument.\(^\text{9}\)Formally, $\text{STAR}(\mathcal{F}) = \{ cf : f \in \mathcal{F}, c \in [0, 1]\}$.\(^\text{10}\)The notation $\tilde{O}(\cdot)$ means $O(\cdot)$ up to logarithmic factors. For parametric classes, $\alpha = 1/2$.\hfill 9
Assumption 2 (Source condition). \( h_0 = (T^*T)^{\beta/2}w_0 \) for some \( w_0 \in \mathcal{H}, \beta \in (0, \infty) \)\(^{11}\)

To interpret Assumption 2, suppose \( T \) admits singular value decomposition \( (\sigma_j, u_j, v_j) \), so that \( Th = \sum_{j=1}^{\infty} \sigma_j \langle h, v_j \rangle_{L^2} u_j \). We impose \( h_0 \in \mathcal{H}^\beta = \{ h \in L_2 : \sum_{j=1}^{\infty} 1_{\sigma_j \neq 0} \cdot \sigma_j^{-2\beta} \langle h, v_j \rangle_{L^2}^2 < \infty \} \). Clearly, \( \mathcal{H}^0 = L_2 \) when each \( \sigma_j \neq 0 \). For \( \beta > 0 \), \( \mathcal{H}^\beta \) is a subset of \( \mathcal{H}^0 \). Due to the singular value penalty \( \sigma_j^{-2\beta} \), it consists of functions that are less aligned with the higher order right singular functions \( (v_j) \). Intuitively, it rules out “rough” functions primarily supported on the tail of the spectrum of \( T \).

We use the source condition to quantify the ill posedness of the inverse problem that defines the nested NPIV \( h_0 \). Analytically, we use it to bound the bias from ridge regularization. See e.g. [Chen and Reiss, 2011] and [Singh, 2020] for comparisons of source conditions employed in the NPIV and proxy variable literatures, respectively.

In particular, define the well posedness \( \text{well}(\beta) = \frac{\min(\beta,1)}{\min(\beta,1)+1} \in (0, 1/2] \). We find that the rate \( \|\hat{h} - h_0\|_2^2 \) depends on \( \text{well}(\beta) \) and an initial rate \( \|\hat{g} - g_0\|_2^2 \). As such, the ill posedness compounds as a product of \( \text{well}(\beta_h) \) and \( \text{well}(\beta_g) \), where \( (\beta_h, \beta_g) \) are source conditions.

**New assumption: Relative ill posedness.** For faster rates of convergence, we place what appears to be a new assumption: the \( g_0 \) inverse problem is relatively well posed compared to the \( h_0 \) inverse problem. Denote the singular values of the conditional expectation operator \( S : g \mapsto E\{g(A)|C' = \cdot \} \) by \( (\sigma'_j) \).

**Assumption 3** (Relative well posedness). \( \sup_j \frac{\sigma_j}{\sigma'_j + \mu'} = O(1) \) for all \( \mu' > 0 \).

We interpret \( \tau_{\mu'}(S,T) = \frac{\sigma_j}{\sigma'_j + \mu'} \) as the relative measure of ill posedness for the conditional expectation operators \( S \) and \( T \), up to a tolerance \( \mu' \). Assumption 3 imposes that the singular values of \( S \), aided by \( \mu' > 0 \), are not too small relative to the singular values of \( T \). If \( \sigma_j \) and \( \sigma'_j \) are of the same order with respect to \( j \), then Assumption 3 trivially holds.

As we will see in Section 5, Assumption 3 improves convergence rates by limiting how the ill posedness of \( g_0 \) transfers to ill posedness of \( h_0 \). We arrive at a somewhat

\(^{11}\)Here, \( T^* \) is the adjoint of \( T \).
surprising result: under this auxiliary condition, the final rate for $h_0$ depends on the minimum of $\text{WELL}(\beta_h)$ and $\text{WELL}(\beta_g)$ rather than their product, which is a dramatic improvement.

Assumption 3 is not necessary for our sequential estimation results. It can be relaxed for our simultaneous estimation results as well, at the cost of slower rates.

4 A nested NPIV estimator for causal inference

We would like a procedure that estimates parameters in nonlinear, heterogeneous causal models using short panel data and possibly proxy variables. We would like this procedure to prevent the ill posedness of the nested inverse problems from compounding too much. Moreover, we would like this procedure to tolerate a moderate level of ill posedness among some inverse problems as long as other inverse problems are sufficiently well posed. If such a procedure were to exist, it would make recent nonparametric identification results fully usable for economists: it would become possible to estimate the long term heterogeneous effects of Project STAR, and to estimate the direct proximal effect of the US Job Corps, while allowing for general nonlinearity and heterogeneity.

Why is inference challenging for functionals of nested NPIV? First, a prior nested NPIV estimator does not appear to exist. We extend known NPIV estimators [Dikkala et al., 2020, Bennett et al., 2023c] to sequential and simultaneous nested NPIV estimators. Second, the rates of convergence for nested NPIV estimators $\hat{h}$ may be much slower than $n^{-1/2}$, yet we wish to obtain a standard error of order $\hat{\sigma}n^{-1/2}$ for the causal estimator $\hat{\theta}$. We use the multiple robust estimating equation and characterize sufficient conditions that involve products of rates [Chernozhukov et al., 2018, Van der Laan and Rose, 2018, Rotnitzky et al., 2021]. The third issue is a theoretical one to which we return in Section 5: it is unclear whether these rate conditions can ever be satisfied, since the ill posedness of $\hat{g}$ compounds into further ill posedness of $\hat{h}$. We ameliorate the issue in two ways: (i) improving rates via a relative well posedness condition; (ii) sharpening the sufficient conditions to involve products of projected
mean square rates and mean square rates [Kallus et al., 2021, Ghassami et al., 2022b, Chernozhukov et al., 2023]. We then verify that our sufficient conditions are satisfied under moderate ill posedness of some inverse problems.

**Overview of the procedure.** Split the observations into equally sized train and test sets, each with \( m = n/2 \) observations. Our procedure consists of two steps, which we state at a high level before filling in the details: (i) nested NPIV: \( \hat{h} \) using train; (ii) causal parameter: \( \hat{\theta} \pm 1.96\hat{\sigma}n^{-1/2} \) using test. The former step is a direct extension of known NPIV procedures. The latter is the well known debiased machine learning meta procedure. Our contribution is to prove, in Section 5, that this combination of familiar ingredients has strong, previously unknown guarantees that can handle moderate ill posedness.

**Step 1: Nested NPIV.** The nested NPIV procedure \( \hat{h} \) is adversarial: it is the best response in a zero sum game against an adversary \( \hat{f} \) that aims to violate the conditional moment.

The inverse problem that defines \( h_0 \) may be viewed as the conditional moment restriction \( \mathbb{E}\{h_0(B) - g_0(A)|C\} = 0 \), which implies a continuum of unconditional moment restrictions \( \mathbb{E}[\{h_0(B) - g_0(A)\} f(C)] = 0 \) for all \( f \in \mathbb{L}_2 \). Let \( \text{LOSS}(f, g, h) = \mathbb{E}_m[\{h(B) - g(A)\} f(C)] \) be the empirical analogue over train. We use the notation \( \mathbb{E}_m(Y) = \frac{1}{m} \sum_{i \in \text{train}} Y_i \).

**Estimator 1** (Sequential nested NPIV). Given observations \((A_i, B_i, C_i)\) in train, an initial estimator \( \hat{g} \) which may be estimated in train, and hyperparameter values \((\lambda, \mu)\),

\[
\hat{h} = \arg\min_{h \in \mathcal{H}} \left[ \sup_{f \in \mathcal{F}} \{2 \cdot \text{LOSS}(f, \hat{g}, \hat{h}) - \text{PENALTY}(f, \lambda)\} + \text{PENALTY}(h, \mu) \right]
\]

where \( \text{PENALTY}(f, \lambda) = \mathbb{E}_m\{f(C)^2\} + \lambda \cdot \|f\|^2_F \) and \( \text{PENALTY}(h, \mu) = \mu \cdot \|h\|^2_H \).

**Estimator 2** (Sequential nested NPIV: Ridge). Given observations \((A_i, B_i, C_i)\) in train, an initial estimator \( \hat{g} \) which may be estimated in train, and a hyperparameter \( \mu \),

\[
\hat{h} = \arg\min_{h \in \mathcal{H}} \left[ \sup_{f \in \mathcal{F}} \{2 \cdot \text{LOSS}(f, \hat{g}, \hat{h}) - \text{PENALTY}(f)\} + \text{PENALTY}(h, \mu) \right]
\]
where \( \text{penalty}(f) = \mathbb{E}_m\{f(C)^2\} \) and \( \text{penalty}(h, \mu) = \mu \cdot \mathbb{E}_m\{h(B)^2\} \).

A virtue of the sequential Estimators 1 and 2 is their agnosticism about the initial estimator \( \hat{g} \), which may be a previous NPIV, \( Y \), or something else. As such, analysis of \( \hat{h} \) will imply analysis of every nuisance that arises in the multiple robust estimation of \( \hat{\theta} \).

Another virtue is that Estimators 1 and 2 allow \( \hat{g} \) to be estimated on the same observations as \( \hat{h} \), preventing further sample splitting and thereby increasing the effective sample size. Previous work that allows for machine learning estimation of nuisances in mediation analysis \cite{Farbmacher2022} and time varying treatment effects \cite{Bodory2022} is not only limited to the exogenous setting, but also requires further sample splitting for \( \hat{g} \) and \( \hat{h} \), which reduces the effective sample size.

Estimator 1 allows for complex regularization, e.g. \( \ell_1 \) norm regularization in sparse linear function spaces, and reproducing kernel Hilbert space (RKHS) norm regularization in RKHSs. Under Assumption 1, we will prove projected mean square error rates. Our analysis of Estimator 1 avoids Assumption 2 and accommodates more regularization types.

Estimator 2 imposes ridge regularization. Under Assumptions 1 and 2, we will prove projected mean square error rates and mean square error rates.

Estimators 1 and 2 are sequential; next, we introduce an estimator that is simultaneous. As before, the inverse problem that defines \( g_0 \) may be viewed as a continuum of unconditional moment restrictions \( \mathbb{E}[\{g_0(A) - Y\}f'(C')] = 0 \) for all \( f' \in \mathbb{L}_2 \). Let \( \text{LOSS}(f', Y, g) = \mathbb{E}_m[\{g(A) - Y\}f'(C')] \) be the empirical analogue over \textsc{train}.

**Estimator 3** (Simultaneous nested NPIV). Given observations \((A_i, B_i, C_i, C'_i)\) in \textsc{train}\footnote{It could also be a previous nested NPIV. Future work may study functionals of higher order nesting of NPIV.}...
and hyperparameter values \((\mu',\mu)\), estimate 

\[
(g, \hat{h}) = \arg\min_{g \in \mathcal{G}, h \in \mathcal{H}} \left[ \sup_{f' \in \mathcal{F}} \{2 \cdot \text{LOSS}(f', Y, g) - \text{PENALTY}(f')\} + \text{PENALTY}(g, \mu') 
+ \sup_{f \in \mathcal{F}} \{2 \cdot \text{LOSS}(f, g, h) - \text{PENALTY}(f)\} + \text{PENALTY}(h, \mu) \right]
\]

using analogous PENALTY notation to Estimator 2.

Estimator 3 imposes ridge regularization. Under Assumptions 1, 2, and 3, we will prove projected mean square rates and mean square rates that are better than those of Estimators 1 and 2. Using relative well posedness, we strictly limit how ill posedness may compound.

**Step 2: Causal estimation and inference.** The second step uses \(\hat{h}\) learned from train, and evaluates it on test according to the multiple robust estimating equation.

For bilinear functionals of nested NPIV, four nuisances appear in the multiple robust estimating equation, which we denote by \((h_1, h_2, h_3, h_4)\). Each nuisance can be expressed as a nested NPIV with some arguments set to counterfactual values; see concrete examples below. Let the argument of \(h_j\) be \(B_j\) for simplicity.

**Estimator 4** (Causal parameter). Given nested NPIV estimators \((\hat{h}_1, \hat{h}_2, \hat{h}_3, \hat{h}_4)\) estimated in train, calculate the empirical influence of observation \(i \in \text{test}\) as

\[
\hat{\psi}_i = \hat{h}_1(B_1i) + \hat{h}_3(B_3i)\{Y_i - \hat{h}_2(B_2i)\} + \hat{h}_4(B_4i)\{\hat{h}_2(B_2i) - \hat{h}_1(B_1i)\}.
\]

This process generates a vector \(\hat{\psi} \in \mathbb{R}^m\). Reversing the roles of train and test, we generate another such vector. Slightly abusing notation, we concatenate the two to obtain a vector \(\hat{\psi} \in \mathbb{R}^n\). We estimate \(\hat{\theta} = \text{MEAN}(\hat{\psi})\), its variance as \(\hat{\sigma}^2 = \text{VAR}(\hat{\psi})\), and its confidence interval as \(\text{CI} = \hat{\theta} \pm 1.96\hat{\sigma}n^{-1/2}\). For causal functions, replace \(\hat{\psi}_i\) with \(\ell_{\nu}\hat{\psi}_i\).

A virtue of Estimator 4 is its simple parametrization in terms of \((h_1, h_2, h_3, h_4)\), each of which can be estimated using Estimators 1, 2, or 3. This parametrization is

\(^{13}\)If \(\mathbb{E}\{h_0(B)|C\} = \mathbb{E}\{g_0(A)|C\}\) and \(\mathbb{E}\{g_0(A)|C'\} = \mathbb{E}(Y|C')\), then \((B_1, B_2, B_3, B_4) = (B, A, C', C)\).
bilinear in the nuisances, facilitating nonasymptotic analysis. We will prove validity of
the confidence interval CI under product rate conditions involving \((\hat{h}_1, \hat{h}_2, \hat{h}_3, \hat{h}_4)\). We will then use our general theory for \(\hat{h}\) to verify these rate conditions while allowing for moderate ill posedness in some of the inverse problems that define \((h_1, h_2, h_3, h_4)\).

**Concrete examples.** We return to our running examples to illustrate \((h_1, h_2, h_3, h_4)\).

**Example 1** (Long term heterogeneous treatment effects). Recall that \(h_0(V, X, M, G) = \mathbb{E}(Y|V, X, M, G)\) is the outcome mechanism and \(P(M|V, X, D, G)\) is the surrogate mechanism. Then \(h_1(V, X) = \int h_0(V, X, m, 1)dP(m|V, X, d, 0)\), \(h_2(V, X, M) = h_0(V, X, M, 1)\), \(h_3(V, X, M, G) = \frac{1}{P(G=1|V, X, M)}\frac{P(d|V, X, M, G=0)P(G=0|V, X, M)}{P(d|V, X, G=0)P(G=0|V, X)}\), and finally \(h_4(V, X, D, G) = \frac{1}{P(d|V, X, G=0)P(G=0|V, X)}\). The nuisances \((h_3, h_4)\) involve the treatment and selection mechanisms. To localize, replace \(\hat{\psi}_i\) with \(\ell_{\nu}(V_i)\hat{\psi}_i\).

**Example 2** (Direct effect with proxies). Recall that \(h_0\) is an outcome confounding bridge that solves \(\mathbb{E}\{h(X, D, W)|X, Z, D = 0\} = \mathbb{E}\{g_0(X, 1, M, W)|X, Z, D = 0\}\), where \(g_0\) solves \(\mathbb{E}\{g(X, D, M, W)|X, Z, D = 1, M\} = \mathbb{E}(Y|X, Z, D = 1, M)\). Now let \(h'_0\) be a treatment confounding bridge that solves \(\mathbb{E}\{h'(X, Z, D, M)|X, D = 1, M, W\} = \mathbb{E}\{g_0'(X, Z, 0)|X, D = 1, M, W\}\), where \(g_0'\) solves \(\mathbb{E}\{g'(X, Z, D)|X, D = 0, W\} = \mathbb{E}\{\frac{1}{P(D=0|X, W)}|X, D = 0, W\}\). Then \(h_1(X, W) = h_0(X, 0, W)\), \(h_2(X, M, W) = g_0(X, 1, M, W)\), \(h_3(Z, X, M, W) = 1_{D=1}h_0'(X, Z, 1, M)\), and \(h_4(X, Z, D) = 1_{D=0}g_0'(X, Z, 0)\).

See Appendix [D] for more examples from the literature, as well as a general method to derive \((h_1, h_2, h_3, h_4)\) in terms of \((h_0, g_0)\) and their dual analogues \((h'_0, g'_0)\). The general derivation follows from the identification of \(\theta_0\) as a bilinear functional.

**Robust performance in simulations using machine learning.** Before demonstrating that our procedure works in theory, we demonstrate that it works in practice via extensive Monte Carlo simulations. We evaluate Estimator [I] by itself, as well as the coverage of the confidence intervals calculated by combining Estimators [I] and [II].

\[\text{Since } \int h_0(V, X, m, 1)dP(m|V, X, d, 0) = \mathbb{E}\{h_0(V, X, M, 1)|V, X, D = d, G = 0\}, h_1 \text{ may be viewed as a nested NPIV that has been partially evaluated.}\]
To begin, we demonstrate robust performance of Estimator 1 across several nonlinear data generating processes (DGPs) for nested NPIV. For simplicity, we focus on the exactly identified setting; \( p = \text{dim}(A) = \text{dim}(B) = \text{dim}(C) = \text{dim}(C') = 10 \). We fix the initial NPIV \( g_0 \) as a cubic function, and let \( h_0 \) be one of four different nonlinear functions, inspired by [Dikkala et al., 2020]. Each sample has \( n = 2000 \) observations.

For each of these four variations of the DGP, we implement three versions of our estimator: a simple RKHS, neural network, or random forest estimator with \( \mathcal{F} = \mathcal{G} = \mathcal{H} \). As benchmarks, we also implement nested 2SLS, with and without regularization.

Table 1 summarizes results of nested NPIV simulations. Each row corresponds to a different nonlinear function \( h_0 \). Each column corresponds to a different estimator: the two benchmarks, followed by three of our estimators. We report the empirical mean square error, averaged across 100 samples.

Table 1 shows that 2SLS performs poorly in all nonlinear DGPs, while regularized 2SLS performs poorly in some of them. Our proposals typically outperform the benchmarks, sometimes in dramatic fashion, despite the nested ill posedness.

Next, we demonstrate robust performance of Estimators 1 and 4 across several nonlinear DGPs for the direct effect with proxies, i.e. Example 2. We modify the simulation design of [Dukes et al., 2023], introducing the same four nonlinearities studied in Table 1. All variables are scalars except \( X \in \mathbb{R}^2 \); see Appendix 1 for details. As before, each sample has \( n = 2000 \) observations. We implement three versions of our

| DGP            | 2SLS  | reg. 2SLS | RKHS  | neural net | random forest |
|----------------|-------|-----------|-------|------------|---------------|
| linear         | 69084.320 | 0.367     | 0.370 | 0.017      | 0.007         |
| piecewise linear | 819340.283 | 0.176     | 0.134 | 0.016      | 0.006         |
| sigmoid        | 222252.265 | 0.066     | 0.148 | 0.017      | 0.006         |
| cubic          | 9222.205  | 63.726    | 0.550 | 0.059      | 0.025         |

Table 1: Nested NPIV simulations across DGPs
estimator as well as two benchmarks.

| metric     | Benchmarks         | Our proposals       |
|------------|--------------------|---------------------|
|            | 2SLS    | reg. 2SLS | RKHS     | neural net | random forest |
| bias       | 0.008   | 0.529     | 0.005    | -0.071     | -0.118        |
| variance   | 29.444  | 79.751    | 28.776   | 31.794     | 25.526        |
| coverage   | 0.950   | 0.210     | 0.940    | 0.880      | 0.800         |
| length     | 0.476   | 0.783     | 0.471    | 0.495      | 0.443         |

Table 2: Coverage simulations: Linear DGP

| metric     | Benchmarks         | Our proposals       |
|------------|--------------------|---------------------|
|            | 2SLS    | reg. 2SLS | RKHS     | neural net | random forest |
| bias       | -0.0137 | 0.540     | -0.023   | -0.038     | -0.136        |
| variance   | 35.321  | 84.980    | 28.818   | 28.204     | 25.085        |
| coverage   | 0.930   | 0.250     | 0.900    | 0.900      | 0.760         |
| length     | 0.521   | 0.808     | 0.472    | 0.466      | 0.439         |

Table 3: Coverage simulations: Piecewise linear DGP

Tables 2, 3, 4, and 5 summarize results of coverage experiments. Each table corresponds to a different nonlinear function \( h_0 \). Each column corresponds to a different estimator: the two benchmarks, followed by three of our estimators. Each row corresponds to a different performance metric: bias of the point estimate, variance of the point estimate, coverage of the confidence interval, and width of the confidence interval, each reported as an average across 100 samples.

The coverage tables show that 2SLS obtains nominal coverage while regularized 2SLS does not. Our estimators often obtain nominal coverage, with the exact variation of the procedure that works well depending on the nonlinearity in the DGP. When both 2SLS and our proposals obtain nominal coverage, our confidence intervals are consistently shorter, demonstrating the gain due to our flexible approach.
### Benchmarks

| metric       | 2SLS | reg. 2SLS | RKHS | neural net | random forest |
|--------------|------|-----------|------|------------|---------------|
| bias         | -0.010 | 0.532    | -0.018 | 0.025     | -0.140        |
| variance     | 34.342 | 83.645   | 28.238 | 25.578    | 25.0344       |
| coverage     | 0.930  | 0.250    | 0.910  | 0.910     | 0.750         |
| length       | 0.514  | 0.802    | 0.466  | 0.443     | 0.439         |

**Table 4:** Coverage simulations: Sigmoid DGP

| metric       | 2SLS | reg. 2SLS | RKHS | neural net | random forest |
|--------------|------|-----------|------|------------|---------------|
| bias         | 13.977 | 0.620    | -0.067 | -1.071    | -0.029        |
| variance     | $3.23 \times 10^9$ | 115.195 | 50.005 | 1011.402 | 27.700        |
| coverage     | 0.940 | 0.270    | 0.910  | 0.560     | 0.930         |
| length       | 18319.470 | 0.921   | 0.619  | 2.586     | 0.461         |

**Table 5:** Coverage simulations: Cubic DGP

In summary, Estimators 1 and 4 work well across nonlinear DGPs. Moreover, several variations of these estimators work well across machine learning function spaces. They repeatedly outperform nested 2SLS in nonlinear, heterogeneous causal models using short panel data and proxy variables.

## 5 Finite sample analysis

In Section 4, we described challenges to inference on functionals on nested NPIV. First, a prior nested NPIV estimator does not appear to exist. We extend known NPIV estimators in a straightforward way, yet we still need to prove rates of convergence for the new \( \hat{h} \) estimators in projected mean square error and mean square error. Second, the rates of convergence for \( \hat{h} \) are slower than \( n^{-1/2} \). We incorporate the multiple robust
estimating equation in the hope of achieving product rate conditions, yet we still need to derive such conditions. Third, the ill posedness of \( \hat{g} \) compounds into further ill posedness of \( \hat{h} \), throttling convergence rates and raising the question of whether the product rate conditions ever be satisfied.

In this section, we prove the answer is yes, and characterize multiple robustness to ill posedness: some inverse problems may be moderately ill posed, as long as others are sufficiently well posed. We prove four nonasymptotic theorems to arrive at this conclusion:

1. Estimator 1: \( \hat{h} \) converges to \( h_0 \) in projected mean square error under Assumption 1;
2. Estimator 2: \( \hat{h} \) converges to \( h_0 \) in mean square error under Assumptions 1 and 2;
3. Estimator 3: \( \hat{h} \) converges to \( h_0 \) in mean square error with better rates under Assumptions 1, 2, and 3;
4. Estimator 4: \( P \{ \theta_0 \in (\hat{\theta} \pm 1.96\hat{\sigma}n^{-1/2}) \} \to 0.95 \) under product rate conditions.

In a corollary, we verify multiple robustness to ill posedness by combining these new results.

### 5.1 Sequential nested NPIV

We formalize our operator notation as follows. Let \( T(h, g) = E\{h(B) - g(A)|C = \cdot\} \), with \( T_h(h) = T(h, 0) \) and \( T_g(g) = T(0, g) \). We abbreviate \( T_h(h) = T(h) \) as in earlier sections. Since \( h_0 \) may be non-unique, we hereafter take \( h_0 \) to be the minimal \( L_2 \) norm solution to \( T(h, g_0) = 0 \). To simplify our results, we assume correct specification of \( T \).

**Assumption 4** (Closedness). \( T(h - h_0, g - g_0) \in \mathcal{F} \) for all \( h \in \mathcal{H} \) and \( g \in \mathcal{G} \).

This condition can be relaxed, incurring an additive approximation error; see our earlier draft. Since \( m = n/2 \), rates in terms of \( m \) may be equivalently stated in terms of \( n \).
Theorem 1 (Rate for Estimator 1). Suppose Assumption 1 holds for $F$, $G$, and $H \times F$; and Assumption 4 holds. Further assume $h_0 \in H$ and $\|T(h - h_0)\|_2^2 \leq \text{LIP}\|h - h_0\|_H^2$ for some Lipschitz constant $\text{LIP} < \infty$. Then with probability $1 - \zeta$, when $\mu \geq \lambda \cdot \text{LIP}$ and $\delta_n = \Omega[\log \log(n) + \log(1/\zeta)]^{1/2} n^{-1/2}$, we have $\|T(\hat{h} - h_0)\|_2^2 = O(R_n)$, where $R_n = \mu \|h_0\|_H^2 + \delta_n^2 + \|\hat{g} - g_0\|_2^2$.

Theorem 1 appears to be the first projected mean square rate for nested NPIV. It does not require a source condition, and it allows for generic regularization. It exactly generalizes known results for NPIV when $\hat{g}(A) = Y$ [Dikkala et al., 2020]. The rate $R_n$ has three terms: bias $\mu \|h_0\|_H^2$, variance $\delta_n^2$, and initial estimation error $\|\hat{g} - g_0\|_2^2$. This third term arises in the nested NPIV problem, and it is new. Only the ill posedness of $\hat{g}$ appears in Theorem 1, because the definition of projected mean square error sidesteps the ill posedness of $\hat{h}$.

Corollary 1 (Rate for Estimator 1). Suppose the conditions of Theorem 1 hold. Set $\mu = O(\delta_n^2)$. Then with probability $1 - \zeta$, $\|T(\hat{h} - h_0)\|_2^2 = O(\delta_n^2 + \|\hat{g} - g_0\|_2^2)$.

Future work may strengthen Theorem 1 and Corollary 1 to mean square rates by placing further approximation assumptions, e.g. a restricted eigenvalue condition [Gautier and Rose, 2011] [Gautier and Tsybakov, 2018].

Theorem 2 (Rate for Estimator 2). Suppose Assumption 1 holds for $F$, $G$, $H$, and $H \times F$; Assumption 2 holds; and Assumption 4 holds. Then with probability $1 - \zeta$, when $\mu = O(1)$ and $\delta_n = \Omega[\log \log(n) + \log(1/\zeta)]^{1/2} n^{-1/2}$, we have $\|T(\hat{h} - h_0)\|_2^2 = O(R_n)$ and $\|\hat{h} - h_0\|_2^2 = O(\mu^{-1} R_n)$, where $R_n = \mu \|w_0\|_2^2 + \delta_n^2 + \|\hat{g} - g_0\|_2^2$. The former conclusion, $\|T(\hat{h} - h_0)\|_2^2 = O(R_n)$, also holds relaxing Assumption 1 for $H \times F$.

Theorem 2 appears to be the first mean square rate for nested NPIV. It exactly generalizes known results for NPIV, recovering state of the art rates in mean square error [Liao et al., 2020] [Bennett et al., 2023b] [Bennett et al., 2023c] and projected mean square error [Dikkala et al., 2020] when $\hat{g}(A) = Y$. It is stronger than state of the art projected mean square results for NPIV since it relaxes Assumption 1 from $H \times F$ to
\(H\), which is of independent interest. The rate \(R_n\) again contains bias \(\mu^{\min(\beta+1.2)} \|w_0\|_2\), variance \(\delta^2_n\), and initial estimation error \(\|\hat{g} - g_0\|_2^2\).

Theorem 2 cleanly separates the ill posedness of \(\hat{g}\) from \(\hat{h}\). The ill posedness of \(\hat{g}\) appears via \(\|\hat{g} - g_0\|_2^2\), which is additively separable from the other terms in \(R_n\). The projected mean square rate \(R_n\) is not affected by the ill posedness of \(\hat{h}\), because its definition sidesteps ill posedness. However, the rate for mean square error is slower than the rate for projected mean square error by a factor of \(\mu^{-1}\), encoding the ill posedness of \(\hat{h}\).

The rates may be optimized by choosing \(\mu\) to balance the bias term with the other terms. To lighten notation, let \(\text{WELL}(\beta) = \min(\beta, 1)+1\) be a measure of well posedness.

\(\text{Corollary 2 (Rate for Estimator 2)}\). Suppose the conditions of Theorem 2 hold.

Take \(\mu = \max(\delta_n, \|\hat{g} - g_0\|_2)\)\(^{\min(\beta, 1)+1}\). Then with probability \(1 - \zeta\), \(\|T(\hat{h} - h_0)\|_2^2 = O\{\max(\delta^2_n, \|\hat{g} - g_0\|_2^2)\}\) and \(\|\hat{h} - h_0\|_2^2 = O\{\max(\delta^2_n, \|\hat{g} - g_0\|_2^2)^{\text{WELL}(\beta)}\}\).

\(\text{Corollary 3 (Compounding ill posedness)}\). Suppose the conditions of Theorem 2 hold for \((\hat{g}, \hat{h})\). Write the larger critical radius as \(\bar{\delta}_n\), the source conditions as \(\bar{\beta} = (\beta_g', \beta_h)\), and the regularizations as \((\mu_g, \mu_h)\). Set \(\mu_g = \delta_n^{\min(\beta, 1)+1}\) and \(\mu_h = \delta_n^{\min(\beta, 1)+1}\)\(^{\text{WELL}(\beta_g')}\). Then with probability \(1 - \zeta\), \(\|T(\hat{h} - h_0)\|_2^2 = O\{\delta_n^{2\text{WELL}(\beta_g')}\}\) and \(\|\hat{h} - h_0\|_2^2 = O\{\delta_n^{2\text{WELL}(\beta_h)\text{WELL}(\beta_g')}\}\).

Corollary 3 demonstrates that ill posedness compounds in a simple way for Estimator 2: our mean square rate is a “base rate” slowed by the ill posedness of \(\hat{g}\) then by the ill posedness of \(\hat{h}\). We refer to \(\bar{\delta}^2_n\) as the “base rate”. It is \(\tilde{O}(n^{-1})\) for parametric classes, and it converges at well known, often optimal regression rates for many nonparametric classes. Our mean square rate for Estimator 2 is the base rate raised to \(\text{WELL}(\beta_g') \cdot \text{WELL}(\beta_h)\), where each expression quantifies the ill posedness of the corresponding inverse problem. At best, \(\beta_g', \beta_h \geq 1\) and the Estimator 2 rate approaches \(O(\delta_n^{3/2})\). Rates do not further improve for higher \(\bar{\beta}\), echoing the saturation effect of ridge regression [Bauer et al., 2007].
5.2 Simultaneous nested NPIV

A natural question is: can rates in Corollary 3 be improved? In particular, can the way that ill posedness compounds be partially ameliorated? We now demonstrate that the answer is yes for Estimator 3 under stronger assumptions.

We further formalize our operator notation. Let $S(g) = \mathbb{E}\{g(A)|C' = \cdot\}$. Since $(g_0, h_0)$ may be non-unique, we hereafter take $(g_0, h_0)$ to be the minimal $L_2$ norm solutions to $T(h, g) = 0$ and $S(g) = \mathbb{E}(Y|C' = \cdot)$. In this notation, we place analogous assumptions for $g_0$ to those previously placed for $h_0$.

**Assumption 5** (Source condition). $g_0 = (S^*S)^{\beta_g/2}w'_g$ for some $w'_g \in \mathcal{G}$, $\beta_g' \in (0, \infty)$; $g_0 = (T^*_gh)^{\beta_h/2}w_g$ for some $w_g \in \mathcal{G}$, $\beta_g \in (0, \infty)$.

**Assumption 6** (Closedness). $S(g - g_0) \in \mathcal{F}$ for all $g \in \mathcal{G}$.

Hereafter, we clarify $h_0 = (T^*_hT_h)^{\beta_h/2}w_h$ in Assumption 2. As before, the correct specification of $S$ can be relaxed.

**Theorem 3** (Rate for Estimator 3). Suppose Assumption 1 holds for $\mathcal{F}$, $\mathcal{G}$, $\mathcal{G} \times \mathcal{F}$, $\mathcal{H}$, and $\mathcal{H} \times \mathcal{F}$; Assumptions 2 and 5 hold; Assumption 3 holds; and Assumptions 4 and 6 hold. Then with probability $1 - \zeta$, when $\mu = \mu' = O(1)$ and $\delta_n = \Omega[\log\log(\log\log(n)) + \log(1/\zeta)]$, we have $\|S(\hat{g} - g_0^*)\| = O(R_n)$, $\|T(\hat{h} - h_0^*, \hat{g} - g_0)\|_2 = O(R_n)$, $\|\hat{g} - g_0^*\| = O(\mu^{-1}R_n)$, and $\|\hat{h} - h_0^*\|_2 = O(\mu^{-1}R_n)$, where

$$R_n = \mu^{\min(\beta_h + 1, 2)}\|w_h\|^2_2 + \mu^{\min(\beta_g' + 1, 2)}\|w'_g\|^2_2 + \mu^{\min(\beta_g + 1, 2)}\|w_g\|^2_2 + \delta^2_n.$$ 

Theorem 3 is a new result for the simultaneous nested NPIV. The rate $R_n$ contains several bias terms $\mu^{\min(\beta_h, 2)}\|w_h\|^2_2 + \mu^{\min(\beta_g', 2)}\|w_g'\|^2_2 + \mu^{\min(\beta_g, 2)}\|w_g\|^2_2$, a variance term $\delta^2_n$, and no initial estimation error.

Theorem 3 cleanly separates the ill posedness of $\hat{g}$ from $\hat{h}$ in a different way than Theorem 2. The ill posedness of $\hat{g}$ appears via additional bias terms, which are additively separable from the other terms in $R_n$. As before, the rate for mean square error is slower than the rate for projected mean square error by a factor of $\mu^{-1}$. The rates may be optimized by choosing $\mu$ to balance the bias terms with variance term.
Corollary 4 (Rate for Estimator 3). Suppose the conditions of Theorem 3 hold. Take
$\mu = \min\{\frac{1}{2}, \frac{1}{4}\}$, where $\beta = \min(\beta_h, \beta_g)$. Then with probability $1 - \zeta$, \[\|T(\hat{\theta} - \theta_0)\|_2^2 = O(\delta_n^2)\] and \[\|\hat{\theta} - \theta_0\|_2^2 = O\left(\frac{\delta_n^2}{n}\right)\].

Comparing Corollaries 3 and 4, we see how Assumption 3 improves rates by re-
stricting how ill posedness may compound. Whereas Corollary 3 gives \[\|\hat{\theta} - \theta_0\|_2^2 = O\left(\frac{\delta_n^2}{n}\right)\] well
\((\beta_h, \beta_g)\), Corollary 4 gives \[\|\hat{\theta} - \theta_0\|_2^2 = O\left(\frac{\delta_n^2}{n}\right)\] well
\((\beta_h \wedge \beta_g)\). The base rate $\delta_n^2$ is throttled less in the latter. By placing an assumption on the relative measure of ill posedness, we ensure that the ill posedness compounds in a much more benign way. Remarkably, it is the minimum rather than the product.

5.3 Causal estimation and inference

Equipped with rates for the nested NPIV $\hat{h}$, we turn to the causal estimator $\hat{\theta}$, whose
nuisance functions are nested NPIVs $(\hat{h}_1, \hat{h}_2, \hat{h}_3, \hat{h}_4)$. To state general results, we assume
the bilinear estimating equation is Neyman orthogonal.

Assumption 7 (Neyman orthogonality). For all $\tilde{h}_1 \in H_1$, $\mathbb{E}[\hat{h}_1(B_1)\{1 - h_4(B_4)\}] = 0$.
For all $\tilde{h}_2 \in H_2$, $\mathbb{E}[\hat{h}_2(B_2)\{h_4(B_4) - h_3(B_3)\}] = 0$. For all $\tilde{h}_3 \in H_3$, $\mathbb{E}[\hat{h}_3(B_3)\{Y - h_2(B_2)\}] = 0$. For all $\tilde{h}_4 \in H_4$, $\mathbb{E}[\hat{h}_4(B_4)\{h_2(B_2) - h_1(B_1)\}] = 0$.

Assumption 7 implies Neyman orthogonality in our bilinear setting. It is straight-
forward to verify Assumption 7 for all of the motivating examples, e.g. long term,
mediated, and time varying treatment effects with or without proxies; see our earlier
draft.

Finally, we place weak regularity conditions.

Assumption 8 (Regularity conditions). (i) The residual variances are bounded: $\mathbb{E}[\{Y - h_2(B_2)\}|B_2] \leq \sigma_y^2$ and $\mathbb{E}[\{h_2(B_2) - h_1(B_1)\}|B_1] \leq \sigma_2^2$. (ii) The balancing weights are bounded: $\|\hat{h}_3\|_\infty \leq \bar{h}_3$ and $\|h_4\|_\infty \leq \bar{h}_4$. (iii) The balancing weights are censored: $\|\hat{h}_3\|_\infty \leq \bar{h}_3'$ and $\|\hat{h}_4\|_\infty \leq \bar{h}_4'$.
Assumption 8(i) is quite weak. Assumption 8(ii) encodes a familiar necessary condition for regular estimation. In Example 1, it imposes that the treatment and selection propensity scores are bounded away from zero and one. Assumption 8(iii) can be achieved by censoring extreme values in a way that is asymptotically negligible.

To state unified results, we introduce some additional notation. Let \( \Phi \) be the standard Gaussian distribution function. Let \( c_{BE} = 0.4748 \) be the Berry-Esseen constant [Shevtsova, 2011]. Let \( \sigma^2, \kappa^3, \text{and } \chi^4 \) be the second, third, and fourth moments of the oracle

\[
h_1(B_1) + h_3(B_3)\{Y - h_2(B_2)\} + h_4(B_4)\{h_2(B_2) - h_1(B_1)\} - \theta_0.
\]

We pointwise approximate causal functions such as Example 1, taking the limit where the bandwidth \( \nu \) of the weighting \( \ell_{\nu} \) vanishes. Fix \( \nu \). Formally, we write \( \theta_0(v) = \lim_{\nu \to 0} \theta_{\nu}(v) \). For each \( \theta_{\nu}(v) \), we define the same quantities as for causal scalars, where now the oracle is

\[
\ell_{\nu}(V)[h_1(B_1) + h_3(B_3)\{Y - h_2(B_2)\} + h_4(B_4)\{h_2(B_2) - h_1(B_1)\}] - \theta_{\nu}(v).
\]

We write the pointwise approximation error as \( \Delta_{\nu}(v) = n^{1/2}\sigma^{-1}\|\theta_{\nu}(v) - \theta_0(v)\|_2 \).

**Theorem 4** (Finite sample Gaussian approximation for Estimator 4). Suppose Assumptions 7, 8(i), and 8(ii) hold. Then with probability \( 1 - \epsilon \),

\[
\sup_{z \in \mathbb{R}} P \left\{ \frac{n^{1/2}}{\sigma}(\hat{\theta} - \theta_0) \leq z \right\} - \Phi(z) \leq c_{BE} (\frac{\kappa}{\sigma})^3 n^{-1/2}\Delta + \frac{\Delta}{(2\pi)^{1/2}} + \epsilon,
\]

where

\[
\Delta = \frac{7L}{2\epsilon\sigma} \left\{ (1 + \bar{h}_4)\|\bar{h}_1 - h_1\|_2 + (\bar{h}_3 + \bar{h}_4)\|\bar{h}_2 - h_2\|_2 + \bar{\sigma}_y\|\bar{h}_3 - h_3\|_2 + \bar{\sigma}_2\|\bar{h}_4 - h_4\|_2
\]

\[
+ n^{1/2}\|\bar{h}_1 - h_1\|_2\|\bar{h}_4 - h_4\|_2 + n^{1/2}\|\bar{h}_2 - h_2\|_2\|\bar{h}_3 - h_3\|_2 + n^{1/2}\|\bar{h}_2 - h_2\|_2\|\bar{h}_4 - h_4\|_2 \right\}.
\]

\(^{15}\)Formally, when pointwise approximating causal functions, the quantities in Assumptions 8 as well as the oracle moments \( (\sigma^2, \kappa^2, \chi^4) \) are each indexed by \( (v, \nu) \). We suppress this indexing to lighten notation and to state unified results. See Appendix G for a more detailed statement.
If in addition Assumption \ref{assumption:8}(iii) holds, then the same holds updating $\Delta$ to be

$$\Delta = \frac{4L}{\epsilon^{1/2}\sigma} \left\{ (1 + \hat{h}_4 + \hat{h}_3')\|\hat{h}_1 - h_1\|_2 + (\hat{h}_3 + \hat{h}_4')\|\hat{h}_2 - h_2\|_2 + \bar{\sigma}_y\|\hat{h}_3 - h_3\|_2 + \sigma_2\|\hat{h}_4 - h_4\|_2 \right\}$$

$$+ \frac{1}{2L^{1/2}\sigma} \left\{ n^{1/2}\|T_1(\hat{h}_1 - h_1)\|_2\|\hat{h}_4 - h_4\|_2 \wedge n^{1/2}\|\hat{h}_1 - h_1\|_2\|T_4(\hat{h}_4 - h_4)\|_2 \right.$$ 

$$+ n^{1/2}\|T_2(\hat{h}_2 - h_2)\|_2\|\hat{h}_3 - h_3\|_2 \wedge n^{1/2}\|\hat{h}_2 - h_2\|_2\|T_3(\hat{h}_3 - h_3)\|_2 \right.$$ 

$$+ n^{1/2}\|T_2(\hat{h}_2 - h_2)\|_2\|\hat{h}_4 - h_4\|_2 \wedge n^{1/2}\|\hat{h}_2 - h_2\|_2\|T_4(\hat{h}_4 - h_4)\|_2 \right\}.$$

For causal functions, the same holds replacing $(\hat{\theta}, \theta_0, \Delta)$ with $\{\hat{\theta}_\nu(v), \theta_0(v), \Delta + \Delta_\nu(v)\}$.

**Theorem 5** (Finite sample variance estimation for Estimator \ref{estimator:4}). Suppose Assumptions \ref{assumption:8}(i) and (iii) hold. Then with probability $1 - \epsilon', |\hat{\sigma}^2 - \sigma^2| \leq \Delta' + 2(\Delta')^{1/2}\{(\Delta'')^{1/2} + \Delta''\}$, where $\Delta'' = \left(\frac{2}{\sigma}\right)^{1/2}\chi^2 n^{-1/2}$ and

$$\Delta' = 7(\hat{\theta} - \theta_0)^2 + \frac{84L}{\epsilon} \left[\|\hat{h}_1 - h_1\|_2^2 + \{(\hat{h}_3')^2 + (\hat{h}_4')^2\}\|\hat{h}_2 - h_2\|_2^2 + \{(\hat{h}_4')^2 + \bar{\sigma}_y^2\}\|\hat{h}_3 - h_3\|_2^2 + \sigma_2^2\|\hat{h}_4 - h_4\|_2^2\right].$$

**Corollary 5** (Confidence interval validity in Estimator \ref{estimator:4}). Suppose Assumptions \ref{assumption:7} and \ref{assumption:8} hold, as well as the moment regularity $\{(\kappa/\sigma)^3 + \chi^2\}n^{-1/2} \to 0$. Suppose the following quantities are $o_p(1)$: the individual rates $(1 + \hat{h}_4/\sigma + \hat{h}_4'/\sigma)\|\hat{h}_1 - h_1\|_2$, $(\hat{h}_3/\sigma + \hat{h}_3'/\sigma + \hat{h}_4/\sigma + \hat{h}_4'/\sigma)\|\hat{h}_2 - h_2\|_2$, $(\hat{h}_4' + \bar{\sigma}_y\|\hat{h}_3 - h_3\|_2, \sigma_2\|\hat{h}_4 - h_4\|_2$; and the product rates

1. $n^{1/2}\sigma^{-1}\left\{\|\hat{h}_1 - h_1\|_2\|\hat{h}_4 - h_4\|_2 \wedge \|T_1(\hat{h}_1 - h_1)\|_2\|\hat{h}_4 - h_4\|_2 \wedge \|\hat{h}_1 - h_1\|_2\|T_4(\hat{h}_4 - h_4)\|_2 \right\}$,

2. $n^{1/2}\sigma^{-1}\left\{\|\hat{h}_2 - h_2\|_2\|\hat{h}_3 - h_3\|_2 \wedge \|T_2(\hat{h}_2 - h_2)\|_2\|\hat{h}_3 - h_3\|_2 \wedge \|\hat{h}_2 - h_2\|_2\|T_3(\hat{h}_3 - h_3)\|_2 \right\}$,

3. $n^{1/2}\sigma^{-1}\left\{\|\hat{h}_2 - h_2\|_2\|\hat{h}_4 - h_4\|_2 \wedge \|T_2(\hat{h}_2 - h_2)\|_2\|\hat{h}_4 - h_4\|_2 \wedge \|\hat{h}_2 - h_2\|_2\|T_4(\hat{h}_4 - h_4)\|_2 \right\}$.

Then $\hat{\theta} \overset{p}{\to} \theta_0$, $\frac{\sqrt{n}}{\sigma}(\hat{\theta} - \theta_0) \overset{d}{\to} \mathcal{N}(0, 1)$, and $\mathbb{P}\{\theta_0 \in (\hat{\theta} \pm c_0 \hat{\sigma}_n^{-1/2})\} \to 1 - a$. For causal functions, if $\Delta_\nu(v) \to 0$ then the same holds replacing $(\hat{\theta}, \theta_0)$ with $\{\hat{\theta}_\nu(v), \theta_0(v)\}$.

Theorem \ref{estimator:4} appears to be the first nonasymptotic Gaussian approximation for long term, mediated, and time varying treatment effects. Similarly, Theorem \ref{estimator:5} appears to be the first nonasymptotic variance guarantee for this class of causal parameters. Whereas previous nonasymptotic results are limited to linear functionals of NPIV \cite{Chernozhukov2023}, our results handle bilinear functionals of nested NPIV.
The results hold with or without proxy variables, and apply to nonparametric causal functionss.

The asymptotic summary, Corollary 5, handles new cases compared to previous asymptotic results: the long term treatment effect, long term heterogeneous treatment effect (Example 1), direct proximal effect (Example 2), and many more; see Appendix D for a partial list. See Appendix C for a more explicit version of Corollary 5 for causal functions, including conditions on how the bandwidth $\nu$ vanishes.

The product rate conditions in Corollary 5 partly ameliorate how the ill posedness of the nested NPIV $h_0$ affects inference for the causal parameter $\theta_0$. Each rate condition multiplies a projected mean square rate with a mean square rate. As demonstrated above, the former sidesteps the ill posedness of $\hat{h}$, extending classic results for inference on functionals of NPIV [Blundell et al., 2007]. Unlike previous work, our results apply to functionals of nested NPIV, and they enable us to characterize a new multiple robustness to ill posedness.

5.4 Multiple robustness to ill posedness

We now combine our main results, demonstrating that our framework is optimistic for causal inference. Theorems 1, 2, and 3 prove rates of convergence for new nested NPIV estimators. Theorem 4 achieves product rate conditions for inference on the causal parameter in terms of nested NPIV rates. We combine these results to show how some inverse problems may be moderately ill posed, as long as others are sufficiently well posed. In other words, we characterize a new multiple robustness to ill posedness.

For all of the leading examples, $(h_1, h_3)$ are nested NPIVs while $(h_2, h_4)$ are NPIVs. To lighten notation, let $\tilde{\beta}_j = (\beta_{jg}, \beta_{jh})$ for the nested NPIVs. Recall $\text{well}(\beta) = \frac{\min(\beta_1^\prime)}{\min(\beta_1^\prime)+1}$.

**Corollary 6** (Multiple robustness to ill posedness). Suppose the conditions of Corollary 3 hold for $(\hat{h}_1, \hat{h}_2, \hat{h}_3, \hat{h}_4)$. Write the largest critical radius as $\bar{\delta}_n = \tilde{O}(n^{-\alpha})$, and the source conditions as $(\tilde{\beta}_1, \tilde{\beta}_2, \tilde{\beta}_3, \beta_4)$. Set the regularizations as in Corollary 3.
Suppose $\sigma \approx n^\gamma$. Then product rate condition of Corollary 5 are satisfied when (i) $\gamma + \alpha \{\text{WELL}(\beta_1) \text{WELL}(\beta_1) + 1\} > 1/2$; (ii) $\gamma + \alpha \{\text{WELL}(\beta_3) \text{WELL}(\beta_3) + 1\} > 1/2$; (iii) $\gamma + \alpha \{\text{WELL}(\beta_2) \lor \text{WELL}(\beta_4) + 1\} > 1/2$.

**Corollary 7** (Multiple robustness to ill posedness). Suppose the conditions of Corollary 4 hold for $(\hat{h}_1, \hat{h}_2, \hat{h}_3, \hat{h}_4)$. Write the largest critical radius as $\bar{\delta}_n = \tilde{O}(n^{-\alpha})$, and the source conditions as $(\bar{\beta}_1, \bar{\beta}_2, \bar{\beta}_3, \bar{\beta}_4)$. Set the regularizations as in Corollary 4.

Suppose $\sigma \approx n^\gamma$. Then product rate condition of Corollary 5 are satisfied when (i) $\gamma + \alpha \{\text{WELL}(\beta_1) \lor \text{WELL}(\beta_4) + 1\} > 1/2$; (ii) $\gamma + \alpha \{\text{WELL}(\beta_2) \lor \text{WELL}(\beta_3) + 1\} > 1/2$; (iii) $\gamma + \alpha \{\text{WELL}(\beta_2) \lor \text{WELL}(\beta_4) + 1\} > 1/2$.

We now interpret the simplified product rate conditions, and confirm that the set of values $(\alpha, \bar{\beta}, \gamma)$ satisfying these conditions is nonempty. For each condition, the right hand side is a constant. Therefore the stated condition is a joint requirement on the critical radius via $\alpha$, the source conditions via $\bar{\beta}$, and the asymptotic variance via $\gamma$.

The quantity $\alpha$ measures the complexity of the function classes. At best, $\alpha = 1/2$ for parametric function classes. For nonparametric classes, $\alpha < 1/2$.

Each quantity $\text{WELL}(\beta)$ measures the ill posedness of an inverse problem. At best, $\beta \geq 1$ and $\text{WELL}(\beta) = 1/2$. For severely ill posed inverse problems, $\beta \to 0$ and $\text{WELL}(\beta) \to 0$. Our conditions allow the well posedness of some inverse problem to compensate the ill posedness of others. Hence Corollaries 6 and 7 formalize multiple robustness to ill posedness.

For causal scalars, under mild regularity conditions, $\sigma \approx 1$ and hence $\gamma = 0$. For causal functions, under the regularity conditions given in Appendix G $\sigma_\nu(\nu) \approx \nu^{-1/2}$ and hence for bandwidth $\nu = n^{-1/5}$ we have $\gamma = 1/10$. Echoing the work of [Kennedy, 2023] and others on heterogeneous treatment effects, we derive product rate conditions that are weaker for causal functions than for causal scalars. Unlike [Kennedy, 2023], we study causal functions in short panel data e.g. long term heterogeneous treatment effects.

Finally, we demonstrate that the set of data generating processes is non-empty. For
simplicity, saturate each source condition with $\beta \geq 1$ and suppose we are studying causal scalars with $\gamma = 0$. Then the single sufficient condition is $\alpha > 2/5$ for Corollary 6 and $\alpha > 1/3$ for Corollary 7 which tolerates nonparametric function classes.

Corollaries 6 and 7 are the culmination of a few technical innovations, which are necessary to obtain optimistic results. First, we require sufficiently fast rates for nested NPIV in which the ill posedness does not compound too much. Second, we require product rate conditions that involve projected mean square rates and mean square rates to partly sidestep some ill posedness. Our fast rates and product rate conditions extend insights from NPIV to the new and harder problem of nested NPIV. In particular, the product rate conditions handle compounded ill posedness, which is new.

In light of the compounded ill posedness, it is not obvious that nested NPIV could ever culminate in causal inference at the rate $n^{-1/2}$. Corollaries 6 and 7 provide what appears to be the first end-to-end results that $n^{-1/2}$ causal inference is possible when a nuisance is a nested NPIV, which is often the case in short panel data models with proxy variables.

5.5 Concrete examples

We return to our running examples to illustrate our theoretical contributions, including multiple robustness to ill posedness.

Example 1 (Long term heterogeneous treatment effects). Recall that $h_0(V, X, M, G) = E(Y | V, X, M, G)$ is the outcome mechanism and $P(M | V, X, D, G)$ is the surrogate mechanism. Write the treatment mechanism as $\pi_0(D | X, G) = P(D | X, G)$ and $\rho_0(D | X, M, G) = P(D | X, M, G)$, and the selection mechanism as $\pi_0'(G | X) = P(G | X)$ and $\rho_0'(G | X, M) = P(G | X, M)$. Assumption 7 holds for the $(h_1, h_2, h_3, h_4)$ previously stated. Suppose the treatment and selection mechanisms as well as their estimators are bounded away from zero and one. Ignoring localization, Assumptions S(ii) and (iii) hold with $\bar{h}_3, \bar{h}_4, \bar{h}_3', \bar{h}_4' \leq 1$, and the rate conditions have interpretable upper bounds:

$$
\|\hat{h}_2 - h_2\|_2 \leq \|\hat{h} - h_0\|_2, \|\hat{h}_3 - h_3\|_2 \leq \|\hat{\pi} - \pi_0\|_2 + \|\hat{\rho}' - \pi_0'\|_2 + \|\hat{\rho}_0\|_2 + \|\hat{\rho}' - \rho_0\|_2,
$$

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and \(\|\hat{h}_4 - h_4\|_2 \lesssim \|\hat{\pi} - \pi_0\|_2 + \|\hat{\pi}' - \pi'_0\|_2\).

All of \((\hat{h}, \hat{\pi}, \hat{\pi}', \hat{\rho}, \hat{\rho}')\) are well posed nonparametric regressions with rates of order \(\delta_n\).

Since \(\hat{h}_1\) is a nested regression of \(\hat{h}\), a simplification of Corollary 2 for nested regression shows that its rate is also of order \(\delta_n\). We may then appeal to Corollary 5.

See Appendix G for localization details. We explicitly characterize how various local objects scale with the bandwidth and their local analogues, e.g. \(h_{1,\nu} \lesssim \nu^{-1}h_1\). In providing these details, we provide what appear to be the first machine learning inference results for long term heterogeneous treatment effects and other causal functions within our class.

**Example 2** (Direct effect with proxies). Recall that \(h_0\) is an outcome confounding bridge with initial NPIV \(g_0\) and \(h'_0\) is a treatment confounding bridge with intial NPIV \(g'_0\). Write the treatment mechanism as \(\pi_0(D|X,Z), \pi'_0(D|X,W), \pi''_0(X,Z,W), \rho_0(D|X,Z,M), \rho'_0(D|X,M,W)\), and \(\rho''_0(D|X,Z,M,W)\). Assumption 7 holds for the \((h_1, h_2, h_3, h_4)\) previously stated. Suppose the treatment mechanism and its estimators are bounded away from zero and one, and the outcome mechanism \((g_0, h_0)\) and its estimators are bounded above. Assumptions 8(ii) and (iii) hold with \(h_3, h_4, h'_3, h'_4 \lesssim 1\), and the rate conditions have interpretable upper bounds: \(\|\hat{h}_1 - h_1\|_2 \lesssim \|\hat{h} - h_0\|_2\), \(\|\hat{h}_2 - h_2\|_2 \lesssim \|\hat{g} - g_0\|_2\), \(\|\hat{h}_3 - h_3\|_2 \lesssim \|\hat{h}' - h'_0\|_2\), and \(\|\hat{h}_4 - h_4\|_2 \lesssim \|\hat{g}' - g'_0\|_2\). Likewise for projected rates.

We may then appeal to Corollaries 6 and 7 to demonstrate multiple robustness to ill posedness. Due to our main result, we provide what appear to be the first machine learning inference results for the direct effect with proxies and other functionals of nested NPIV. See Appendix D for more examples of new results relative to the literature.

6 Case studies: Project STAR and US Job Corps

**Long term heterogeneous treatment effects of Project STAR.** Equipped with theoretical guarantees, we now return to a motivating real world issue: how to flexibly
measure long term treatment effects by combining short term experimental data with
long term observational data, which we have studied as the running Example 1. We
replicate an influential program evaluation [Athey et al., 2020] that combines Project
STAR experimental data with NYC observational data to ask: what is the long term
average treatment effect of kindergarten class size on test scores later in life? We ask an
additional question: is there meaningful heterogeneity in those long term effects? Our
empirical results represent a realistic use case of our method. We document substantial
heterogeneity, with students at the bottom of their kindergarten classes benefiting the
most.

[Athey et al., 2020] propose a parametric method for long term average treatment
effects. The authors validate their results through an intuitive exercise, which we extend.
Though Project STAR data include kindergarten class size $D$, elementary school test
scores $M$, and middle school test scores $Y$, we suppose that the economist sees $(D, M)$
but not $Y$. The economist combines the short term experimental $(D, M)$ from Project
STAR with the long term observational $(M, Y)$ from NYC to estimate the long term
average treatment effect. These estimates may be validated by comparing them with
the “oracle” long term average treatment effect that an “oracle” who sees $(D, Y)$ in the
Project STAR data would obtain.

A similar exercise may be conducted in a closely related variation of the problem.
In this variation, the economist sees $(D, M)$ but not $Y$ in Project STAR, and $(D, M, Y)$
in NYC. Both variations of the problem [Athey et al., 2019, Athey et al., 2020] belong
to our class, as well as their generalizations to causal functions.

Figure 1 demonstrates that our semiparametric approach to long term average treat-
ment effect estimation performs well in the validation exercise. Following [Athey et al., 2020],
we fix $M$ as third grade test scores and take $Y$ to be third, fourth, fifth, sixth, seventh,
or eighth grade test scores. Across choices of $Y$, i.e. across horizons of extrapolation,
both variations of our long term average treatment recover the oracle estimates.

Figure 2 goes deeper, from average effects to heterogeneous effects with respect to
student aptitude. In particular, we examine heterogeneity with respect to prior ability
Figure 1: Long term average treatment effect of class size on test score over different horizons

$V$, measured in percentiles before the intervention. For simplicity, we continue to fix $M$ as third grade test scores and now fix $Y$ to be eighth grade test scores.

Figure 2 demonstrates that the students at the bottom of their kindergarten class benefit the most from enrollment in a small kindergarten class. The results are statistically significant, with pointwise confidence intervals that exclude zero. Students at the top of their kindergarten class size may have a slightly negative long term effect, though the pointwise confidence interval includes zero so the evidence is inconclusive. This empirical insight appears to be new. Insights like these are only possible due to our new theoretical results for causal functions such as long term heterogeneous treatment effects.

Direct proximal treatment effect of US Job Corps. Using our new multiple robustness to ill posedness, we return to another motivating real world issue: how to flexibly measure direct treatment effects while using proxies for unobserved confounding, which we have studied as the running Example 2. We replicate another influential program evaluation [Dukes et al., 2023] to ask: what is the direct effect of job training on arrests later in life, i.e. the effect that is not through the mechanism of employment? The answer sheds light on the production technology of worker skills. We extend
Figure 2: Long term heterogeneous treatment effects of class size on test score with respect to prior ability

previous parametric estimation to semiparametric estimation. Our flexible method documents a significant, negative direct effect. Again, these empirical results represent a realistic use case of our method: causal estimation in short panel data models with proxy variables.

[Dukes et al., 2023] propose a parametric method for the direct proximal treatment effect. The authors continue an extensive literature on the non-employment effects of the US Job Corps. The treatment $D$ is job training in the year following randomization, the mechanism $M$ is employment two years after randomization, and the outcome $Y$ is arrests four years after randomization. The auxiliary variables $(Z, W)$ are assumed to be relevant to unobserved motivation $U$, and also to satisfy exclusion restrictions: time spent with the Job Corps recruiter $Z$ does not directly cause employment or arrests, and pre-training expectations $W$ are not directly caused by training or employment. The final estimate is a scalar with a confidence interval.

Figure 3 compares the previous parametric approach with our semiparametric approach. The previous parametric approach found statistically insignificant effects, possibly due to simultaneous mis-specification of the parametric models for the outcome confounding bridge and treatment confounding bridge. By allowing for flexible nonpara-
metric estimation of the confounding bridges as nested NPIVs, our approach incurs a smaller approximation error. In this setting, it appears to improve statistical precision, suggesting a negative and significant direct effect of job training arrests. This empirical result is only possible due to our new theoretical results for bilinear functionals of nested NPIV.

7 Conclusion

A growing literature identifies parameters in nonlinear, heterogeneous causal models using short panel data and proxy variables. These identifications have not been fully usable for economists because they introduce a new statistical problem: nested nonparametric instrumental variable regression (nested NPIV). This paper provides what appears to be the first analysis of nested NPIV. Our nonasymptotic results are optimistic for causal inference, tolerating moderate ill posedness among some inverse problems. Our new estimators detect long term heterogeneous treatment effects of Project STAR, and direct proximal effects of the US Job Corps. The former empirical insight appears to be new. Future work may extend our results to long panel data models with higher order nested NPIV.
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38
A Sequential nested NPIV proof

A.1 Preliminaries

Let \( \alpha > 0 \) and define \( L_\alpha(h, g) = \max_{f \in \mathcal{F}} \mathbb{E}[2\{h(B) - g(A)\}f(C) - \alpha f(C)^2] \). Let \( f_h = T(h - h_0, 0) \) and \( f_g = T(0, g - g_0) \) so that \( f_h + f_g = T(h - h_0, g - g_0) \).

**Lemma 1** (Maximization identity). If \( f_h, f_g \in \mathcal{F} \) for any \( h \in \mathcal{H} \) and \( g \in \mathcal{G} \), then

\[
L_\alpha(h, g) = \frac{1}{\alpha} \mathbb{E}[2\{h(B) - g(A)\}(f_h + f_g)(C) - (f_h + f_g)^2(C)] = \frac{1}{\alpha} \|T(h - h_0, g - g_0)\|_2^2.
\]

In particular, since \( \mathbb{E}[\{h_0(B) - g_0(A)\}f(C)] = 0 \),

\[
L_\alpha(h_0, g_0) = \frac{1}{\alpha} \mathbb{E}[2\{h_0(B) - h_0(B)\}f_h(C) - f_h^2(C)] = \frac{1}{\alpha} \|T(h - h_0, 0)\|_2^2,
\]

\[
L_\alpha(h_0, g_0) = \frac{1}{\alpha} \mathbb{E}[2\{g_0(A) - g(A)\}f_g(C) - f_g^2(C)] = \frac{1}{\alpha} \|T(0, g - g_0)\|_2^2.
\]

**Proof.** By the law of iterated expectations, write

\[
L_\alpha(h, g) = \max_{f \in \mathcal{F}} \mathbb{E}[2\{h(B) - h_0(B) + g_0(A) - g(A)\}f(C) - \alpha f(C)^2]
\]

\[
= \max_{f \in \mathcal{F}} \mathbb{E}\{2 \cdot T(h - h_0, g - g_0)f(C)\} - \alpha \mathbb{E}\{f(C)^2\}
\]

\[
= \max_{f \in \mathcal{F}} 2\langle T(h - h_0, g - g_0), f \rangle_2 - \alpha \langle f, f \rangle_2.
\]

Taking the Gateaux derivative with respect to \( f \), we see that the first order condition is

\[
2T(h - h_0, g - g_0) - 2\alpha f^* = 0.
\]

Rearranging, \( f^* = \frac{1}{\alpha} T(h - h_0, g - g_0) \). Substitute \( f^* \) into initial and final expressions in the display, and recall \( T(h - h_0, g - g_0) = f_h + f_g \).

**Lemma 2** (High probability events). Suppose Assumption \( \square \) holds for \( \mathcal{F}, \mathcal{G} \), and \( \mathcal{H} \times \mathcal{F} \).

With probability \( 1 - \zeta \), when \( \delta_n = \Omega(\{\log \log(n) + \log(1/\zeta)\}^{1/2}n^{-1/2}) \),

\[
|\langle \mathbb{E}_n - \mathbb{E} \rangle[2\{h(B) - g(A)\}f(C) - f(C)^2] = O(\delta_n g - g_0\|_2 + \delta_n \|f\|_2 + \delta^2_n)|.
\]

**Proof.** See Appendix \( \square \)
Lemma 3 (High probability events under weaker conditions). Suppose Assumption 1 holds for $\mathcal{F}$, $\mathcal{G}$, and $\mathcal{H}$. With probability $1 - \zeta$, when $\delta_n = \Omega([\log \log(n) + \log(1/\zeta)]^{1/2} n^{-1/2})$, for a data independent hypothesis $h_\ast \in \mathcal{H}$,

$$\left| (\mathbb{E}_n - \mathbb{E}) [2\{h(B) - g(A)\} f(C) - f(C)^2] \right| = O(\delta_n \|h - h_\ast\|_2 + \delta_n \|\hat{g} - g_\ast\|_2 + \delta_n \|f\|_2 + \delta_n^2).$$

Proof. See Appendix E. $\square$

Let $\|h\|_{2,n}^2 = \mathbb{E}_n \{h(B)^2\}$, $I_n = 2\mu(\|h\|_{2,n}^2 - \|h_\ast\|_{2,n}^2)$, and $I = 2\mu(\|h\|_2^2 - \|h_\ast\|_2^2)$ for some data independent $h_\ast \in \mathcal{H}$.

Lemma 4 (High probability event for regularization). Suppose Assumption 1 holds for $\mathcal{H}$. With probability $1 - \zeta$, when $\delta_n = \Omega([\log \log(n) + \log(1/\zeta)]^{1/2} n^{-1/2})$, for a data independent hypothesis $h_\ast \in \mathcal{H}$, $|I_n - I| = O(\mu \delta_n \|h - h_\ast\|_2 + \mu \delta_n^2)$.

Proof. See Appendix E. $\square$

Remark 1 (AM-GM inequality). If $a = O(b \cdot c)$ then $a \leq \frac{b^2}{2} + O(c^2)$.

A.2 Estimator 2

We study the ridge regularized estimator and its population analogue:

$$\hat{h} = \arg\min_{h \in \mathcal{H}} \max_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2\{h(B) - \hat{g}(A)\} f(C) - f(C)^2 \right] + \mu \mathbb{E}_n \{h(B)^2\},$$

$$h_\mu = \arg\min_{h \in \mathcal{H}} \max_{f \in \mathcal{F}} \mathbb{E} \left[ 2\{h(B) - g_0(A)\} f(C) - f(C)^2 \right] + \mu \mathbb{E} \{h(B)^2\}.$$

Lemma 5 (From weak to strong metric). For any $\mu > 0$,

$$\|T(\hat{h} - h_\mu)\|_2^2 + 2\mu \|\hat{h} - h_\mu\|_2^2 = \|T(h - h_0)\|_2^2 - \|T(h_\mu - h_0)\|_2^2 + 2\mu (\|\hat{h}\|_2^2 - \|h_\mu\|_2^2).$$

Proof. To lighten notation, let $h_{(\tau)} = h_\mu + \tau(\hat{h} - h_\mu)$. Define $W(\tau) = \|T\{h_{(\tau)} - h_0\}\|_2^2 + 2\mu \|h_{(\tau)}\|_2^2$. Clearly $W(\tau)$ is quadratic in $\tau$ and strongly convex. By Lemma 1

$$W(\tau) = L_1\{h_{(\tau)}, g_0\} + 2\mu \|h_{(\tau)}\|_2^2 = \max_{f \in \mathcal{F}} \mathbb{E} \left[ 2\{h_{(\tau)}(B) - g_0(A)\} f(C) - f(C)^2 \right] + 2\mu \|h_{(\tau)}\|_2^2$$

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which is minimized at $\tau = 0$ by the definition of $h_{2\mu}$. Therefore by an exact Taylor expansion, $\frac{1}{2}\partial_{\tau}^2 W(0) = \partial_{\tau} W(0) + \frac{1}{2} \partial_{\tau}^2 W(0) = W(1) - W(0)$. The derivatives of $W(\tau)$ are

$$\partial_{\tau} W(\tau) = 2\langle T\{h(\tau) - h_0\}, T(\hat{h} - h_{2\mu})\rangle_2 + 4\mu\langle h(\tau), \hat{h} - h_{2\mu}\rangle_2$$

and $\partial_{\tau}^2 W(\tau) = 2\|T(\hat{h} - h_{2\mu})\|_2^2 + 4\mu\|\hat{h} - h_{2\mu}\|_2^2$. Substituting in $\partial_{\tau}^2 W(0), W(1)$, and $W(0)$ into the Taylor expansion yields the result.

\textbf{Lemma 6} (Relating weak metrics). Suppose the conditions of Lemmas 1 and 2 hold. With probability $1 - \zeta$, when $\delta_n = \Omega[\{\log \log(n) + \log(1/\zeta)\}^{1/2}n^{-1/2}]$, $\|T(\hat{h} - h_0)\|^2_2 - \|T(h_\ast - h_0)\|^2_2 \leq 8\|T(h_\ast - h_0)\|^2_2 + 2\mu(\|h_\ast\|^2_{2,n} - \|\hat{h}\|^2_{2,n}) + O\{\|\hat{g} - g_0\|^2_2 + \delta_n\|T(\hat{h} - h_\ast)\|^2_2 + \delta_n^2\}.$

\textit{Proof.} We proceed in steps.

1. By Lemma 1

$$\|T(\hat{h} - h_0)\|^2_2 = L_1(\hat{h}, g_0) = \mathbb{E} \left[ 2\left\{ \hat{h}(B) - h_0(B) \right\} f_\hat{h}(C) - f_{\hat{h}}(C)^2 \right]$$

$$= \mathbb{E} \left[ 2\left\{ \hat{h}(B) - \hat{g}(A) + \hat{g}(A) - g_0(A) \right\} f_\hat{h}(C) - f_{\hat{h}}(C)^2 \right].$$

2. Focusing on the third and fourth term, by Lemma 1 Cauchy Schwarz, and AM-GM

$$\mathbb{E}[2\{\hat{g}(A) - g_0(A)\}f_\hat{h}(C)] \leq 2\|\hat{g} - g_0\|_2\|T(\hat{h} - h_0)\|_2 \leq 2\|\hat{g} - g_0\|^2_2 + \frac{1}{2}\|T(\hat{h} - h_0)\|^2_2.$$ 

3. Focusing on the remaining terms, by Lemma 2 with probability $1 - \zeta$

$$\mathbb{E} \left[ 2\left\{ \hat{h}(B) - \hat{g}(A) \right\} f_\hat{h}(C) - f_{\hat{h}}(C)^2 \right]$$

$$\leq \mathbb{E}_n \left[ 2\left\{ \hat{h}(B) - \hat{g}(A) \right\} f_\hat{h}(C) - f_{\hat{h}}(C)^2 \right] + O(\delta_n\|\hat{g} - g_0\|_2 + \delta_n\|f_\hat{h}\|_2 + \delta_n^2).$$

(a) Consider the empirical expectation. By Assumption 4, the definition of $\hat{h}$, Lemma 2, and the AM-GM inequality $O(\delta_n\|f\|_2) \leq \frac{1}{2}\|f\|^2_2 + O(\delta_n^2)$, with
Collecting results,

\[
\mathbb{E}_n \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_{\hat{h}}(C) - f_{\hat{h}}(C)^2 \right] \leq \sup_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f(C) - f(C)^2 \right]
\]

\leq \sup_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2 \left\{ h_*(B) - \hat{g}(A) \right\} f(C) - f(C)^2 \right] + \mu(\|h_*\|_{2,n} - \|\hat{h}\|_{2,n})

\leq \sup_{f \in \mathcal{F}} \mathbb{E} \left[ 2 \left\{ h_*(B) - \hat{g}(A) \right\} f(C) - f(C)^2 \right] + O(\delta_n \|\hat{g} - g_0\|_2 + \delta_n^2) + \mu(\|h_*\|_{2,n} - \|\hat{h}\|_{2,n}).

By triangle inequality, Lemma 1, and Jensen’s inequality

\[
\sup_{f \in \mathcal{F}} \mathbb{E} \left[ 2 \left\{ h_*(B) - \hat{g}(A) \right\} f(C) - \frac{1}{2} f(C)^2 \right]
\]

\leq \sup_{f \in \mathcal{F}} \mathbb{E} \left[ 2 \left\{ h_*(B) - g_0(B) \right\} f(C) - \frac{1}{4} f(C)^2 \right] + \sup_{f \in \mathcal{F}} \mathbb{E} \left[ 2 \left\{ h_0(A) - \hat{g}(A) \right\} f(C) - \frac{1}{4} f(C)^2 \right]

= L_{1/4}(h_*, g_0) + L_{1/4}(h_*, \hat{g}) = 4\|T(h_* - h_0, 0)\|_2^2 + 4\|T(0, \hat{g} - g_0)\|_2^2
\]

\leq 4\|T(h_* - h_0)\|_2^2 + 4\|\hat{g} - g_0\|_2^2.

In summary, \( \mathbb{E}_n \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_{\hat{h}}(C) - f_{\hat{h}}(C)^2 \right] \) is bounded by

\[
4\|T(h_* - h_0)\|_2^2 + O(\|\hat{g} - g_0\|_2^2 + \delta_n^2) + \mu(\|h_*\|_{2,n} - \|\hat{h}\|_{2,n}).
\]

(b) Consider the penultimate term. By Lemma 1, triangle inequality, and AM-GM inequality,

\[
O(\delta_n \|f_{\hat{h}}\|_2) = O(\delta_n \|T(\hat{h} - h_0)\|_2) = O(\delta_n \|T(\hat{h} - h_*)\|_2 + \delta_n \|T(h_* - h_0)\|_2)
\]

\leq \frac{1}{2} \|T(h_* - h_0)\|_2^2 + O(\delta_n \|T(\hat{h} - h_*)\|_2^2 + \delta_n^2).

In summary, we bound \( \mathbb{E} \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_{\hat{h}}(C) - f_{\hat{h}}(C)^2 \right] \) by

\[
\frac{9}{2} \|T(h_* - h_0)\|_2^2 + \mu(\|h_*\|_{2,n} - \|\hat{h}\|_{2,n}) + O(\|\hat{g} - g_0\|_2^2 + \delta_n \|T(\hat{h} - h_*)\|_2^2 + \delta_n^2).
\]

4. Collecting results,

\[
\|T(\hat{h} - h_0)\|_2^2 \leq \frac{1}{2} \|T(\hat{h} - h_0)\|_2^2 + \frac{9}{2} \|T(h_* - h_0)\|_2^2 + \mu(\|h_*\|_{2,n} - \|\hat{h}\|_{2,n})
\]

\[
+ O(\|\hat{g} - g_0\|_2^2 + \delta_n \|T(\hat{h} - h_*)\|_2^2 + \delta_n^2). \square
\]
Lemma 7 (Relating weak metrics under weaker conditions). Suppose the conditions of Lemmas 1 and 3 hold. With probability $1 - \zeta$, when $\delta_n = \Omega[\{\log \log(n) + \log(1/\zeta)\}^{1/2}n^{-1/2}]$, $\|T(\hat{h} - h_0)\|_2^2 - \|T(h_* - h_0)\|_2^2 \leq 8\|T(h_* - h_0)\|_2^2 + 2\mu(\|h_*\|_{2,n}^2 - \|\hat{h}\|_{2,n}^2) + O\{\|\hat{g} - g_0\|_2^2 + \delta_n\|T(\hat{h} - h_*)\|_2 + \delta_n\|\hat{h} - h_*\|_2^2 + \delta_n^2\}.$

Proof. The argument is identical to Lemma 6 using Lemma 3 instead of 2. \qed

Lemma 8 (Regularization bias; Lemma 3 of Bennett et al., 2023d). If Assumption 2 holds then $\|h_* - h_0\|_2^2 \leq \|w_0\|_2^2\mu^{\min(\beta,2)}$ and $\|T(h_* - h_0)\|_2^2 \leq \|w_0\|_2^2\mu^{\min(\beta+1,2)}$.

Proof of Theorem 3. We consolidate both versions of the result, either placing the stronger assumption on the product space ($\gamma = 0$) or not ($\gamma = 1$). Take $h_* = h_{2\mu}$.

1. By Lemmas 5, 6, 7, and 4 AM-GM inequality, and $\mu + \gamma = O(1)$, we bound the quantity $\|T(\hat{h} - h_{2\mu})\|_2^2 + 2\mu\|\hat{h} - h_{2\mu}\|_2^2$ by

\[
\|T(\hat{h} - h_0)\|_2^2 - \|T(h_{2\mu} - h_0)\|_2^2 + 2\mu(\|\hat{h}\|_2^2 - \|h_{2\mu}\|_2^2) \\
\leq 8\|T(h_{2\mu} - h_0)\|_2^2 + 2\mu(\|h_{2\mu}\|_{2,n}^2 - \|\hat{h}\|_{2,n}^2) + 2\mu(\|\hat{h}\|_2^2 - \|h_{2\mu}\|_2^2) \\
+ O\{\|\hat{g} - g_0\|_2^2 + \delta_n\|T(\hat{h} - h_{2\mu})\|_2 + \gamma\|\hat{h} - h_{2\mu}\|_2 + \delta_n^2\} \\
= 8\|T(h_{2\mu} - h_0)\|_2^2 - I_n + I + O\{\|\hat{g} - g_0\|_2^2 + \delta_n\|T(\hat{h} - h_{2\mu})\|_2 + \gamma\|\hat{h} - h_{2\mu}\|_2 + \delta_n^2\} \\
\leq 8\|T(h_{2\mu} - h_0)\|_2^2 + O\{\|\hat{g} - g_0\|_2^2 + \delta_n\|T(\hat{h} - h_{2\mu})\|_2 + (\mu + \gamma)\|\hat{h} - h_{2\mu}\|_2 + \delta_n^2\} \\
\leq 8\|T(h_{2\mu} - h_0)\|_2^2 + \frac{1}{2}\|T(\hat{h} - h_{2\mu})\|_2^2 + O\{\|\hat{g} - g_0\|_2^2 + (\sqrt{\mu + \gamma})^2\|\hat{h} - h_{2\mu}\|_2 + \delta_n^2\} \\
\leq 8\|T(h_{2\mu} - h_0)\|_2^2 + \frac{1}{2}\|T(\hat{h} - h_{2\mu})\|_2^2 + \frac{\mu + \gamma}{2}\|\hat{h} - h_{2\mu}\|_2^2 + O\|\hat{g} - g_0\|_2^2 + \delta_n^2)\).
\]

Rearranging yields

\[
\frac{1}{2}\|T(\hat{h} - h_{2\mu})\|_2^2 + \frac{3\mu - \gamma}{2}\|\hat{h} - h_{2\mu}\|_2^2 \leq 8\|T(h_{2\mu} - h_0)\|_2^2 + O\|\hat{g} - g_0\|_2^2 + \delta_n^2),
\]

hence

\[
\|T(\hat{h} - h_{2\mu})\|_2^2 \leq 16\|T(h_{2\mu} - h_0)\|_2^2 + O\|\hat{g} - g_0\|_2^2 + \delta_n^2),
\]

\[
\|\hat{h} - h_{2\mu}\|_2^2 \leq \frac{16}{3\mu - \gamma}\|T(h_{2\mu} - h_0)\|_2^2 + \frac{2}{3\mu - \gamma} \cdot O\|\hat{g} - g_0\|_2^2 + \delta_n^2).
\]

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2. For the weak metric result, we use triangle inequality and Lemma 8

\[ \|T(\hat{h} - h_0)\|_2^2 \leq 2\|T(\hat{h} - h_{2\mu})\|_2^2 + 2\|T(h_{2\mu} - h_0)\|_2^2 \]

\[ \leq 18\|T(h_{2\mu} - h_0)\|_2^2 + O(\|\hat{g} - g_0\|_2^2 + \delta_n^2) \]

\[ = O\left\{ \|w_0\|_2^2 \mu^{\min(\beta+1,2)} + \|\hat{g} - g_0\|_2^2 + \delta_n^2 \right\} \]

3. For the strong metric result, we use triangle inequality and Lemma 8

\[ \|\hat{h} - h_0\|_2^2 \leq 2\|\hat{h} - h_{2\mu}\|_2^2 + 2\|h_{2\mu} - h_0\|_2^2 \]

\[ \leq \frac{32}{3\mu - \gamma}\|T(h_{2\mu} - h_0)\|_2^2 + \frac{2}{3\mu - \gamma} \cdot O(\|\hat{g} - g_0\|_2^2 + \delta_n^2) \]

\[ = O\left\{ \frac{\|w_0\|_2^2 \mu^{\min(\beta+1,2)}}{\mu - \gamma/3} + \|w_0\|_2^2 \mu^{\min(\beta,2)} + \frac{\|\hat{g} - g_0\|_2^2 + \delta_n^2}{\mu - \gamma/3} \right\} \]

When \( \gamma = 0 \), \( \|\hat{h} - h_0\|_2^2 = \{ \|w_0\|_2^2 \mu^{\min(\beta,1)} + \mu^{-1}\|\hat{g} - g_0\|_2^2 + \mu^{-1}\delta_n^2 \} \).

A.3 Estimator 1

We now study

\[ \hat{h} = \arg\min_{h \in \mathcal{H}} \max_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2\{h(B) - \hat{g}(A)\}f(C) - f(C)^2 \right] - \lambda\|f\|_x^2 + \mu\|h\|_h^2. \]

**Lemma 9** (Relating weak metrics). Suppose the conditions of Lemma 6 hold. With probability \( 1 - \zeta \), when \( \delta_n = \Omega[\log \log(n) + \log(1/\zeta)]^{1/2}n^{-1/2} \), \( \|T(\hat{h} - h_0)\|_2^2 - \|T(h_* - h_0)\|_2^2 \leq 8\|T(h_* - h_0)\|_2^2 + 2\mu(\|h_*\|_{\mathcal{H}}^2 - \|\hat{h}\|_{\mathcal{H}}^2) + \lambda\text{LIP}\|h - h_0\|_{\mathcal{H}} + O\{\|\hat{g} - g_0\|_2^2 + \delta_n\|T(h - h_0)\|_2^2 + \delta_n^2\}. \)

**Proof.** We proceed in steps similar to Lemma 6

1. As before, \( \|T(\hat{h} - h_0)\|_2^2 = \mathbb{E} \left[ \left\{ \hat{h}(B) - \hat{g}(A) + \hat{g}(A) - g_0(A) \right\} f_\lambda(C) - f_\lambda(C)^2 \right] \).

2. As before, \( \mathbb{E}[2\{\hat{g}(A) - g_0(A)\}f_\lambda(C)] \leq 2\|\hat{g} - g_0\|_2^2 + \frac{1}{2}\|T(\hat{h} - h_0)\|_2^2. \)

3. As before, with probability \( 1 - \zeta \), we bound \( \mathbb{E} \left[ \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_\lambda(C) - f_\lambda(C)^2 \right] \) by

\[ \mathbb{E}_n \left[ \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_\lambda(C) - f_\lambda(C)^2 \right] + O(\delta_n\|\hat{g} - g_0\|_2^2 + \delta_n\|f_\lambda\|_2^2 + \delta_n^2). \]
(a) Consider the empirical expectation. By Assumption 4, the definition of \( \hat{h} \), Lemma 2 and the AM-GM inequality \( O(\delta_n\|f\|_2) \leq \frac{1}{2}\|f\|_2^2 + O(\delta_n^2) \), with probability \( 1 - \zeta \),

\[
\mathbb{E}_n \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_h(C) - f_h(C)^2 \right] - \lambda \|f_h\|_F^2 \\
\leq \sup_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f(C) - f(C)^2 \right] - \lambda \|f\|_F^2 \\
\leq \sup_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2 \left\{ h_*(B) - \hat{g}(A) \right\} f(C) - f(C)^2 \right] + \mu(\|h_*\|_{\mathcal{H}}^2 - \|\hat{h}\|_{\mathcal{H}}^2) - \lambda \|f\|_F^2 \\
\leq \sup_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2 \left\{ h_*(B) - \hat{g}(A) \right\} f(C) - f(C)^2 \right] + O(\delta_n\|\hat{g} - g_0\|_2 + \delta_n\|f\|_2 + \delta_n^2) \\
+ \mu(\|h_*\|_{\mathcal{H}}^2 - \|\hat{h}\|_{\mathcal{H}}^2) - \lambda \|f\|_F^2 \\
\leq \sup_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2 \left\{ h_*(B) - \hat{g}(A) \right\} f(C) - \frac{1}{2} f(C)^2 \right] + O(\delta_n\|\hat{g} - g_0\|_2 + \delta_n^2) + \mu(\|h_*\|_{\mathcal{H}}^2 - \|\hat{h}\|_{\mathcal{H}}^2). 
\]

As before,

\[
\sup_{f \in \mathcal{F}} \mathbb{E}_n \left[ 2 \left\{ h_*(B) - \hat{g}(A) \right\} f(C) - \frac{1}{2} f(C)^2 \right] \leq 4\|T(h_* - h_0)\|_2^2 + 4\|\hat{g} - g_0\|_2^2. 
\]

Moreover, \( \|f_h\|_F^2 = \|T(h_0 - h_0)\|_2^2 \leq \lip \|\hat{h} - h_0\|_{\mathcal{H}}^2 \). We conclude that the quantity \( \mathbb{E}_n \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_h(C) - f_h(C)^2 \right] \) is bounded by

\[
4\|T(h_* - h_0)\|_2^2 + O(\delta_n\|\hat{g} - g_0\|_2 + \delta_n^2) + \mu(\|h_*\|_{\mathcal{H}}^2 - \|\hat{h}\|_{\mathcal{H}}^2) + \lambda \lip \|\hat{h} - h_0\|_{\mathcal{H}}^2. 
\]

(b) Consider the penultimate term. As before, \( O(\delta_n\|f_h\|_2) \leq \frac{1}{2}\|T(h_* - h_0)\|_2^2 + O(\delta_n\|T(h_* - h_0)\|_2^2) \).

In summary, we bound \( \mathbb{E}_n \left[ 2 \left\{ \hat{h}(B) - \hat{g}(A) \right\} f_h(C) - f_h(C)^2 \right] \) by

\[
\frac{9}{2}\|T(h_* - h_0)\|_2^2 + \mu(\|h_*\|_{\mathcal{H}}^2 - \|\hat{h}\|_{\mathcal{H}}^2) + \lambda \lip \|\hat{h} - h_0\|_{\mathcal{H}}^2 + O(\delta_n\|\hat{g} - g_0\|_2 + \delta_n\|T(h_* - h_0)\|_2 + \delta_n^2). 
\]

4. Collecting results,

\[
\|T(h_* - h_0)\|_2^2 \leq \frac{1}{2}\|T(h_* - h_0)\|_2^2 + \frac{9}{2}\|T(h_* - h_0)\|_2^2 + \mu(\|h_*\|_{\mathcal{H}}^2 - \|\hat{h}\|_{\mathcal{H}}^2) + \lambda \lip \|\hat{h} - h_0\|_{\mathcal{H}}^2 \\
+ O\{\delta_n\|\hat{g} - g_0\|_2 + \delta_n\|T(h_* - h_0)\|_2 + \delta_n^2\}. \square
Proof of Theorem [1] Take $h_*=h_0$. By Lemma 9, we bound $\|T(\hat{h} - h_0)\|_2^2$ by

$$2\mu(\|h_0\|_H^2 - \|\hat{h}\|_H^2) + \text{LIP}(\|\hat{h} - h_0\|_H^2 + O\{\|\hat{g} - g_0\|_2^2 + \delta_n\|T(\hat{h} - h_0)\|_2 + \delta_n^2\}).$$

Since $\text{LIP}(\|\hat{h} - h_0\|_H^2 + \|h_0\|_H^2) \leq 2\text{LIP}(\|\hat{h}\|_H^2 + \|h_0\|_H^2)$, we have

$$\|T(\hat{h} - h_0)\|_2^2 \leq 4\mu\|h_0\|_H^2 + O\{\|\hat{g} - g_0\|_2^2 + \delta_n\|T(\hat{h} - h_0)\|_2 + \delta_n^2\}. $$

By AM-GM inequality,

$$\|T(\hat{h} - h_0)\|_2^2 \leq 4\mu\|h_0\|_H^2 + \frac{1}{2}\|T(\hat{h} - h_0)\|_2^2 + O\{\|\hat{g} - g_0\|_2^2 + \delta_n^2\}. \quad \square$$

B Simultaneous nested NPIV proof

B.1 Preliminaries

Let $\alpha > 0$, $L'_\alpha(g) = \max_{f' \in F} E[2\{g(A) - Y\} f'(C') - \alpha f'(C')^2]$, and $f'_g = S(g - g_0)$.

Lemma 10 (Maximization identity). If $f'_g \in F$ for any $g \in G$, then

$$L'_\alpha(g) = \frac{1}{\alpha} E[2\{g(A) - Y\} f'_g(C') - (f'_g)^2(C')] = \frac{1}{\alpha} \|S(g - g_0)\|_2^2.$$

Proof. By the law of iterated expectations, write

$$L'_\alpha(g) = \max_{f \in F} E[2\{g(A) - g_0(A)\} f(C') - \alpha f(C')^2]$$

$$= \max_{f \in F} E\{2 \cdot S(g - g_0) f(C')\} - \alpha E\{f(C')^2\}$$

$$= \max_{f \in F} 2\langle S(g - g_0), f \rangle_2 - \alpha \langle f, f \rangle_2.$$

Taking the Gateaux derivative with respect to $f$, we see that the first order condition is $2S(g - g_0) - 2\alpha f^* = 0$. Rearranging, $f^* = \frac{1}{\alpha} S(g - g_0)$. Substitute $f^*$ into initial and final expressions in the display, and recall $S(g - g_0) = f'_g$. \quad \square

Lemma 11 (High probability events). Suppose Assumption 1 holds for $F$, $G \times F$, and $H \times F$. With probability $1 - \zeta$, when $\delta_n = \Omega(\{\log \log(n) + \log(1/\zeta)\}^{1/2} n^{-1/2})$,

$$|E_n - E|2\{g(A) - Y\} f'(C') - f'(C')^2| = O(\delta_n\|f\|_2 + \delta_n^2),$$

$$|E_n - E|2\{h(B) - g(A)\} f(C) - f(C)^2| = O(\delta_n\|f\|_2 + \delta_n^2).$$

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**Proof.** See Appendix E. 

Let \( \|g\|_2^2 = \mathbb{E}_n \{g(A)^2\} \), \( I'_n = 2\mu'(\|g\|_2^2 - \|g_*\|_2^2) \), and \( I' = 2\mu'(\|g\|_2^2 - \|g_*\|_2^2) \) for some data independent \( g_* \in \mathcal{G} \).

**Lemma 12** (High probability event for regularization). Suppose Assumption \( \Box \) holds for \( \mathcal{G} \). With probability \( 1 - \zeta \), when \( \delta_n = \Omega([\log \log(n) + \log(1/\zeta)]^{1/2}n^{-1/2}) \), for a data independent hypothesis \( g_* \in \mathcal{G} \), \( |I'_n - I'| = O(\mu'\delta_n\|g - g_*\|_2^2 + \mu'\delta_n^2) \).

**Proof.** See Appendix E. 

### B.2 Estimator 3

We study the ridge regularized estimator and its population analogue:

\[
(\hat{g}, \hat{h}) = \arg \min_{g \in \mathcal{G}, h \in \mathcal{H}, f' \in \mathcal{F}} \max \mathbb{E}_n \left[ 2\{g(A) - Y\}f'(C') - f'(C')^2 \right] + \mu' \mathbb{E}_n \{g(A)^2\}
+ \max_{f' \in \mathcal{F}} \mathbb{E}_n \left[ 2\{h(B) - g(A)\}f(C) - f(C)^2 \right] + \mu \mathbb{E}_n \{h(B)^2\},
\]

\( \{g(2\mu', 2\mu), h(2\mu', 2\mu)\} = \arg \min_{g \in \mathcal{G}, h \in \mathcal{H}, f' \in \mathcal{F}} \max \mathbb{E}_n \left[ 2\{g(A) - Y\}f'(C') - f'(C')^2 \right] + 2\mu' \mathbb{E}\{g(A)^2\}
+ \max_{f' \in \mathcal{F}} \mathbb{E}_n \left[ 2\{h(B) - g(A)\}f(C) - f(C)^2 \right] + 2\mu \mathbb{E}\{h(B)^2\}. \)

**Lemma 13** (From weak to strong metric). For any \( \mu', \mu > 0 \),

\[
\|S\{\hat{g} - g_{(2\mu', 2\mu)}\}\|_2^2 + 2\mu'\|\hat{g} - g_{(2\mu', 2\mu)}\|_2^2 + \|T\{\hat{h} - h_{(2\mu', 2\mu)}, \hat{g} - g_{(2\mu', 2\mu)}\}\|_2^2 + 2\mu\|\hat{h} - h_{(2\mu', 2\mu)}\|_2^2
= \|S(\hat{g} - g_0)\|_2^2 - \|S\{g_{(2\mu', 2\mu)} - g_0\}\|_2^2 + 2\mu'\|\hat{g}\|_2^2 - \|g_{(2\mu', 2\mu)}\|_2^2)
+ \|T(\hat{h} - h_0, \hat{g} - g_0)\|_2^2 - \|T\{h_{(2\mu', 2\mu)} - h_0, g_{(2\mu', 2\mu)} - g_0\}\|_2^2 + 2\mu\|\hat{h}\|_2^2 - \|h_{(2\mu', 2\mu)}\|_2^2). \]

**Proof.** To lighten notation, let \( g_{(\tau)} = g_{(2\mu', 2\mu)} + \tau\{\hat{g} - g_{(2\mu', 2\mu)}\} \) and \( h_{(\tau)} = h_{(2\mu', 2\mu)} + \tau\{\hat{h} - h_{(2\mu', 2\mu)}\} \). Define

\[
W(\tau) = \|S\{g_{(\tau)} - g_0\}\|_2^2 + 2\mu'\|g_{(\tau)}\|_2^2 + \|T\{h_{(\tau)} - h_0, g_{(\tau)} - g_0\}\|_2^2 + 2\mu\|h_{(\tau)}\|_2^2. \]
Clearly $W(\tau)$ is quadratic in $\tau$ and strongly convex. By Lemmas\[1\] and\[10\]
\[
W(\tau) = L_1\{g(\tau)\} + 2\mu\|g(\tau)\|_2^2 + L_1\{h(\tau), g(\tau)\} + 2\mu\|h(\tau)\|_2^2
\]
\[
= \max_{f' \in F} \mathbb{E}\left[2\{g(\tau)(A) - Y\}f'(C') - f'(C')^2\right] + 2\mu\|g(\tau)\|_2^2
\]
\[
+ \max_{f' \in F} \mathbb{E}\left[2\{h(\tau)(B) - g(\tau)(A)\}f(C) - f(C)^2\right] + 2\mu\|h(\tau)\|_2^2
\]
which is minimized at $\tau = 0$ by the definition of $\{g(2\mu', 2\mu), h(2\mu', 2\mu)\}$. Therefore by an exact Taylor expansion, $\frac{1}{2}\partial_\tau^2 W(0) = \partial_\tau W(0) + \frac{1}{2}\partial_\tau^2 W(0) = W(1) - W(0)$. The derivatives are
\[
\partial_\tau W(\tau) = 2\{S\{g(\tau) - g_0\}, S\{\hat{g} - g(2\mu', 2\mu)\}\} + 4\mu\langle g(\tau), \hat{g} - g(2\mu', 2\mu)\rangle
\]
\[
+ 2\{T\{h(\tau) - h_0, g(\tau) - g_0\}, T\{\hat{h} - h(2\mu', 2\mu), \hat{g} - g(2\mu', 2\mu)\}\} + 4\mu\langle h(\tau), \hat{h} - h(2\mu', 2\mu)\rangle
\]
\[
\partial_\tau^2 W(\tau) = 2\|S\{\hat{g} - g(2\mu', 2\mu)\}\|_2^2 + 4\mu\|\hat{g} - g(2\mu', 2\mu)\|_2^2
\]
\[
+ 2\|T\{\hat{h} - h(2\mu', 2\mu), \hat{g} - g(2\mu', 2\mu)\}\|_2^2 + 4\mu\|\hat{h} - h(2\mu', 2\mu)\|_2^2.
\]
Substituting in $\partial_\tau^2 W(0)$, $W(1)$, and $W(0)$ into the Taylor expansion yields the result. \[\Box\]

**Lemma 14** (Relating weak metrics). Suppose the conditions of Lemmas\[1\] and\[10\] hold. With probability $1 - \zeta$, when $\delta_n = \Omega[\{\log \log(n) + \log(1/\zeta)\}]^{1/2}n^{-1/2}$,
\[
\|S(\hat{g} - g_0)\|_2^2 - \|S(g_* - g_0)\|_2^2 + \|T(\hat{h} - h_0, \hat{g} - g_0)\|_2^2 - \|T(h_* - h_0, g_* - g_0)\|_2^2
\]
\[
\leq \frac{3}{2}\|S(g_* - g_0)\|_2^2 + \frac{3}{2}\|T(h_* - h_0, g_* - g_0)\|_2^2 + 2\mu\|g_*\|_2^2 - \|\hat{g}\|_2^2
\]
\[
+ O\{\delta_n\|S(\hat{g} - g_0)\|_2^2 + \delta_n\|T(\hat{h} - h_0, \hat{g} - g_0)\|_2^2 + \delta_n^2}\}.
\]

**Proof.** We proceed in steps similar to Lemma\[6\]

1. By Lemma\[10\] $\|S(\hat{g} - g_0)\|_2^2 = L_1(\hat{g}) = \mathbb{E}\left[2\{\hat{g}(A) - Y\}f'_a(C') - f'_a(C')^2\right]$. By Lemma\[1\] $\|T(\hat{h} - h_0, \hat{g} - g_0)\|_2^2 = L_1(\hat{h}, \hat{g}) = \mathbb{E}\left[2\{\hat{h}(B) - \hat{g}(A)\}(f_{\hat{h}} + f_{\hat{g}})(C) - (f_{\hat{h}} + f_{\hat{g}})^2(C)\right]$. 48
2. By Lemma 11 with probability $1 - \zeta$,

\[
\mathbb{E}[2\{\hat{g}(A) - Y\}f'_{\hat{g}}(C') - f'_{\hat{g}}(C')] \\
\leq \mathbb{E}_n[2\{\hat{g}(A) - Y\}f'_{\hat{g}}(C') - f'_{\hat{g}}(C')] + O(\delta_n\|f'_{\hat{g}}\|_2 + \delta_n^2), \\
\mathbb{E}\left[2\left\{\hat{h}(B) - \hat{g}(A)\right\}(f_{\hat{h}} + f_{\hat{g}})(C) - (f_{\hat{h}} + f_{\hat{g}})^2(C)\right] \\
\leq \mathbb{E}_n\left[2\left\{\hat{h}(B) - \hat{g}(A)\right\}(f_{\hat{h}} + f_{\hat{g}})(C) - (f_{\hat{h}} + f_{\hat{g}})^2(C)\right] + O(\delta_n\|f_{\hat{h}} + f_{\hat{g}}\|_2 + \delta_n^2).
\]

3. By Assumptions 4 and 6

\[
\mathbb{E}_n\left[2\{\hat{g}(A) - Y\}f'_{\hat{g}}(C') - f'_{\hat{g}}(C')^2\right] \leq \sup_{f' \in \mathcal{F}} \mathbb{E}_n\left[2\{\hat{g}(A) - Y\}f'(C') - f'(C')^2\right] \\
\mathbb{E}_n\left[2\left\{\hat{h}(B) - \hat{g}(A)\right\}(f_{\hat{h}} + f_{\hat{g}})(C) - (f_{\hat{h}} + f_{\hat{g}})^2(C)\right] \leq \sup_{f' \in \mathcal{F}} \mathbb{E}_n\left[2\left\{\hat{h}(B) - \hat{g}(A)\right\}f(C) - f(C)^2\right].
\]

4. By the definition of $(\hat{g}, \hat{h})$, Lemma 11, AM-GM inequality, and Lemmas 1 and 10, with probability $1 - \zeta$,

\[
\sup_{f' \in \mathcal{F}} \mathbb{E}_n\left[2\{\hat{g}(A) - Y\}f'(C') - f'(C')^2\right] + \sup_{f' \in \mathcal{F}} \mathbb{E}_n\left[2\left\{\hat{h}(B) - \hat{g}(A)\right\}f(C) - f(C)^2\right] \\
\leq \sup_{f' \in \mathcal{F}} \mathbb{E}_n\left[2\{g_*(A) - Y\}f'(C') - f'(C')^2\right] + \sup_{f' \in \mathcal{F}} \mathbb{E}_n\left[2\{h_*(B) - g_*(A)\}f(C) - f(C)^2\right] \\
+ \mu'(\|g_*\|_{2,n}^2 - \|\hat{g}\|_{2,n}^2) + \mu(\|h_*\|_{2,n}^2 - \|\hat{h}\|_{2,n}^2) \\
\leq \sup_{f' \in \mathcal{F}} \mathbb{E}\left[2\{g_*(A) - Y\}f'(C') - \frac{1}{2}f'(C')^2\right] + \sup_{f' \in \mathcal{F}} \mathbb{E}\left[2\{h_*(B) - g_*(A)\}f(C) - \frac{1}{2}f(C)^2\right] \\
+ \mu'(\|g_*\|_{2,n}^2 - \|\hat{g}\|_{2,n}^2) + \mu(\|h_*\|_{2,n}^2 - \|\hat{h}\|_{2,n}^2) + O(\delta_n^2) \\
= L_{1/2}(g_*) + L_{1/2}(h_*, g_*) + \mu'(\|g_*\|_{2,n}^2 - \|\hat{g}\|_{2,n}^2) + \mu(\|h_*\|_{2,n}^2 - \|\hat{h}\|_{2,n}^2) + O(\delta_n^2) \\
= 2\|S(g_* - g_0)\|_2^2 + 2\|T(h_* - h_0, g_* - g_0)\|_2^2 + \mu'(\|g_*\|_{2,n}^2 - \|\hat{g}\|_{2,n}^2) + \mu(\|h_*\|_{2,n}^2 - \|\hat{h}\|_{2,n}^2) + O(\delta_n^2).
\]
5. By Lemmas 1 and 10, triangle inequality, and AM-GM inequality,

\[ O(\delta_n\|f'_2\|_2) = O(\delta_n\|S(\hat{g} - g_0)\|_2) = O(\delta_n\|S(\hat{g} - g_\ast)\|_2 + \delta_n\|S(g_\ast - g_0)\|_2) \]

\[ \leq \frac{1}{2}\|S(g_\ast - g_0)\|_2^2 + O(\delta_n\|S(\hat{g} - g_\ast)\|_2 + \delta_n^2) \];

\[ O(\delta_n\|f'_h+ f'_\gamma\|_2) = O(\delta_n\|T(\hat{h} - h_0, \hat{\gamma} - g_0)\|_2) \]

\[ = O(\delta_n\|T(\hat{h} - h_\ast, \hat{\gamma} - g_\ast)\|_2 + \delta_n\|T(h_\ast - h_0, g_\ast - g_0)\|_2) \]

\[ \leq \frac{1}{2}\|T(h_\ast - h_0, g_\ast - g_0)\|_2^2 + O(\delta_n\|T(\hat{h} - h_\ast, \hat{\gamma} - g_\ast)\|_2 + \delta_n^2). \]

6. Collecting results,

\[ \|S(\hat{g} - g_0)\|_2^2 + \|T(\hat{h} - h_0, \hat{\gamma} - g_0)\|_2^2 \]

\[ \leq 2\|S(g_\ast - g_0)\|_2^2 + \|T(h_\ast - h_0, g_\ast - g_0)\|_2^2 + \mu'(\|g_\ast\|_2^2, \|\hat{g}\|_2^2) + \mu(\|h_\ast\|_2^2 - \|\hat{h}\|_2^2) + O(\delta_n^2) \]

\[ + \frac{1}{2}\|S(g_\ast - g_0)\|_2^2 + O(\delta_n\|S(\hat{g} - g_\ast)\|_2 + \delta_n^2) \]

\[ + \frac{1}{2}\|T(h_\ast - h_0, g_\ast - g_0)\|_2^2 + O(\delta_n\|T(\hat{h} - h_\ast, \hat{\gamma} - g_\ast)\|_2 + \delta_n^2) \]

\[ = \frac{5}{2}\|S(g_\ast - g_0)\|_2^2 + \frac{5}{2}\|T(h_\ast - h_0, g_\ast - g_0)\|_2^2 + \mu'(\|g_\ast\|_2^2, \|\hat{g}\|_2^2) + \mu(\|h_\ast\|_2^2 - \|\hat{h}\|_2^2) \]

\[ + O(\delta_n\|S(\hat{g} - g_\ast)\|_2 + \delta_n\|T(\hat{h} - h_\ast, \hat{\gamma} - g_\ast)\|_2 + \delta_n^2). \]

**Lemma 15** (Regularization bias). Suppose Assumptions 2, 3 and 5 hold. Then

\[ \|h_{\mu', \mu} - h_0\|_2^2 = O\left\{ \|w_h\|_2^2 \min(\beta_h, 2) + \|w'_h\|_2^2 \min(\beta'_h, 2) \right\} \]

\[ \|T_h(h_{\mu', \mu} - h_0)\|_2^2 = O\left\{ \|w_h\|_2^2 \min(\beta_h+1, 2) + \|w'_h\|_2^2 \min(\beta'_h+1, 2) \right\} \]

\[ \|g_{\mu', \mu} - g_0\|_2^2 = O\left\{ \|w_h\|_2^2 \min(\beta_h, 2) + \|w'_h\|_2^2 \min(\beta'_h, 2) \right\} \]

\[ \|S(g_{\mu', \mu} - g_0)\|_2^2 = O\left\{ \|w_h\|_2^2 \min(\beta_h+1, 2) + \|w'_h\|_2^2 \min(\beta'_h+1, 2) \right\} \]

\[ \|T_g(g_{\mu', \mu} - g_0)\|_2^2 = O\left\{ \|w_h\|_2^2 \min(\beta_h+1, 2) + \|w'_h\|_2^2 \min(\beta'_h+1, 2) \right\}. \]

**Proof.** See Appendix F \[ \square \]

**Proof of Theorem 3** We proceed in steps similar to Theorem 2. Take \((g_\ast, h_\ast) = \{g(2\mu', \mu), h(2\mu', \mu)\} \).
1. By Lemmas 13, 14, 12 and 4 AM-GM inequality, and \( \mu', \mu = O(1) \), we bound

\[
\| S\{ \hat{g} - g(2\mu', 2\mu) \}\|^2 + 2\mu' \| \hat{g} - g(2\mu', 2\mu) \|^2 + \| T\{ \hat{h} - h(2\mu', 2\mu), \hat{g} - g(2\mu', 2\mu) \}\|^2 + 2\mu \| \hat{h} - h(2\mu', 2\mu) \|^2 \\
= \| S\{ \hat{g} - g_0 \}\|^2 - \| S\{ g(2\mu', 2\mu) - g_0 \}\|^2 + 2\mu' \{ \| \hat{g} \|^2 - \| g(2\mu', 2\mu) \|^2 \} \\
+ \| T\{ \hat{h} - h_0, \hat{g} - g_0 \}\|^2 - \| T\{ h(2\mu', 2\mu) - h_0, g(2\mu', 2\mu) - g_0 \}\|^2 + 2\mu \{ \| \hat{h} \|^2 - \| h(2\mu', 2\mu) \|^2 \} \\
\leq \frac{3}{2} \| S\{ g(2\mu', 2\mu) - g_0 \}\|^2 + \frac{3}{2} \| T\{ h(2\mu', 2\mu) - h_0, g(2\mu', 2\mu) - g_0 \}\|^2 \\
+ 2\mu' \{ \| g(2\mu', 2\mu) \|^2 - \| g(2\mu', 2\mu) \|^2 \} \\
+ 2\mu \{ \| h(2\mu', 2\mu) \|^2 - \| h(2\mu', 2\mu) \|^2 \} \\
+ O[\delta_n, \| g(2\mu', 2\mu) \|^2] + \| h(2\mu', 2\mu) \|^2 + \| g(2\mu', 2\mu) \|^2 \\
= \frac{3}{2} \| S\{ g(2\mu', 2\mu) - g_0 \}\|^2 + \frac{3}{2} \| T\{ h(2\mu', 2\mu) - h_0, g(2\mu', 2\mu) - g_0 \}\|^2 \\
- \| f'_n + f' - f_n + O[\delta_n, \| g(2\mu', 2\mu) \|^2] + \| h(2\mu', 2\mu) \|^2 + \| g(2\mu', 2\mu) \|^2 \\
= \frac{3}{2} \| S\{ g(2\mu', 2\mu) - g_0 \}\|^2 + \frac{3}{2} \| T\{ h(2\mu', 2\mu) - h_0, g(2\mu', 2\mu) - g_0 \}\|^2 \\
+ O[\sqrt{\mu'}^2 \delta_n, \| \hat{g} - g(2\mu', 2\mu) \|^2 + \sqrt{\mu^2} \delta_n, \| \hat{h} - h(2\mu', 2\mu) \|^2 \\
+ \delta_n, \| S\{ \hat{g} - g(2\mu', 2\mu) \}\|^2 + \| h(2\mu', 2\mu) \|^2 + \| g(2\mu', 2\mu) \|^2 \\
\leq \frac{3}{2} \| S\{ g(2\mu', 2\mu) - g_0 \}\|^2 + \frac{3}{2} \| T\{ h(2\mu', 2\mu) - h_0, g(2\mu', 2\mu) - g_0 \}\|^2 \\
+ \frac{\mu'}{2} \| \hat{g} - g(2\mu', 2\mu) \|^2 + \frac{\mu}{2} \| \hat{h} - h(2\mu', 2\mu) \|^2 \\
+ \frac{1}{2} \| S\{ \hat{g} - g(2\mu', 2\mu) \}\|^2 + \frac{1}{2} \| T\{ \hat{h} - h(2\mu', 2\mu), \hat{g} - g(2\mu', 2\mu) \}\|^2 \}
\]

Rearranging yields

\[
\frac{1}{2} \| S\{ \hat{g} - g(2\mu', 2\mu) \}\|^2 + \frac{1}{2} \| T\{ \hat{h} - h(2\mu', 2\mu), \hat{g} - g(2\mu', 2\mu) \}\|^2 \\
+ \frac{3\mu'}{2} \| \hat{g} - g(2\mu', 2\mu) \|^2 + \frac{3\mu}{2} \| \hat{h} - h(2\mu', 2\mu) \|^2 \\
\leq \frac{3}{2} \| S\{ g(2\mu', 2\mu) - g_0 \}\|^2 + \frac{3}{2} \| T\{ h(2\mu', 2\mu) - h_0, g(2\mu', 2\mu) - g_0 \}\|^2 + O(\delta^2_n). \]
2. For the weak metric result, we use triangle inequality and Lemma 15:

\[ \|S\{\hat{g} - g(2\mu',2\mu)\}\|^2_2, \|T\{\hat{h} - h(2\mu',2\mu), \hat{g} - g(2\mu',2\mu)\}\|^2_2 \]

\[ \leq 3\|S\{g(2\mu',2\mu) - g_0\}\|^2_2 + 3\|T\{h(2\mu',2\mu) - h_0, g(2\mu',2\mu) - g_0\}\|^2_2 + O(\delta_n^2) \]

\[ \|\hat{g} - g(2\mu',2\mu)\|^2_2 \leq (\mu')^{-1}\|S\{g(2\mu',2\mu) - g_0\}\|^2_2 + (\mu')^{-1}\|T\{h(2\mu',2\mu) - h_0, g(2\mu',2\mu) - g_0\}\|^2_2 + O(\delta_n^2) \]

\[ \|\hat{h} - h(2\mu',2\mu)\|^2_2 \leq \mu^{-1}\|S\{g(2\mu',2\mu) - g_0\}\|^2_2 + \mu^{-1}\|T\{h(2\mu',2\mu) - h_0, g(2\mu',2\mu) - g_0\}\|^2_2 + O(\mu^{-1}\delta_n^2). \]

2. For the weak metric result, we use triangle inequality and Lemma 15:

\[ \|S\{\hat{g} - g_0\}\|^2_2 \leq 2\|S\{\hat{g} - g(2\mu',2\mu)\}\|^2_2 + 2\|S\{g(2\mu',2\mu) - g_0\}\|^2_2 \]

\[ \leq 8\|S\{g(2\mu',2\mu) - g_0\}\|^2_2 + 6\|T\{h(2\mu',2\mu) - h_0, g(2\mu',2\mu) - g_0\}\|^2_2 + O(\delta_n^2) \]

\[ = O\{\|\mu\|_2^{\min(\beta,1,2)} + \|\mu'\|_2^{\min(\beta',1,2)} + \|\delta\|_2^{\min(\beta,1,2)} + \delta_n^2\} \]

\[ = O(R_n), \]

\[ \|T\{\hat{h} - h_0, \hat{g} - g_0\}\|^2_2 \leq 2\|T\{\hat{h} - h(2\mu',2\mu), \hat{g} - g(2\mu',2\mu)\}\|^2_2 + 2\|T\{h(2\mu',2\mu) - h_0, g(2\mu',2\mu) - g_0\}\|^2_2 \]

\[ \leq 6\|S\{g(2\mu',2\mu) - g_0\}\|^2_2 + 8\|T\{h(2\mu',2\mu) - h_0, g(2\mu',2\mu) - g_0\}\|^2_2 + O(\delta_n^2) \]

\[ = O(R_n). \]
3. For the strong metric result, we use triangle inequality and Lemma \[15\]

\[
\|\hat{g} - g_0\|_2^2 \leq 2\|\hat{g} - g_{(2\mu', 2\mu)}\|_2^2 + 2\|g_{(2\mu', 2\mu)} - g_0\|_2^2 \\
\leq 2(\mu')^{-1}S\{g_{(2\mu', 2\mu)} - g_0\}\|_2^2 + 2(\mu')^{-1}\|T\{h_{(2\mu', 2\mu)} - h_0, g_{(2\mu', 2\mu)} - g_0\}\|_2^2 \\
+ 2\|g_{(2\mu', 2\mu)} - g_0\|_2^2 + O(\mu'\delta_n^2) \\
= O\{(\mu')^{-1}R_n + \|w_h\|_2^2 \mu_{\min(\beta_h, 2)} + \|w_g\|_2^2 (\mu')^{\min(\beta_g, 2)} \land \|w_g\|_2^2 (\mu')^{\min(\beta_g, 2)} + (\mu')^{-1}\delta_n^2\} \\
= O\{(\mu')^{-1}R_n + \|w_h\|_2^2 \mu_{\min(\beta_h, 2)}\},
\]

\[
\|\hat{h} - h_0\|_2^2 \leq 2\|\hat{h} - h_{(2\mu', 2\mu)}\|_2^2 + 2\|h_{(2\mu', 2\mu)} - h_0\|_2^2 \\
\leq 2\mu^{-1}S\{g_{(2\mu', 2\mu)} - g_0\}\|_2^2 + 2\mu^{-1}\|T\{h_{(2\mu', 2\mu)} - h_0, g_{(2\mu', 2\mu)} - g_0\}\|_2^2 \\
+ 2\|h_{(2\mu', 2\mu)} - h_0\|_2^2 + O(\mu^{-1}\delta_n^2) \\
= O\{\mu^{-1}R_n + \|w_h\|_2^2 \mu_{\min(\beta_h, 2)} + \|w_g\|_2^2 (\mu')^{\min(\beta_g, 2)} \land \|w_g\|_2^2 (\mu')^{\min(\beta_g, 2)} + \mu^{-1}\delta_n^2\} \\
= O\{\mu^{-1}R_n + \|w_g\|_2^2 (\mu')^{\min(\beta_g, 2)} \land \|w_g\|_2^2 (\mu')^{\min(\beta_g, 2)}\}.
\]

4. In particular, when \(\mu = \mu'\), \(\|\hat{g} - g_0\|_2 = O(\mu^{-1}R_n)\) and \(\|\hat{h} - h_0\|_2 = O(\mu^{-1}R_n)\) where

\[
R_n = \|w_h\|_2^2 \mu_{\min(\beta_h + 1, 2)} + \|w_g\|_2^2 \mu_{\min(\beta_g + 1, 2)} + \|w_g\|_2^2 \mu_{\min(\beta_g + 1, 2)} + \delta_n^2.
\]

C Causal estimation and inference proof

C.1 Neyman orthogonality

In this appendix, we lighten notation in a few ways. We denote the norm \(\mathcal{R}(h) = \|h - h_0\|_2^2\) and \(\mathcal{P}(h) = \|T(h - h_0)\|_2^2\), where the operator \(T\) is relative to the definition of \(h_0\). We write the nuisances as \((\nu_0, \delta_0, \alpha_0, \eta_0) = (h_1, h_2, h_3, h_4)\). Let \(W\) concatenate all of the random variables in an observation. Let \(\psi_0(w) = \psi(w, \theta_0, \nu_0, \delta_0, \alpha_0, \eta_0\) where

\[
\psi(w, \theta, \nu, \delta, \alpha, \eta) = \nu(w) + \alpha(w)\{y - \delta(w)\} + \eta(w)\{\delta(w) - \nu(w)\} - \theta.
\]

Let \(s(w), t(w), u(w), v(w)\) be functions and let \(\tau, \zeta \in \mathbb{R}\) be scalars. The Gateaux derivative of \(\psi(w, \theta, \nu, \delta, \alpha, \eta)\) with respect to its argument \(\nu\) in the direction \(s\) is
\{\partial_{\nu}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(u) = \frac{\partial}{\partial \nu}\psi(w,\theta,\nu+\tau s,\delta,\alpha,\eta)|_{\tau=0}. The cross derivative of \psi(w,\theta,\nu,\delta,\alpha,\eta) with respect to its arguments \((\nu, \delta)\) in the directions \((s, t)\) is \(\{\partial_{\nu,\delta}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(s, t) = \frac{\partial^2}{\partial \nu \partial \delta}\psi(w,\theta,\nu+\tau s,\delta+\zeta t,\alpha,\eta)|_{\tau=0,\zeta=0}.\)

**Lemma 16** (Calculation of derivatives). The first derivatives are \(\{\partial_{\nu}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(s) = s(w)\{1-\eta(w)\}, \{\partial_{\delta}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(t) = t(w)\{\eta(w)-\alpha(w)\}, \{\partial_{\alpha}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(u) = u(w)\{y-\delta(w)\},\) and \(\{\partial_{\eta}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(v) = v(w)\{\delta(w)-\nu(w)\}.\) The second derivatives are \(\{\partial^2_{\nu,\delta}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(s, t) = 0, \{\partial^2_{\nu,\alpha}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(s, u) = 0, \{\partial^2_{\nu,\eta}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(s, v) = -v(w)s(w), \{\partial^2_{\delta,\alpha}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(t, u) = -u(w)t(w), \{\partial^2_{\delta,\eta}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(t, v) = v(w)t(w),\) and \(\{\partial^2_{\alpha,\eta}\psi(w,\theta,\nu,\delta,\alpha,\eta)\}(u, v) = 0.\)

**Proof.** The result is immediate from the definition of Gateaux differentiation. \(\square\)

**Lemma 17** (Neyman orthogonality). If Assumption \(7\) holds then \(\psi\) is Neyman orthogonal with respect to \((\nu, \delta, \alpha, \eta)\).

**Proof.** The result is immediate from the first derivatives in Lemma 16. \(\square\)

**Lemma 18** (Verifying Neyman orthogonality). Examples 1 and 2, as well as those in Appendix D, are Neyman orthogonal.

**Proof.** By the law of iterated expectations, it is straightforward to verify Assumption \(7\) for each example. By Lemma 17 this suffices for Neyman orthogonality. \(\square\)

### C.2 Gaussian approximation

Partition the observations into \(L\) folds. Denote the \(\ell\)th fold by \(I_\ell\). Train \((\hat{\nu}_\ell, \hat{\delta}_\ell, \hat{\alpha}_\ell, \hat{\eta}_\ell)\) on observations in \(I_\ell\). Let \(n_\ell = |I_\ell| = n/L\) be the number of observations in \(I_\ell\). Denote by \(E_\ell(\cdot) = n_\ell^{-1}\sum_{i\in I_\ell}\cdot\) the average over observations in \(I_\ell\). Denote by \(E_n(\cdot) = n^{-1}\sum_{i=1}^n\cdot\) the average over all observations in the sample.

We define the foldwise target as \(\hat{\theta}_\ell = E_\ell[\hat{\nu}_\ell(W) + \hat{\delta}_\ell(W)\{Y - \hat{\delta}_\ell(W)\} + \hat{\eta}_\ell(W)\{\hat{\delta}_\ell(W) - \hat{\nu}_\ell(W)\}].\) We define the foldwise oracle as \(\hat{\theta}_\ell = E_\ell[\nu_0(W) + \alpha_0(W)\{Y - \delta_0(W)\} + \eta_0(W)\{\delta_0(W) - \nu_0(W)\}].\) We define the overall target as \(\hat{\theta} = \frac{1}{L}\sum_{\ell=1}^L \hat{\theta}_\ell.\) We define the overall oracle as \(\hat{\theta} = \frac{1}{L}\sum_{\ell=1}^L \hat{\theta}_\ell.\) Finally, let \((\bar{\alpha}, \bar{\eta}, \bar{\alpha}', \bar{\eta}', \bar{\sigma}_1, \bar{\sigma}_2) = (\bar{h}_3, \bar{h}_4, \bar{h}_3', \bar{h}_4', \bar{\sigma}_y, \bar{\sigma}_2).\)
Lemma 19 (Taylor expansion). Let \( s = \tilde{\nu}_t - \nu_0, \) \( t = \tilde{\delta}_t - \delta_0, \) \( u = \tilde{\alpha} - \alpha_0, \) and \( v = \tilde{\eta} - \eta_0. \) Then \( n^{1/2}(\tilde{\theta}_t - \bar{\theta}_t) = \sum_{j=1}^{7} \Delta_j \) where the first derivative terms are \( \Delta_1 = n^{1/2}E_{\ell}[s(W)\{1-\eta_0(W)\}], \) \( \Delta_2 = n^{1/2}E_{\ell}[t(W)\{\eta_0(W)-\alpha_0(W)\}], \) \( \Delta_3 = n^{1/2}E_{\ell}[u(W)\{Y-\delta_0(W)\}], \) \( \Delta_4 = n^{1/2}E_{\ell}[v(W)\{\delta_0(W)-\nu_0(W)\}], \) and the second derivative terms are \( \Delta_5 = n^{1/2}E_{\ell}\{-s(W)v(W)\}, \) \( \Delta_6 = n^{1/2}E_{\ell}\{-t(W)u(W)\}, \) \( \Delta_7 = n^{1/2}E_{\ell}\{t(W)v(W)\}. \)

Proof. An exact Taylor expansion gives \( \psi(w, \theta_0, \tilde{\nu}_t, \tilde{\delta}_t, \tilde{\alpha}_t, \tilde{\eta}_t) - \psi_0(w) \) equal to

\[
\begin{align*}
\{\partial_{\nu_0}(w)\}(s) + \{\partial_{\delta_0}(w)\}(t) + \{\partial_{\alpha_0}(w)\}(u) + \{\partial_{\psi_0}(w)\}(v) \\
\quad + \frac{1}{2}\{\partial_{s,s}^2(\psi_0(w))\}(s,t) + \frac{1}{2}\{\partial_{s,t}^2(\psi_0(w))\}(s,u) + \frac{1}{2}\{\partial_{s,\nu}^2(\psi_0(w))\}(s,v) \\
\quad + \frac{1}{2}\{\partial_{t,\nu}^2(\psi_0(w))\}(t,u) + \frac{1}{2}\{\partial_{t,t}^2(\psi_0(w))\}(t,v) + \frac{1}{2}\{\partial_{\nu,\nu}^2(\psi_0(w))\}(u,v).
\end{align*}
\]

Averaging over observations in \( I_\ell, \) \( \tilde{\theta}_t - \bar{\theta}_t = E_{\ell}\{\psi(W, \theta_0, \tilde{\nu}_t, \tilde{\delta}_t, \tilde{\alpha}_t, \tilde{\eta}_t)\} - E_{\ell}\{\psi_0(W)\}. \)

Finally appeal to Lemma 16.

Lemma 20 (Residuals). Suppose the conditions of Theorem 1 hold. Then with probability \( 1 - \epsilon/L, \) the first derivative terms have the bounds

\( |\Delta_1| \leq t_1 = \left( \frac{7L}{\epsilon} \right)^{1/2}(1 + \tilde{\eta})\{\mathcal{R}(\tilde{\nu}_t)\}^{1/2}, \)

\( |\Delta_2| \leq t_2 = \left( \frac{7L}{\epsilon} \right)^{1/2}(\tilde{\alpha} + \tilde{\eta})\{\mathcal{R}(\tilde{\delta}_t)\}^{1/2}, \)

\( |\Delta_3| \leq t_3 = \left( \frac{7L}{\epsilon} \right)^{1/2}\tilde{\sigma}_1\{\mathcal{R}(\tilde{\alpha}_t)\}^{1/2}, \)

\( |\Delta_4| \leq t_4 = \left( \frac{7L}{\epsilon} \right)^{1/2}\tilde{\sigma}_2\{\mathcal{R}(\tilde{\eta}_t)\}^{1/2} \)

while the second derivative terms have the bounds

\( |\Delta_5| \leq t_5 = \frac{7L}{2\epsilon}\{n\mathcal{R}(\tilde{\nu}_t)\mathcal{R}(\tilde{\eta}_t)\}^{1/2}, \)

\( |\Delta_6| \leq t_6 = \frac{7L}{2\epsilon}\{n\mathcal{R}(\tilde{\delta}_t)\mathcal{R}(\tilde{\alpha}_t)\}^{1/2}, \)

\( |\Delta_7| \leq t_7 = \frac{7L}{2\epsilon}\{n\mathcal{R}(\tilde{\delta}_t)\mathcal{R}(\tilde{\eta}_t)\}^{1/2}. \)

Proof. For simplicity, we focus on one first derivative term and one second derivative term; the rest are similar.

1. Markov inequality implies \( \mathbb{P}( |\Delta_1| > t_1 ) \leq \frac{\mathbb{E}(\Delta_1^2)}{t_1^2} \) and \( \mathbb{P}( |\Delta_5| > t_5 ) \leq \frac{\mathbb{E}(\Delta_5^2)}{t_5^2}. \)

2. The law of iterated expectations implies \( \mathbb{E}(\Delta_1^2) = \mathbb{E}(\mathbb{E}(\Delta_1^2 \mid I_{\ell})) \) and \( \mathbb{E}(\Delta_5^2) = \mathbb{E}(\mathbb{E}(\Delta_5^2 \mid I_{\ell})). \)

3. Conditional on \( I_{\ell}, (s, t, u, v) \) are nonrandom. Moreover, observations within fold \( I_{\ell} \) are independent and identically distributed. Hence by Assumption 7, \( \mathbb{E}(\Delta_1^2 \mid I_{\ell}) \)
equals

\[ \mathbb{E}\left( \left[ n_\ell^{1/2} \mathbb{E}_\ell \{s(W) - s(W)\eta_0(W)\}\right]^2 \mid I_\ell^c \right) \]

\[ = \mathbb{E}\left[ \frac{n_\ell}{n_\ell^2} \sum_{i,j \in I_\ell} \{s(W_i) - s(W_i)\eta_0(W_i)\}\{s(W_j) - s(W_j)\eta_0(W_j)\} \mid I_\ell^c \right] \]

\[ = \frac{n_\ell}{n_\ell^2} \sum_{i,j \in I_\ell} \mathbb{E}\{s(W_i) - s(W_i)\eta_0(W_i)\}\{s(W_j) - s(W_j)\eta_0(W_j)\} \mid I_\ell^c \]

\[ = \frac{n_\ell}{n_\ell^2} \sum_{i \in I_\ell} \mathbb{E}\{s(W_i) - s(W_i)\eta_0(W_i)\}^2 \mid I_\ell^c \] = \mathbb{E}[s(W)^2(1 - \eta_0(W))^2 \mid I_\ell^c] \leq (1 + \bar{\eta})^2 \mathcal{R}(\hat{\nu}_\ell).

By Cauchy Schwarz, \( \mathbb{E}(\|\Delta_5\| \mid I_\ell^c) = \frac{n_\ell^{1/2}}{2} \mathbb{E}\{|-s(W)\nu(W)| \mid I_\ell^c\} \) is bounded by

\[ \frac{n_\ell^{1/2}}{2} \left[ \mathbb{E}\{s(W)^2 \mid I_\ell^c\}\right]^{1/2} \mathbb{E}\{\nu(W)^2 \mid I_\ell^c\}^{1/2} = \frac{n_\ell^{1/2}}{2} \{\mathcal{R}(\hat{\nu}_\ell)\}^{1/2} \{\mathcal{R}(\bar{\eta}_\ell)\}^{1/2}. \]

4. Collecting results gives \( \mathbb{P}(\|\Delta_4\| > t_1) \leq \frac{(1 + \bar{\eta})^2 \mathcal{R}(\hat{\nu}_\ell)}{t_1^2} = \frac{\epsilon}{2L} \) and \( \mathbb{P}(\|\Delta_5\| > t_5) \leq \frac{n_\ell^{1/2}(\mathcal{R}(\hat{\nu}_\ell))^{1/2}(\mathcal{R}(\bar{\eta}_\ell))^{1/2}}{2t_5} = \frac{\epsilon}{2L}. \) Therefore with probability \( 1 - \epsilon/L, \) \( |\Delta_5| \leq t_1 = (\frac{7L}{4\epsilon})^{1/2}(1 + \bar{\eta})\{\mathcal{R}(\hat{\nu}_\ell)\}^{1/2} \) and \( |\Delta_5| \leq t_5 = \frac{7L}{2\epsilon}n_\ell^{1/2}\{\mathcal{R}(\hat{\nu}_\ell)\}^{1/2}\{\mathcal{R}(\bar{\eta}_\ell)\}^{1/2}. \)

**Lemma 21** (Residuals: Alternative path). Suppose the conditions of Theorem 4 hold.

Then with probability \( 1 - \epsilon/L, \) the first derivative terms have the bounds of Lemma 20, while the second derivative terms have the bounds

\[ |\Delta_5| \leq t_5 = \left( \frac{7L}{4\epsilon} \right)^{1/2}(\bar{\eta} + \bar{\eta}')\{\mathcal{R}(\hat{\nu}_\ell)\}^{1/2} + (4L)^{-1/2}\{n\mathcal{P}(\hat{\nu}_\ell)\mathcal{R}(\bar{\eta}_\ell)\}^{1/2} \wedge \{n\mathcal{R}(\hat{\nu}_\ell)\mathcal{P}(\bar{\eta}_\ell)\}^{1/2}, \]

\[ |\Delta_6| \leq t_6 = \left( \frac{7L}{4\epsilon} \right)^{1/2}(\bar{\alpha} + \bar{\alpha}')\{\mathcal{R}(\hat{\delta}_\ell)\}^{1/2} + (4L)^{-1/2}\{n\mathcal{P}(\hat{\delta}_\ell)\mathcal{R}(\bar{\alpha}_\ell)\}^{1/2} \wedge \{n\mathcal{R}(\hat{\delta}_\ell)\mathcal{P}(\bar{\alpha}_\ell)\}^{1/2}, \]

\[ |\Delta_7| \leq t_7 = \left( \frac{7L}{4\epsilon} \right)^{1/2}(\bar{\eta} + \bar{\eta}')\{\mathcal{R}(\hat{\delta}_\ell)\}^{1/2} + (4L)^{-1/2}\{n\mathcal{P}(\hat{\delta}_\ell)\mathcal{R}(\bar{\eta}_\ell)\}^{1/2} \wedge \{n\mathcal{R}(\hat{\delta}_\ell)\mathcal{P}(\bar{\eta}_\ell)\}^{1/2}. \]

**Proof.** See Lemma 20 for \((t_1, t_2, t_3, t_4). \) We focus on \( t_5; (t_6, t_7) \) are similar.

1. Write \( 2\Delta_5 \ell = n_\ell^{1/2} \mathbb{E}_\ell \{-s(W)v(W)\} = \Delta_5\ell + \Delta_5'\ell \) where \( \Delta_5\ell = n_\ell^{1/2} \mathbb{E}_\ell \{-s(W)v(W) + \mathbb{E}\{s(W)v(W) \mid I_\ell^c\}\} \) and \( \Delta_5'\ell = n_\ell^{1/2} \mathbb{E}\{-s(W)v(W) \mid I_\ell^c\}. \)

2. Consider the former term. By Markov inequality, \( \mathbb{P}(\|\Delta_5\ell\| > t) \leq \frac{\mathbb{E}(\Delta_5^2\ell)}{t^2}. \) By the law of iterated expectations, \( \mathbb{E}(\Delta_5^2\ell) = \mathbb{E}\{\mathbb{E}(\Delta_5^2 \mid I_\ell^c)\}. \) We bound the conditional
moment. Conditional on \( I^c_\ell \), \((s, t, u, v)\) are nonrandom. Moreover, observations within fold \( I_\ell \) are independent and identically distributed. Since each summand in \( \Delta_{j\ell} \) \((j = 5, 6, 7)\) has conditional mean zero by construction, \( \mathbb{E}(\Delta_{j\ell}^2 | I^c_\ell) \) equals

\[
\mathbb{E}\left\{ \left( n^2_\ell \mathbb{E}[ -s(W)v(W) + \mathbb{E}\{ s(W)v(W) | I^c_\ell \} \right]^2 | I^c_\ell \right\} 
= \mathbb{E}\left( \frac{n^2_\ell}{n^2_\ell} \sum_{i,j \in I_\ell} [-s(W_i)v(W_i) + \mathbb{E}\{ s(W_i)v(W_i) | I^c_\ell \}][-s(W_j)v(W_j) + \mathbb{E}\{ s(W_j)v(W_j) | I^c_\ell \}] | I^c_\ell \right) 
= \frac{n^4_\ell}{n^2_\ell \sum_{i,j \in I_\ell} \mathbb{E}([-s(W_i)v(W_i) + \mathbb{E}\{ s(W_i)v(W_i) | I^c_\ell \}][-s(W_j)v(W_j) + \mathbb{E}\{ s(W_j)v(W_j) | I^c_\ell \}] | I^c_\ell \right) 
= \mathbb{E}([-s(W)v(W) - \mathbb{E}\{ s(W)v(W) | I^c_\ell \}^2 | I^c_\ell \] 
\leq \mathbb{E}\{ s(W)^2v(W)^2 | I^c_\ell \} \leq (\tilde{\eta} + \tilde{\eta}')^2 R(\hat{\nu}_\ell).
\]

Collecting results gives \( \mathbb{P}(|\Delta_{5\ell}| > t) \leq \frac{(\tilde{\eta} + \tilde{\eta}')^2 R(\hat{\nu}_\ell)}{t^2} = \frac{t}{4L}. \) Therefore with probability \( 1 - 3\epsilon/(7L) \), \(|\Delta_{5\ell}| \leq t = (\frac{7L}{4L})^{1/2}(\tilde{\eta} + \tilde{\eta}')\{R(\hat{\nu}_\ell)\}^{1/2}.

3. Consider the latter term. Specializing to nonparametric confounding bridges, if \( \mathbb{E}\{ h_0(B)|C \} = \mathbb{E}\{ g_0(A)|C \} \) and \( \mathbb{E}\{ g_0(A)|C' \} = \mathbb{E}(Y| C') \), then the arguments of \((\nu, \delta, \alpha, \eta)\), and hence \((s, t, u, v)\), are \((B, A, C', C)\), respectively. Therefore \( \mathbb{E}\{ -s(W)v(W) | I^c_\ell \} = \mathbb{E}[\mathbb{E}\{ -s(B) | C, I^c_\ell \}v(C) | I^c_\ell \] is bounded by

\[
\{\mathbb{E}\{\mathbb{E}\{ s(B) | C, I^c_\ell \}^2 | I^c_\ell \}\}^{1/2}[\mathbb{E}\{ v(C)^2 | I^c_\ell \}]^{1/2} = \{P(\hat{\nu}_\ell)\}^{1/2}\{R(\hat{\eta}_\ell)\}^{1/2}.
\]

Hence \( \Delta_{5\ell} \leq n^{1/2}_\ell \{P(\hat{\nu}_\ell)\}^{1/2}\{R(\hat{\eta}_\ell)\}^{1/2} = L^{-1/2}\{nP(\hat{\nu}_\ell)R(\hat{\eta}_\ell)\}^{1/2}. \) Likewise \( \Delta_{5\ell} \leq n^{1/2}_\ell \{R(\hat{\nu}_\ell)\}^{1/2}\{P(\hat{\eta}_\ell)\}^{1/2} = L^{-1/2}\{nP(\hat{\nu}_\ell)P(\hat{\eta}_\ell)\}^{1/2}.

4. Combining terms yields the desired result. \( \square \)

**Lemma 22** (Oracle approximation). Suppose the conditions of Theorem 4 hold. Then with probability \( 1 - \epsilon, \frac{n^{1/2}_\ell}{\sigma}|\hat{\theta} - \theta| \leq \Delta \) where \( \Delta \) equals

\[
\frac{7L}{2\epsilon\sigma} \left[ \left( 1 + \tilde{\eta} \right)\{R(\hat{\nu}_\ell)\}^{1/2} + \left( \tilde{\alpha} + \tilde{\eta} \right)\{R(\hat{\delta}_\ell)\}^{1/2} + \tilde{\sigma}_1\{R(\hat{\alpha}_\ell)\}^{1/2} + \tilde{\sigma}_2\{R(\hat{\eta}_\ell)\}^{1/2} 
\right.
\left. + \left\{ nR(\hat{\nu}_\ell)R(\hat{\eta}_\ell) \right\}^{1/2} + \left\{ nR(\hat{\delta}_\ell)R(\hat{\alpha}_\ell) \right\}^{1/2} + \left\{ nR(\hat{\delta}_\ell)R(\hat{\eta}_\ell) \right\}^{1/2} \right].
\]
Proof. We proceed in steps.

1. By Lemma 19, write \( n^{1/2}(\hat{\theta} - \bar{\theta}) = n_{i/2}^{1/2} \frac{1}{L} \sum_{\ell=1}^{L} n_{\ell}^{1/2}(\hat{\theta}_\ell - \bar{\theta}) = L^{1/2} \frac{1}{L} \sum_{\ell=1}^{L} \sum_{j=1}^{3} \Delta_{jk}. \)

2. Define the events \( \mathcal{E}_\ell = \{ \text{for all } j \in \{1, \ldots, 7\}, \ |\Delta_{jk}| \leq t_j \} \), \( \mathcal{E} = \cap_{\ell=1}^{L} \mathcal{E}_\ell \), and \( \mathcal{E}^c = \cup_{\ell=1}^{L} \mathcal{E}_\ell^c \). Hence by the union bound and Lemma 20, \( \mathbb{P}(\mathcal{E}^c) \leq \sum_{\ell=1}^{L} \mathbb{P}(\mathcal{E}_\ell^c) \leq L_{\ell}^c = \epsilon. \)

3. Therefore with probability \( 1 - \epsilon, \)
\[
n^{1/2}|\hat{\theta} - \bar{\theta}| \leq L^{1/2} \frac{1}{L} \sum_{\ell=1}^{L} \sum_{j=1}^{7} |\Delta_{jk}| \leq L^{1/2} \frac{1}{L} \sum_{\ell=1}^{L} \sum_{j=1}^{7} t_j = L^{1/2} \sum_{j=1}^{7} t_j.
\]

Finally, we simplify \( (t_j) \). Note that \( 7^{1/2} < 7/2 \) and that for \( \epsilon \leq 1, \epsilon^{-1/2} \leq \epsilon^{-1}. \)

Lemma 23 (Oracle approximation: Alternative path). Suppose the conditions of Theorem 4 hold. Then with probability \( 1 - \epsilon, \frac{n^{1/2}}{\sigma} |\hat{\theta} - \bar{\theta}| \leq \Delta \) where \( \Delta \) equals
\[
4L \epsilon^{1/2} \sigma \left[ (1 + \bar{\eta} + \bar{\eta}') \{ \mathcal{R}(\hat{\nu}_\ell) \}^{1/2} + (\bar{\alpha} + \bar{\alpha}' + \bar{\eta} + \bar{\eta}') \{ \mathcal{R}(\hat{\delta}_\ell) \}^{1/2} + \bar{\sigma}_1 \{ \mathcal{R}(\hat{\alpha}_\ell) \}^{1/2} + \bar{\sigma}_2 \{ \mathcal{R}(\hat{\eta}_\ell) \}^{1/2} + \sum_{\ell=1}^{L} \left[ \mathbb{E}(\hat{\nu}_\ell) \mathcal{R}(\hat{\eta}_\ell) \right]^{1/2} + \mathbb{E}(\hat{\delta}_\ell) \mathcal{R}(\hat{\eta}_\ell) \right]^{1/2}.
\]

Proof. As in Lemma 22, Lemmas 19 and 21 imply that with probability \( 1 - \epsilon, n^{1/2}|\hat{\theta} - \bar{\theta}| \leq L^{1/2} \sum_{j=1}^{3} t_j \). Note \( 7^{1/2} + (7/4)^{1/2} < 4 \) when combining terms.

Proof of Theorem 4 The steps of Chernozhukov et al., 2023, Theorem 1 generalize to our setting, using our new \( \Delta \) defined in Lemmas 22 and 23.

C.3 Variance estimation

Recall that \( \mathbb{E}(\cdot) = \frac{1}{n} \sum_{i \in I_\ell} (\cdot) \) means the average over observations in \( I_\ell \) and \( \mathbb{E}(\cdot) = \frac{1}{n} \sum_{i=1}^{n} (\cdot) \) means the average over all observations in the sample. For \( i \in I_\ell \), define \( \psi_0(W_i) = \psi(W_i, \theta_0, \nu_0, \delta_0, \alpha_0, \eta_0) \) and \( \hat{\psi}(W_i) = \psi(W_i, \hat{\theta}, \hat{\nu}_\ell, \hat{\delta}_\ell, \hat{\alpha}_\ell, \hat{\eta}_\ell) \).
Lemma 24 (Foldwise second moment). \( \mathbb{E}_t[\{\hat{\psi}(W) - \psi_0(W)\}^2] \leq 7\left\{ (\hat{\theta} - \theta_0)^2 + \sum_{j=8}^{13} \Delta_j t \right\} \), where \( \Delta_8t = \mathbb{E}_t\{s(W_i)^2\} \), \( \Delta_9t = \mathbb{E}_t[u(W_i)^2\{Y - \delta_0(W_i)\}^2] \), \( \Delta_{10}t = \mathbb{E}_t[v(W_i)^2\{\delta_0(W_i) - \nu_0(W_i)\}^2] \), \( \Delta_{11}t = \mathbb{E}_t[\hat{\alpha}_\ell(W_i)^2t(W_i)^2] \), \( \Delta_{12}t = \mathbb{E}_t[\hat{\eta}_\ell(W_i)^2t(W_i)^2] \), \( \Delta_{13}t = \mathbb{E}_t[\hat{\eta}_\ell(W_i)^2u(W_i)^2] \).

Proof. Write \( \hat{\psi}(W) - \psi_0(W) \) equal to

\[
\begin{align*}
\hat{\psi}_\ell(W_i) + \hat{\alpha}_\ell(W_i)\{Y_i - \hat{\delta}_\ell(W_i)\} &+ \hat{\eta}_\ell(W_i)\{\hat{\delta}_\ell(W_i) - \hat{\psi}_\ell(W_i)\} - \hat{\theta} \\
&\quad - [\nu_0(W) + \alpha_0(W_i)\{Y_i - \delta_0(W_i)\} + \eta_0(W_i)\{\delta_0(W_i) - \nu_0(W_i)\} - \theta_0] \\
&\quad \pm \hat{\alpha}_\ell\{Y - \delta_0(W_i)\} \pm \hat{\eta}_\ell\{\delta_0(W_i) - \nu_0(W_i)\} \\
&\quad = (\theta_0 - \hat{\theta}) + s(W_i) + u(W_i)\{Y - \delta_0(W_i)\} + v(W_i)\{\delta_0(W_i) - \nu_0(W_i)\} \\
&\quad - \hat{\alpha}_\ell(W_i)t(W_i) + \hat{\eta}_\ell(W_i)t(W_i) - \hat{\eta}_\ell(W_i)u(W_i).
\end{align*}
\]

Apply parallelogram law across the seven terms, and take \( \mathbb{E}_t(\cdot) \) of both sides.  

Lemma 25 (Residuals). Suppose the conditions of Theorem 5 hold. Then with probability \( 1 - \epsilon'/2L \), \( |\Delta_8t| \leq t_8 = \frac{12L}{\epsilon'}\mathcal{R}(\hat{\psi}_\ell) \), \( |\Delta_9t| \leq t_9 = \frac{12L}{\epsilon'}\sigma_\ell^2\mathcal{R}(\hat{\alpha}_\ell) \), \( |\Delta_{10}t| \leq t_{10} = \frac{12L}{\epsilon'}\sigma_\ell^2\mathcal{R}(\hat{\eta}_\ell) \), \( |\Delta_{11}t| \leq t_{11} = \frac{12L}{\epsilon'}(\bar{\alpha}')^2\mathcal{R}(\hat{\alpha}_\ell) \), \( |\Delta_{12}t| \leq t_{12} = \frac{12L}{\epsilon'}(\bar{\eta}')^2\mathcal{R}(\hat{\eta}_\ell) \), \( |\Delta_{13}t| \leq t_{13} = \frac{12L}{\epsilon'}(\bar{\eta}')^2\mathcal{R}(\hat{\eta}_\ell) \).

Proof. The steps are analogous to Lemma 20.  

Lemma 26 (Oracle approximation). Suppose the conditions of Lemma 25 hold. Then with probability \( 1 - \epsilon'/2 \), \( \mathbb{E}_n[\{\hat{\psi}(W) - \psi_0(W)\}^2] \leq \Delta' \) where

\[
\Delta' = 7(\hat{\theta} - \theta_0)^2 + \frac{84L}{\epsilon'}\left[\mathcal{R}(\hat{\psi}_{\ell}) + \{(\bar{\alpha}')^2 + (\bar{\eta}')^2\}\mathcal{R}(\hat{\alpha}_{\ell}) + \{(\bar{\eta}')^2 + \sigma_\ell^2\}\mathcal{R}(\hat{\eta}_{\ell}) + \sigma_\ell^2\mathcal{R}(\hat{\eta}_{\ell})\right].
\]

Proof. The steps are analogous to Lemma 22 appealing to Lemmas 24 and 25.  

Lemma 27 (Markov inequality). If \( \chi < \infty \), then with probability \( 1 - \epsilon'/2 \), \( \mathbb{E}_n\{\psi_0(W)^2\} - \sigma^2 \leq \Delta'' = (\frac{3}{2})^{1/2} \frac{n^{1/2}}{\chi^{1/2}}. \)

Proof. The steps of Chernozhukov et al., 2023 Proposition S11 generalize to our setting, using our new moments.
Proof of Theorem 5. The steps of Chernozhukov et al., 2023, Theorem 3 generalize to our setting, using our new \((\Delta', \Delta'')\) defined in Lemmas 26 and 27, respectively.

Proof of Corollary 5. By Theorem 4, \(\hat{\theta} \overset{p}{\rightarrow} \theta_0\) and \(\lim_{n \rightarrow \infty} \mathbb{P}\{\theta_0 \in \left(\hat{\theta} \pm \frac{\sigma}{n^{1/2}}\right)\} = 1 - a\). For the desired result, it suffices that \(\hat{\sigma}^2 \overset{p}{\rightarrow} \sigma^2\), which follows from Theorem 5.

D Additional examples

The class of causal estimands that we study includes several more important examples. For each of these examples, we provide what appear to be the first nonasymptotic results guaranteeing inference while allowing for machine learning estimation. These examples all involve dynamic confounding. Future work may apply our results to structural models with other types of confounding, e.g. strategic considerations.

The initial examples are short panel data models with proxy variables, demonstrating the importance of our nested NPIV analysis.

Example 3 (Long term effect with proxies). Let \(h_0\) be an outcome confounding bridge that solves the inverse problem \(\mathbb{E}\{h(X, D, S_1, S_2)|X, D, S_1, S_2, G = 1\} = \mathbb{E}(Y|X, D, S_1, S_2, G = 1)\). Under proxy variable assumptions, Ghassami et al., 2022b, Imbens et al., 2022,

\[
\text{LONG} = \mathbb{E}\{Y(d)|G = 0\} = \mathbb{E}\{h_0(X, D, S_2, S_3)|D = d, G = 0\}.
\]

Let \(h'_0\) be a treatment confounding bridge that solves the inverse problem

\[
\mathbb{E}\{h'(X, D, S_1, S_2)|X, D, S_2, S_3, G = 1\} = \frac{\mathbb{P}(X, S_2, S_3|D, G = 0)}{\mathbb{P}(X, S_2, S_3|D, G = 1)}.
\]

Then \(h_1(X, D, S_1, S_2, G) = \frac{1_{D = d, G = 0}}{\mathbb{P}(D = d, G = 0)} h_0(X, D, S_1, S_2)\), \(h_2(X, D, S_1, S_2) = h_0(X, D, S_1, S_2)\), \(h_3(X, D, S_1, S_2, G) = \frac{1_{D = d, G = 1}}{\mathbb{P}(D = d, G = 1)} h_0(X, D, S_1, S_2)\), and \(h_4 = 0\).

Example 4 (Time varying effect with proxies). Let \(h_0\) be an outcome confounding bridge that solves the inverse problem

\[
\mathbb{E}\{h(X_1, D_1, W_1, D_2)|X_1, Z_1, D_1\} = \mathbb{E}\{g_0(X_1, D_1, W_1, X_2, D_2, W_2)|X_1, Z_1, D_1\}
\]
where \( g_0 \) solves the inverse problem
\[
\mathbb{E}\{g(X_1, D_1, W_1, X_2, D_2, W_2)|X_1, Z_1, D_1, X_2, Z_2, D_2\} = \mathbb{E}(Y|X_1, Z_1, D_1, X_2, Z_2, D_2).
\]
Under proxy variable assumptions \cite{Ying et al., 2023},
\[
\text{TIME} = \mathbb{E}\{Y^{(d_1,d_2)}\} = \mathbb{E}\left\{\int h_0(X_1, d_1, w_1, d_2)d\mathbb{P}(w_1|X_1)\right\}.
\]
Let \( h'_0 \) be a treatment confounding bridge that solves the inverse problem
\[
\mathbb{E}\{h'(X_1, Z_1, D_1, X_2, Z_2, D_2)|X_1, D_1, W_1, X_2, D_2, W_2\} = \frac{\mathbb{E}\{g'_0(X_1, Z_1, D_1)|X_1, D_1, W_1, X_2, W_2\}}{\mathbb{P}(d_2|X_1, D_1, W_1, X_2, W_2)}
\]
where \( g'_0 \) solves the inverse problem \( \mathbb{E}\{g(X_1, Z_1, D_1)'|X_1, D_1, W_1\} = \frac{1}{\mathbb{P}(d_1|X_1, W_1)} \). Then
\[
h_1(X_1) = \int h_0(X_1, d_1, w_1, d_2)d\mathbb{P}(w_1|X_1), \quad h_2(X_1, W_1) = h_0(X_1, d_1, W_1, d_2), \quad h_3(X_1, Z_1, D_1, X_2, Z_2, D_2) = 1_{D_1=d_1, D_2=d_2}h'_0(X_1, Z_1, D_1, X_2, Z_2, D_2), \quad \text{and} \quad h_4(X_1, Z_1, D_1) = 1_{D_1=d_1}g'_0(X_1, Z_1, D_1).
\]

The subsequent examples are short panel data models in which we care about causal functions, demonstrating the importance of our nonasymptotic semiparametric analysis.

**Example 5** (Direct heterogeneous treatment effects). Let \( h_0(V, X, D, M) = \mathbb{E}(Y|V, X, D, M) \) be the outcome mechanism and let \( \mathbb{P}(M|V, X, D) \) be the mediation mechanism. Under exogeneity assumptions \cite{Robins and Greenland, 1992, Pearl, 2001, Imai et al., 2010}, the direct heterogeneous treatment effects are
\[
\text{DIRECT}(v) = \mathbb{E}\left[Y^{(1,M^{(0)})}|V = v\right] = \lim_{\nu \to 0} \mathbb{E}\left\{\int \ell_\nu(V)h_0(V, X, 1, m)d\mathbb{P}(m|V, X, 0)\right\}.
\]
Let \( \mathbb{P}(D|V, X) \) and \( \mathbb{P}(D|V, X, M) \) be the treatment mechanism. Then
\[
h_1(V, X) = \int h_0(V, X, 1, m)d\mathbb{P}(m|V, X, 0), \quad h_2(V, X, M) = h_0(V, X, 1, M), \quad h_3(V, X, D, M) = \frac{1_{D=1}}{\mathbb{P}(1|V, X, M)}\frac{\mathbb{P}(0|V, X, M)}{\mathbb{P}(0|V, X)},
\]
and
\[
h_4(V, X, D) = \frac{1_{D=0}}{\mathbb{P}(0|V, X)} \text{[Tchetgen Tchetgen and Spirtser, 2012].}
\]
To localize, let
\[
h_{1,\nu}(V, X) = \ell_\nu(V)h_1(V, X) \quad \text{and} \quad h_{2,\nu}(V, X, M) = \ell_\nu(V)h_2(V, X, M).
\]

**Example 6** (Time varying heterogeneous treatment effects). Let \( h_0(V, X_1, D_1, X_2, D_2) = \mathbb{E}(Y|V, X_1, D_1, X_2, D_2) \) be the outcome mechanism and let \( \mathbb{P}(X_2|X_1, D_1) \) be the covariate mechanism. Under exogeneity assumptions \cite{Robins, 1986}, the time varying heterogeneous treatment effects are
\[
\text{TIME}(v) = \mathbb{E}\{Y^{(d_1,d_2)}|V = v\} = \lim_{\nu \to 0} \mathbb{E}\left\{\int \ell_\nu(V)h_0(V, X_1, d_1, x_2, d_2)d\mathbb{P}(x_2|V, X_1, d_1)\right\}.
\]
Let $\mathbb{P}(D_1|V, X)$ and $\mathbb{P}(D_2|V, X_1, D_1, X_2)$ be the treatment mechanism. Then $h_1(V, X_1) = \int h_0(V, X_1, d_1, x_2, d_2) \mathbb{P}(x_2|V, X_1, d_1)\, d\mathbb{P}(x_2|V, X_1, d_1), h_2(V, X_1, X_2) = h_0(V, X_1, d_1, X_2, d_2), h_3(V, X_1, D_1, X_2, D_2) = \frac{1_{D_1=d_1}1_{D_2=d_2}}{\mathbb{P}(d_1|V, X_1)\mathbb{P}(d_2|V, X_1, D_2, X_2)}$, and $h_4(V, X_1, D_1) = \frac{1_{D_1=d_1}}{\mathbb{P}(d_1|V, X_1)}$ [Scharfstein et al., 1999]. To localize, let $h_1(\nu, V, X_1) = \ell(\nu)h_1(V, X_1)$ and $h_2(\nu, V, X_1, X_2) = \ell(\nu)h_2(V, X_1, X_2)$.

### E High probability events

Consider the concatenated space $\mathcal{Q} = \prod_{j=1}^{J} \mathcal{Q}_j$ of vector valued functions $q(W) = \{q_1(W), ..., q_J(W)\}^\top$, where each component is almost surely bounded above. Let $\ell\{W; q(W)\}$ be a loss function.

**Lemma 28** (Concentration; Lemma 14 of [Foster and Syrgkanis, 2023]). Suppose Assumption 1 holds for each $\mathcal{Q}_j$. Further suppose $\ell$ is $O(1)$ Lipschitz in its second argument with respect to $\ell_2$ norm. With probability $1 - \zeta$, for any fixed $q_0 \in \mathcal{Q}$ independent of data and for all $q \in \mathcal{Q}$, when $\delta_n = \Omega[\{J \log \log(n) + \log(1/\zeta)\}^{1/2}n^{-1/2}]$,

$$\left|\mathbb{E}_{n} - \mathbb{E}\right|\ell\{W; q(W)\} - \ell\{W; q_0(W)\}| = O\left(J \delta_n \sum_{j=1}^{J} \|q_j - q_{j,0}\|_2 + J\delta_n^2\right).$$

#### E.1 Sequential approach

**Proof of Lemma 28**. We appeal to Lemma 28 for each term in the empirical process.

1. Consider $(\mathbb{E}_{n} - \mathbb{E})\{h(B)f(C)\}$. Let $q(W) = h(B)f(C), q_0(W) = 0$, and $\ell\{W, q(W)\} = h(B)f(C)$, which has derivative 1 in its second argument. Then $|(\mathbb{E}_{n} - \mathbb{E})\{h(B)f(C) - 0\}| = O(\delta_n\|h\|_2+\delta_n^2) = O(\delta_n\|f\|_2+\delta_n^2)$ since $\mathcal{H}$ is almost surely bounded.

2. Consider $(\mathbb{E}_{n} - \mathbb{E})\{g(A)f(C)\}$. Let $q(W) = \{g(A), f(C)\}, q_0(W) = \{g_0(A), 0\}$, and $\ell\{W, q(W)\} = g(A)f(C)$, which has derivative $\{f(X), g(A)\}$ in its second argument. Then $|(\mathbb{E}_{n} - \mathbb{E})\{g(A)f(C) - 0\}| = O(\delta_n\|g - g_0\|_2+\delta_n\|f\|_2+\delta_n^2)$.

3. Consider $(\mathbb{E}_{n} - \mathbb{E})\{f(C)^2\}$. Let $q(W) = f(C), q_0(W) = 0$, and $\ell\{W, q(W)\} = f(C)^2$, which has derivative $2f(C)$ in its second argument. Then $|(\mathbb{E}_{n} - \mathbb{E})\{f(C)^2 - 0\}| = O(\delta_n\|f\|_2+\delta_n^2)$.
Proof of Lemma 3. The proof is identical to Lemma 2 except for the first empirical process \((\mathbb{E}_n - \mathbb{E})\{h(B)f(C)\}\). Let \(q(W) = \{h(B), f(C)\}, q_0(W) = \{h_*(B), 0\}\), and \(\ell\{W, q(W)\} = h(B)f(C)\), which has derivative \(\{f(X), h(B)\}\) in its second argument. Then by Lemma 28 \(|(\mathbb{E}_n - \mathbb{E})\{h(B)f(C) - 0\}| = O(\delta_n\|h - h_*\|_2 + \delta_n\|f\|_2 + \delta_n^2)\). □

Proof of Lemma 4. Let \(q(W) = h(B)\), \(q_0(W) = h_*(B)\), and \(\ell\{W, q(W)\} = h(B)^2\), which has derivative \(2h(B)\) in its second argument. Then by Lemma 28 \(|h\|_2^2 - \|h_*\|_2^2 - (\|h\|_2^2 - \|h_*\|_2^2) = |(\mathbb{E}_n - \mathbb{E})\{h(B)^2 - h_*(B)^2\}| = O(\delta_n\|h - h_*\|_2 + \delta_n^2)\). □

E.2 Simultaneous approach

Proof of Lemma 11. We appeal to Lemma 28 for each term in the former empirical process, similar to Lemma 2:

1. Consider \((\mathbb{E}_n - \mathbb{E})\{g(A)f'(C')\}\). Let \(q(W) = g(A)f'(C')\), \(q_0(W) = 0\), and \(\ell\{W, q(W)\} = g(A)f'(C')\), which has derivative \(1\) in its second argument. Then \(|(\mathbb{E}_n - \mathbb{E})\{g(A)f'(C') - 0\}| = O(\delta_n\|g f'\|_2 + \delta_n^2) = O(\delta_n\|f'\|_2 + \delta_n^2)\) since \(G\) is almost surely bounded.

2. Consider \((\mathbb{E}_n - \mathbb{E})\{Y f'(C')\}\). Let \(q(W) = f'(C')\), \(q_0(W) = 0\), and \(\ell\{W, q(W)\} = Y f'(C')\), which has derivative \(Y\) in its second argument. Then \(|(\mathbb{E}_n - \mathbb{E})\{Y f'(C') - 0\}| = O(\delta_n\|f'\|_2 + \delta_n^2)\).

3. As before, \(|(\mathbb{E}_n - \mathbb{E})\{f'(C')^2 - 0\}| = O(\delta_n\|f'\|_2 + \delta_n^2)\).

Next we turn to the latter empirical process.

1. As before, \(|(\mathbb{E}_n - \mathbb{E})\{h(B)f(C) - 0\}| = O(\delta_n\|f\|_2 + \delta_n^2)\).

2. Similarly, \(|(\mathbb{E}_n - \mathbb{E})\{g(A)f(C) - 0\}| = O(\delta_n\|f\|_2 + \delta_n^2)\).

3. As before, \(|(\mathbb{E}_n - \mathbb{E})\{f(C)^2 - 0\}| = O(\delta_n\|f\|_2 + \delta_n^2)\).
Proof of Lemma 12. Identical to Lemma 4.

F Regularization bias

F.1 Sequential approach

To lighten notation, we study $h_\mu = h_s$.

Proof of Lemma 8. We state the proof for completeness.

1. By Lemma 1, $h_s = \arg\min_{h \in \mathcal{H}} L_1(h, g_0) + \mu\|h\|^2_2 = \|T(h - h_0)\|^2_2 + \mu\|h\|^2_2$. Taking the Gateaux derivative, the first order condition yields $2T^*T(h_s - h_0) + 2\mu h_s = 0$ and hence $h_s = (T^*T + \mu)^{-1}(T^*T)h_0$. Hence

$$h_s - h_0 = (T^*T + \mu)^{-1}(T^*T - (T^*T + \mu))h_0 = -\mu(T^*T + \mu)^{-1}h_0.$$

Using $h_0 = (T^*T)^{3/2}w_0$,

$$\|h_s - h_0\|^2_2 = \|-\mu(T^*T + \mu)^{-1}(T^*T)^{3/2}w_0\|^2_2 \leq \mu^2\|(T^*T + \mu)^{-2}(T^*T)^{3/2}\|_{op} \|w_0\|^2_2,$$

$$\|T(h_s - h_0)\|^2_2 = \|-\mu(T^*T + \mu)^{-1}(T^*T)^{3/2}w_0\|^2_2 \leq \mu^2\|T^2(T^*T + \mu)^{-2}(T^*T)^{3/2}\|_{op} \|w_0\|^2_2.$$

2. We show $\mu^2\|(T^*T + \mu)^{-2}(T^*T)^{3/2}\|_{op} = \mu^2 \sup_j \frac{\sigma_j^{2\beta}}{\sigma_j^{\beta+\mu}} \leq \mu^{\min(\beta, 2)}$.

(a) If $\beta \geq 2$ then it suffices to show $\sup_j \frac{\sigma_j^{2\beta}}{\sigma_j^{\beta+\mu}} \leq 1$. Clearly $\frac{\sigma_j^{2\beta}}{\sigma_j^{\beta+\mu}} \leq \frac{1}{\sigma_j^{\beta-2}} \leq 1$ since $\beta \geq 2$ and $\sup_j \sigma_j \leq 1$.

(b) If $\beta < 2$ then it suffices to show $f(x) = \mu^2 \frac{x^\beta}{(x+\mu)^\beta} \leq \mu^\beta$. The first order condition yields $x* = \frac{\beta \mu}{2-\beta}$ and $f(x*) = \frac{1}{4}(2-\beta)^{2-\beta} \beta^\beta \mu^\beta \leq \mu^\beta$ since $\beta < 2$.

3. Finally, we show $\mu^2\|T^2(T^*T + \mu)^{-2}(T^*T)^{3/2}\|_{op} = \mu^2 \sup_j \frac{\sigma_j^{2(\beta+1)}}{\sigma_j^{\beta+\mu}} \leq \mu^{\min(\beta+1, 2)}$.

(a) If $\beta + 1 \geq 2$ then it suffices to show $\sup_j \frac{\sigma_j^{2(\beta+1)}}{\sigma_j^{\beta+\mu}} \leq 1$. Clearly $\frac{\sigma_j^{2(\beta+1)}}{\sigma_j^{\beta+\mu}} \leq \frac{\sigma_j^{2(\beta+1-2)}}{\sigma_j^{\beta+1}} \leq 1$ since $\beta \geq 1$ and $\sup_j \sigma_j \leq 1$. 

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(b) If \( \beta + 1 < 2 \) then it suffices to show \( f(x) = \mu^2 \frac{x^{(\beta+1)}}{(x+\mu)^2} \leq \mu^{\beta+1} \). The first order condition yields \( x_* = \frac{(\beta+1)\mu}{1-\beta} \) and \( f(x_*) = \mu^2 \left\{ \frac{(\beta+1)\mu}{1-\beta} \right\}^{\beta+1} \left\{ \frac{(\beta+1)\mu}{1-\beta} + \mu \right\}^{-2} \leq \mu^{\beta+1} \) since \( \beta < 1 \).

\[ \square \]

### F.2 Simultaneous approach

To lighten notation, we study \( \{g_{\mu',\mu}, h_{\mu',\mu}\} = (g_*, h_*) \). We use the notation \( T(h, g) = T_h(h) + T_g(g) \) where \( T_h(h) = T(h, 0) \) and \( T_g(g) = T(0, g) \)

**Lemma 29** (Rewriting regularization bias). We have

\[
g_* - g_0 = (I - A_GA_H)^{-1}(G_1 - A_GH_1) \\
h_* - h_0 = (I - A_HA_G)^{-1}(H_1 - A_HG_1)
\]

where

\[
G_1 = -\mu' (S^*S + T_g^*T_g + \mu')^{-1} g_0 \\
H_1 = -\mu (T_h^*T_h + \mu)^{-1} h_0 \\
A_G = (S^*S + T_g^*T_g + \mu')^{-1} T_g^*T_h \\
A_H = (T_h^*T_h + \mu)^{-1} T_h^*T_g.
\]

If Assumptions 2 and 5 hold then

\[
G_1 = -\mu' (S^*S + T_g^*T_g + \mu')^{-1} (S^*S)^{\beta_g/2} w_g' \\
= -\mu' (S^*S + T_g^*T_g + \mu')^{-1} (T_g^*T_g)^{\beta_g/2} w_g \\
H_1 = -\mu (T_h^*T_h + \mu)^{-1} (T_h^*T_h)^{\beta_h/2} w_h.
\]

**Proof.** By Lemmas 1 and 10

\[
(g_*, h_*) = \arg\min_{g \in G, h \in H} L'_1(g) + L_1(h, g) + \mu' \|g\|^2 + \mu \|h\|^2 \\
= \|S(g - g_0)\|^2 + \|T(h - h_0, g - g_0)\|^2 + \mu' \|g\|^2 + \mu \|h\|^2 \\
= \|S(g - g_0)\|^2 + \|T_h(h - h_0)\|^2 + \|T_g(g - g_0)\|^2 + 2(T_h(h - h_0), T_g(g - g_0)) + \mu' \|g\|^2 + \mu \|h\|^2.
\]
Taking the Gateaux derivative, the first order conditions yield, after dividing by two,

$$(S^*S + T^*_gT_g)(g_* - g_0) + T^*_gT_h(h_* - h_0) + \mu'g_* = 0$$

$$T^*_hT_h(h_* - h_0) + T^*_hT_g(g_* - g_0) + \mu h_* = 0.$$ 

Rearranging each expression,

$$g_* = (S^*S + T^*_gT_g + \mu')^{-1}\{(S^*S + T^*_gT_g)g_0 - T^*_gT_h(h_* - h_0)\}$$

$$h_* = (T^*_hT_h + \mu)^{-1}\{T^*_hT_hh_0 - T^*_hT_g(g_* - g_0)\}.$$

Hence

$$g_* - g_0 = (S^*S + T^*_gT_g + \mu')^{-1}\{-\mu'g_0 - T^*_gT_h(h_* - h_0)\} = G_1 - A_G(h_* - h_0)$$

$$h_* - h_0 = (T^*_hT_h + \mu)^{-1}\{-\mu h_0 - T^*_hT_g(g_* - g_0)\} = H_1 - A_H(g_* - g_0).$$

Rearranging yields the former the result. The latter is immediate. ☐

**Proof of Lemma 15.** We suppress the index $j$ to lighten notation.

1. By Lemma [29]

$$A_G \preceq \frac{\sigma^2_T}{\sigma^2_T + \sigma^2_\gamma + \mu'} \leq 1, \quad A_H \preceq \frac{\sigma^2_T}{\sigma^2_T + \mu} \leq 1,$$

$$(I - A_GA_H)^{-1} \preceq \frac{(\sigma^2_T + \mu)(\sigma^2_\gamma + \sigma^2_\sigma + \mu')}{\sigma^2_T(\sigma^2_\gamma + \mu') + \mu(\sigma^2_\gamma + \sigma^2_\sigma + \mu')} \leq \frac{\sigma^2_T + \sigma^2_\gamma + \mu'}{\sigma^2_\gamma + \mu'} = 1 + \frac{\sigma^2_T}{\sigma^2_\gamma + \mu'},$$

$$G_1 \preceq -\mu'\|w'_g\|_2 \frac{\sigma^2_\gamma}{\sigma^2_\gamma + \sigma^2_\sigma + \mu'} \preceq -\mu'\|w'_g\|_2 \frac{\sigma^2_\gamma}{\sigma^2_\gamma + \sigma^2_\sigma + \mu'}, \quad H_1 \preceq -\mu\|w_h\|_2 \frac{\sigma^2_\gamma}{\sigma^2_T + \mu}. $$

2. To bound $\|h_* - h_0\|_2^2$, it suffices to control

$$\|(I - A_HA_G)^{-1}H_1\|_2 \leq \|H_1\|_2 \leq \mu\|w_h\|_2 \frac{\sigma^2_\gamma}{\sigma^2_T + \mu},$$

$$\|(I - A_GA_H)^{-1}A_HG_1\|_2 \leq \|G_1\|_2 \leq \mu'\|w'_g\|_2 \frac{\sigma^2_\gamma}{\sigma^2_\gamma + \sigma^2_\sigma + \mu'} \wedge \mu'\|w'_g\|_2 \frac{\sigma^2_\gamma}{\sigma^2_T + \mu'}.$$

3. To bound $\|T_h(h_* - h_0)\|_2^2$, it suffices to control

$$\|T_h(I - A_HA_G)^{-1}H_1\|_2 \leq \|T_hH_1\|_2 \leq \mu\|w_h\|_2 \frac{\sigma^2_\gamma}{\sigma^2_T + \mu},$$

$$\|T_h(I - A_GA_H)^{-1}A_HG_1\|_2 \leq \|T_hG_1\|_2 \leq \mu'\|w'_g\|_2 \frac{\sigma^2_\gamma}{\sigma^2_T + \mu'}.$$
4. To bound \( \|g_* - g_0\|_2^2 \), it suffices to control
\[
\|(I - AGA_H)^{-1}G_1\|_2 \leq \|G_1\|_2 \leq \mu'\|w_2'\|_2 \frac{\sigma^{\beta_g}_S}{\sigma^2_S + \mu'} \land \mu'\|w_g\|_2 \frac{\sigma^{\beta_g}_S}{\sigma^2_T + \mu'},
\]
\[
\|(I - AGA_H)^{-1}AGH_1\|_2 \leq \|H_1\|_2 \leq \mu\|w_h\|_2 \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu}.
\]

5. To bound \( \|S(g_* - g_0)\|_2^2 \), it suffices to control
\[
\|S(I - AGA_H)^{-1}G_1\|_2 \leq \|SG_1\|_2 \leq \mu'\|w_2'\|_2 \frac{\sigma^{\beta_g}_S}{\sigma^2_S + \mu'} \land \mu'\|w_g\|_2 \frac{\sigma^{\beta_g}_S}{\sigma^2_T + \mu'} \leq \mu\|w_h\|_2 \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu}
\]
since by AM-GM inequality,
\[
\frac{\sigma^2_S}{\sigma^2_S + \sigma^2_T + \mu'} \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu'} = \frac{\sigma_S\sigma_T}{\sigma^2_S + \sigma^2_T + \mu'} \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu'} \leq \frac{1}{2} \frac{\sigma^2_S + \sigma^2_T}{\sigma^2_S + \sigma^2_T + \mu'} \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu'} \leq \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu}.
\]

6. To bound \( \|T_g(g_* - g_0)\|_2^2 \), it suffices to control
\[
\|T_g(I - AGA_H)^{-1}G_1\|_2 \leq \|T_gG_1\|_2 \leq \mu'\|w_2'\|_2 \frac{\sigma^{\beta_g}_T}{\sigma^2_T + \mu'},
\]
\[
\|T_g(I - AGA_H)^{-1}AGH_1\|_2 \leq \|T_hH_1\|_2 \leq \mu\|w_h\|_2 \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu}.
\]

7. Finally bound these expressions using the same algebra as Lemma 8.

\[
\text{G Causal functions}
\]

\textbf{G.1 Main result}

We revisit causal functions to clarify how the main inference result encompasses them. We pointwise approximate the causal function \( \theta_0(u) \) with the local functional \( \theta_\nu(u) \).

\textbf{Theorem 6} (Key quantities for causal functions in Estimator 4). Suppose that Assumption 7 holds. Suppose bounded balancing weight, residual variance, density, derivative, and kernel conditions defined below hold. Then for the local functional \( \theta_\nu \), suppressing

\[
|S\|_\infty \leq 1, \quad |H\|_\infty \leq 1, \quad |A\|_\infty \leq 1, \quad |A^T G_1 \|_\infty \leq 1, \quad |A^T H_1 \|_\infty \leq 1.
\]

We have
\[
\|T_g(I - AGA_H)^{-1}G_1\|_2 \leq \|T_gG_1\|_2 \leq \mu'\|w_2'\|_2 \frac{\sigma^{\beta_g}_T}{\sigma^2_T + \mu'},
\]
\[
\|T_g(I - AGA_H)^{-1}AGH_1\|_2 \leq \|T_hH_1\|_2 \leq \mu\|w_h\|_2 \frac{\sigma^{\beta_h}_T}{\sigma^2_T + \mu}.
\]
the index \(v, \kappa_\nu / \sigma_\nu \lesssim \nu^{-1/6}, \sigma_\nu \lesssim \nu^{-1/2}, \kappa_\nu \lesssim \nu^{-2/3}, \chi_\nu \lesssim \nu^{-3/4}, \) and \(\sigma_{1,\nu} \lesssim \nu^{-1}\bar{s}, \sigma_{2,\nu} \lesssim \nu^{-1}\bar{s}_2, \Delta_\nu \lesssim n^{1/2}\nu^{a_1/2}, \) where \(a_1\) is the order of differentiability defined below. Moreover, \(\|\tilde{h}_{1,\nu} - h_{1,\nu}\|_2 \lesssim \nu^{-1}\|\tilde{h}_1 - h_1\|_2, \|T_1(\tilde{h}_{1,\nu} - h_{1,\nu})\|_2 \lesssim \nu^{-1}\|T_1(h_1 - \tilde{h}_1)\|_2, \|\tilde{h}_{2,\nu} - h_{2,\nu}\|_2 \lesssim \nu^{-1}\|\tilde{h}_2 - h_2\|_2, \|T_1(\tilde{h}_{2,\nu} - h_{2,\nu})\|_2 \lesssim \nu^{-1}\|T_1(h_2 - \tilde{h}_2)\|_2.\)

Corollary 8 (Confidence interval validity in Estimator 4 Causal functions). Suppose Assumptions 7 and 8 hold as well as the regularity conditions of Theorem 4. Finally assume the following are \(o_p(1):\) the bandwidth rates \(n^{1/2}\nu^{-3/2}\) and \(n^{1/2}\nu^{a_1/2};\) the individual rates \((\nu^{-1} + \nu^{-1/2}\hat{h}_4 + \nu^{-1/2}\hat{h}_5)(\hat{h}_1 - h_1)\|_2, (\nu^{-1/2}\hat{h}_3 + \nu^{-1/2}\hat{h}_4 + \nu^{-1/2}\hat{h}_5 + \nu^{-1/2}\hat{h}_6)(\hat{h}_2 - h_2)\|_2, (\hat{h}_4 + \nu^{-1}\bar{s}_y)(\hat{h}_3 - h_3)\|_2, \nu^{-1}\bar{s}_2(\hat{h}_4 - h_4)\|_2;\) and the product rates

1. \(\nu^{-1/2}n^{1/2}\{\|\hat{h}_1 - h_1\|_2\|\hat{h}_4 - h_4\|_2 and T_2(\hat{h}_2 - h_2)\|_2, \|\hat{h}_3 - h_3\|_2\|\hat{h}_2 - h_2\|_2, \|T_3(\hat{h}_3 - h_3)\|_2\};\)

2. \(\nu^{-1/2}n^{1/2}\{\|\hat{h}_2 - h_2\|_2\|\hat{h}_4 - h_4\|_2 and T_2(\hat{h}_2 - h_2)\|_2, \|\hat{h}_3 - h_3\|_2\|\hat{h}_2 - h_2\|_2, \|T_3(\hat{h}_3 - h_3)\|_2\};\)

3. \(\nu^{-1/2}n^{1/2}\{\|\hat{h}_2 - h_2\|_2\|\hat{h}_4 - h_4\|_2 and T_2(\hat{h}_2 - h_2)\|_2, \|\hat{h}_4 - h_4\|_2\|\hat{h}_2 - h_2\|_2, \|T_4(\hat{h}_4 - h_4)\|_2\}.

Then \(\hat{\theta}_\nu \xrightarrow{p} \theta_0, \frac{\sqrt{n}}{\sigma_\nu}(\hat{\theta}_\nu - \theta_0) \xrightarrow{d} \mathcal{N}(0, 1),\) and \(\mathbb{P}\{\theta_0 \in (\hat{\theta}_\nu \pm c_\alpha \bar{s}_\nu n^{-1/2})\} \to 1 - \alpha.\)

G.2 Extended notation

While proving this result, we use the notation of Appendix C. We emphasize which quantities are diverging sequences for local functionals by indexing with the bandwidth \(h.\) We study a function of the variable \(V \subset W, i.e. \theta_0(v),\) which we approximate with \(\theta_{0,h}(v) = \mathbb{E}\{\ell_h(V)\nu_0(W)\} = \mathbb{E}\{\nu_{0,h}(W)\}.\) Denote the localized moment function

\[
\psi_h(W; \theta_h, \nu_h, \delta_h, \alpha, \eta) = \nu_h(W) + \alpha(W)\{Y_h - \delta_h(W)\} + \eta(W)\{\delta_h(W) - \nu_h(W)\} - \theta_h
\]

where \(\nu_h(W) = \ell_h(V)\nu(W), \delta_h(W) = \ell_h(V)\delta(W),\) and \(Y_h = \ell_h(V)Y.\) To use Theorem 4, we reduce the rates for the localized nuisances \((\hat{\nu}_h, \hat{\delta}_h)\) to the rates for the global nuisances \((\hat{\nu}, \hat{\delta}).\) Intuitively, we expect the former to be slower than the latter.

The moments of the localized moment function are \(0 = \mathbb{E}\{\psi_{0,h}(W)\}, \sigma_h^2 = \mathbb{E}\{\psi_{0,h}(W)^2\}, \kappa_h^3 = \mathbb{E}\{|\psi_{0,h}(W)|^3\},\) and \(\chi_h^4 = \mathbb{E}\{\psi_{0,h}(W)^4\}.\) The moments \((\sigma_h, \kappa_h, \chi_h)\) are indexed
by \( h \), so a complete analysis must also characterize how these parameters diverge as bandwidth \( h \) vanishes. Doing so will verify the regularity condition on moments and also pin down the nonparametric rate of Gaussian approximation \( \sigma_h n^{-1/2} \).

Finally, the residual variances must also be updated. With localization, they become \( \mathbb{E}[(Y_h - \delta_{0,h}(W))^2 | W] \leq \sigma_{1,h}^2 \) and \( \mathbb{E}[(\delta_{0,h}(W) - \nu_{0,h}(W_1))^2 | W_1] \leq \bar{\sigma}_{2,h}^2 \). A complete analysis must also characterize how these parameters diverge as bandwidth \( h \) vanishes.

We restate the conclusions of Theorem 6 that we wish to prove in this alternative notation. Suppose that the global residual variances are finite. Suppose bounded balancing weight, residual, density, derivative, and kernel conditions hold. Then for local functionals, \( \kappa_h/\sigma_h \lesssim h^{-1/6}, \sigma_h \approx h^{-1/2}, \kappa_h \lesssim h^{-2/3}, \chi_h \approx h^{-3/4} \) and \( \bar{\sigma}_{1,h} \lesssim h^{-1} \bar{\sigma}_1, \bar{\sigma}_{2,h} \lesssim h^{-1} \bar{\sigma}_2, \Delta_h \lesssim n^{1/2} h^{s+1/2} \) where \( s \) is the order of differentiability. Moreover, \( \mathcal{R}(\hat{\nu}_{\ell,h}) \lesssim h^{-2} \mathcal{R}(\hat{\nu}_{\ell}), \mathcal{P}(\hat{\nu}_{\ell,h}) \lesssim h^{-2} \mathcal{P}(\hat{\nu}_{\ell}), \mathcal{R}(\hat{\delta}_{\ell,h}) \lesssim h^{-2} \mathcal{R}(\hat{\delta}_{\ell}), \mathcal{P}(\hat{\delta}_{\ell,h}) \lesssim h^{-2} \mathcal{P}(\hat{\delta}_{\ell}). \)

### G.3 Oracle moments

To lighten notation, we write \( \ell = \ell_h \). We also suppress the arguments of functions and define \( U_0 = \nu_0 - \mathbb{E}(\nu_0), U_1 = Y - \delta_0, U_2 = \delta_0 - \nu_0 \) so that \( \psi_{0,h} = \ell \cdot (U_0 + \alpha_0 U_1 + \eta_0 U_2) \). Finally, we lighten notation by defining \( \|W\|_{p,q} = \{\mathbb{E}(W^q)\}^{1/q} \).

**Lemma 30** (Oracle moments for local functionals). Suppose there exist

\[
(\alpha, \bar{\alpha}, \eta, \bar{\eta}, \sigma_0, \bar{\sigma}_0, \sigma_1, \bar{\sigma}_1, \sigma_2, \bar{\sigma}_2, f, \bar{f}, \bar{f}', h_0)
\]

bounded away from zero and above such that the following conditions hold.

1. Control of balancing weights: \( \alpha \leq \|\alpha_0\|_\infty \leq \bar{\alpha}, \eta \leq \|\eta_0\|_\infty \leq \bar{\eta} \).

2. Control of residual moments: for \( q \in \{2, 3, 4\}, \sigma_0 \leq \|U_0||W|_{p,q} \leq \bar{\sigma}_0, \sigma_1 \leq \|U_1||W|_{p,q} \leq \bar{\sigma}_1, \sigma_2 \leq \|U_2||W|_{p,q} \leq \bar{\sigma}_2 \).

3. Bounded density: the density \( f_V \) obeys, for all \( v' \in N_{h_0}(v) = (v' : |v' - v| \leq h_0) \),

\[
\bar{f} \leq f_V(v') \leq \bar{f} \text{ and } |\partial f_V(v')| \leq \bar{f}'.
\]

Then \( \frac{\kappa_h}{\sigma_h} \lesssim h^{-1/6}, \sigma_h \approx h^{-1/2}, \kappa_h \lesssim h^{-2/3}, \chi_h \lesssim h^{-3/4} \).
Proof. We extend [Chernozhukov et al., 2022b] Lemma 3.4. We proceed in steps.

1. Observe that $\sigma_h^2 = \mathbb{E}\{\ell^2 \cdot (U_0^2 + \sigma_0^2 U_1^2 + \eta_0^2 U_2) + 2\alpha_0 U_0 U_1 + 2\eta_0 U_0 U_2 + 2\alpha_0 \eta_0 U_1 U_2\}$ equals $\mathbb{E}\{\ell^2 \cdot (U_0^2 + \sigma_0^2 U_1^2 + \eta_0^2 U_2)\}$ by Assumption 7. In particular, we use $\mathbb{E}\{\alpha(W) - \alpha_0(W)\} U_1 = 0$ and $\mathbb{E}\{\eta(W) - \eta_0(W)\} U_2 = 0$. Hence

$$ \sigma_h^2 \leq \sigma_0^2 + \alpha^2 \sigma_1^2 + \eta^2 \sigma_2^2 ||\ell||_{P,2}.$$  

Moreover, $||\psi_{0,h}||_{P,q} \leq (\sigma_0 + \alpha \sigma_1 + \eta \sigma_2) ||\ell||_{P,q}$. In summary, $||\ell||_{P,2} \lesssim \sigma_h \lesssim ||\ell||_{P,2}$ and $||\psi_{0,h}||_{P,q} \lesssim ||\ell||_{P,q}$.

2. Consider the change of variables $u = (v' - v)/h$ so that $du = h^{-1} dv'$. Hence

$$ ||\ell||_{P,q}^q \omega^q = ||\ell\omega||_{P,q}^q = \int h^{-q} \left| K \left( \frac{v' - v}{h} \right) \right|^q f_V(v') dv' = \int h^{-(q-1)} |K(u)|^q f_V(v - uh) du.$$  

It follows that $h^{-(q-1)/q} f^1 f^{1/q} (\int |K|^q)^{1/q} \leq ||\ell||_{P,q} \omega \leq h^{-(q-1)/q} \tilde{f}^{1/q} (\int |K|^q)^{1/q}$. Further, we have that $\omega = \int h^{-1} K \left( \frac{v' - v}{h} \right) f_V(v') dv' = \int K(u) f_V(v - vh) du$ and $\int K(u) f_V(v - uh) du = \int K(u) f_V(v) du = f_V(v)$. Using the Taylor expansion in $h$ around $h = 0$ and the Holder inequality, there exist some $\tilde{h} \in [0, h]$ such that

$$ |\omega - f_V(v)| \leq h \int K(u) \partial_v f_V(v - vh) du \leq h \tilde{f} \int |u| K(u) du.$$  

Hence there exists some $h_1 \in (h, h_0)$ depending only on $(K, \tilde{f}, \tilde{f}, \tilde{f})$ such that $f/2 \leq \omega \leq 2 \tilde{f}$. In summary,

$$ h^{-(q-1)/q} f^1 f^{1/q} (\int |K|^q)^{1/q} \frac{1}{2f} \leq ||\ell||_{P,q} \leq h^{-(q-1)/q} \tilde{f}^{1/q} (\int |K|^q)^{1/q} \frac{2}{f},$$  

which implies $h^{-(q-1)/q} \lesssim ||\ell||_{P,q} \lesssim h^{-(q-1)/q}$.

3. For all $h < h_1$, $\sigma_h \lesssim ||\ell||_{P,2}$, $||\psi_{0,h}||_{P,2} \lesssim ||\ell||_{P,q}$, $||\ell||_{P,q} \lesssim h^{-(q-1)/q}$. \hfill $\square$

G.4 Residual variances and learning rates

Lemma 31 (Residual variance for local functionals). Suppose there exist $(\tilde{\sigma}_1, \tilde{\sigma}_2, \bar{f}, \bar{f}, \bar{f}', h_0, \bar{K})$ bounded away from zero and above such that the following conditions hold.
1. Bounded residual variance: \[ \|U_1|W\|_{\mathbb{F},2} \leq \bar{\sigma}_1, \|U_2|W\|_{\mathbb{F},2} \leq \bar{\sigma}_2. \]

2. Bounded density: the density \( f_V \) obeys, for all \( v' \in N_{h_0}(v) \), \( 0 < f \leq f_V(v') \leq \bar{f}, \) \( |\partial f_V(v')| \leq \bar{f}. \)

3. Bounded kernel: \( |K(u)| \leq \bar{K}. \)

Then \( \bar{\sigma}_{h,1} \lesssim h^{-1} \bar{\sigma}_1 \) and \( \bar{\sigma}_{h,2} \lesssim h^{-1} \bar{\sigma}_2. \)

**Proof.** Write \( \bar{\sigma}_{1,h} = \|\ell \cdot U_1|W\|_{\mathbb{F},2} \leq \|\ell\|_{\infty} \|U_1|W\|_{\mathbb{F},2}. \) By the proof of Lemma \( 30 \) \( \|\ell\|_{\infty} = \left\| \frac{1}{h_0} K\left(\frac{v'-v}{h}\right) \right\|_{\infty} \leq \bar{K} \frac{1}{h_0} \leq \bar{K} \frac{2}{h}. \) Therefore \( \bar{\sigma}_{1,h} \leq \bar{K} \frac{2}{h} \cdot \bar{\sigma}_h \lesssim h^{-1} \bar{\sigma}_1. \) The argument for \( \bar{\sigma}_{2,h} \) is identical. \( \square \)

A natural choice of estimator \( \hat{\nu}_h \) for \( \nu_{0,h} \) is the localization \( \ell_h \) times an estimator \( \hat{\nu} \) for \( \nu_0. \) We prove that this choice translates global nuisance parameter rates into local nuisance parameter rates under mild regularity conditions.

**Lemma 32 (Translating global rates to local rates).** Suppose the conditions of Lemma \( 31 \) hold. Then \( \mathcal{R}(\hat{\nu}_{\ell,h}) \lesssim h^{-2} \mathcal{R}(\hat{\nu}_\ell), \mathcal{P}(\hat{\nu}_{\ell,h}) \lesssim h^{-2} \mathcal{P}(\hat{\nu}_\ell), \mathcal{R}(\hat{\delta}_{\ell,h}) \lesssim h^{-2} \mathcal{R}(\hat{\delta}_\ell), \mathcal{P}(\hat{\delta}_{\ell,h}) \lesssim h^{-2} \mathcal{P}(\hat{\delta}_\ell). \)

**Proof.** We generalize [Chernozhukov et al., 2023] Lemma 10]. Write \( \mathcal{R}(\hat{\nu}_{\ell,h}) = \mathbb{E}\{\|\ell_h(W_i)\hat{\nu}_\ell(W) - \ell_h(W_i)\nu_0(W)\|^2 | I\}. \) From the proof of Lemma \( 31 \) \( \|\ell_h\|_{\infty} \lesssim h^{-1}. \) The remaining results are identical. \( \square \)

### G.5 Approximation error

Finally, we characterize the finite sample approximation error \( \Delta_h = n^{1/2}\sigma^{-1}|\theta_{0,h} - \theta_0| \) where \( \theta_0 = \lim_{h \to 0} \theta_{0,h}. \) Here, \( \Delta_h \) is bias from approximating a causal function using sequence of local functionals. We define \( m(v) = \mathbb{E}\{\nu_0(W) | V = v\} \) to lighten notation.

**Lemma 33 (Approximation error from localization [Chernozhukov et al., 2022b]).** Suppose there exist constants \( (h_0, s, \bar{g}_s, \bar{f}_s, \bar{f}, \bar{g}) \) bounded away from zero and above such that the following conditions hold.
1. Differentiability: on $N_{ho}(v) = \{v' : |v' - v| \leq h_0\}$, $m(v')$ and $f_V(v')$ are differentiable to the integer order $d$.

2. Bounded derivatives: let $s = d \wedge o$ where $o$ is the order of the kernel $K$. Let $\partial^s_v$ denote the $s$ order derivative $\partial^s/(\partial v)^s$. Assume $\sup_{v' \in N_{ho}(v)}\|\partial^s_v(m(v')f_V(v'))\|_{op} \leq \bar{g}_s$, $\sup_{v' \in N_{ho}(v)}\|\partial^s_v f_V(v')\|_{op} \leq \bar{f}_s$, $\inf_{v' \in N_{ho}(v)} f_V(v') \geq \underline{f}$. Then there exist constants $(C, h_1)$ depending only on $(h_0, K, \bar{g}_s, \bar{f}_s, \underline{f}, \bar{g})$ such that for all $h_1 \in (h, h_0)$, $|\theta_{0,h} - \theta_0| \leq C h^s$. In summary, $\Delta_h \lesssim n^{1/2} h^{s+1/2}$.

H Multiple robustness to ill posedness

H.1 Sequential approach

Proof of Corollary 1. The result is immediate from Theorem 1. \hfill \Box

Proof of Corollary 2. To lighten notation, let $\bar{r} = \max\{\delta_n, \|\hat{g} - g_0\|_2\}$. We minimize the mean square bound in Theorem 2: $\|\hat{h} - h_0\|^2 = O(\mu_{\min}(\beta, 1)\|w_0^*\|^2 + \mu^{-1}\bar{r}^2)$.

In the case $\beta \geq 1$, the first order condition is $\|w_0^*\|^2 - \mu^{-2}\bar{r}^2 = 0$, suggesting $\mu \asymp \bar{r}$, $R_n \asymp \mu^2 + \bar{r}^2 \asymp \bar{r}^2$, and $\mu^{-1}R_n \asymp \bar{r}$.

In the case $\beta < 1$, the first order condition is $\mu^{\beta - 1}\beta\|w_0^*\|^2 - \mu^{-2}\bar{r}^2 = 0$, suggesting $\mu \asymp \bar{r}^{\frac{2}{\beta+1}}$, $R_n \asymp \mu^{\beta+1} + \bar{r}^2 \asymp \bar{r}^2$, and $\mu^{-1}R_n \asymp \bar{r}^2 - \frac{2}{\beta+1} \bar{r}^{\frac{2}{\beta+1}}$. \hfill \Box

Proof of Corollary 3. By Corollary 2 we set $\mu_g = \frac{\delta_n}{\delta_n^{\text{well}}(\beta_g)}$ to obtain $\|\hat{g} - g_0\|^2 = O\{\delta_n^{\text{well}}(\beta_g)\}$, which dominates $\delta_n^2$. Hence $\bar{r}^2 = \delta_n^{\text{well}}(\beta_g)$. Thus by Corollary 2 we set $\mu_h = \frac{\delta_n}{\delta_n^{\text{well}}(\beta_h)}$ to obtain $\|T(\hat{h} - h_0^*)\|^2 = O(\bar{r}^2)$ and $\|\hat{h} - h_0^*\|^2 = O\{\bar{r}^{\text{well}}(\beta_h)\}$. \hfill \Box

Proof of Corollary 4. To begin, recall the rates we have derived. By Corollary 2, $\|T(\hat{g} - g_0)\|^2 = O(\delta_n)$ and $\|\hat{g} - g_0\|^2 = O\{\delta_n^{\text{well}}(\beta_g)\}$. By Corollary 3, $\|T(\hat{h} - h_0^*)\|^2 = O\{\delta_n^{\text{well}}(\beta_h)\}$ and $\|\hat{h} - h_0^*\|^2 = O\{\delta_n^{\text{well}}(\beta_h^{\text{well}}(\beta_g))\}$. 

\[72\]
1. The first product rate condition of Corollary 5 is satisfied when
\[ n^{1/2} \sigma^{-1} \{ \| T_1(\hat{h}_1 - h_1)\|_2 \| \hat{h}_4 - h_4\|_2 \} = o_p(1). \]
Since \( h_1 \) is a nested NPIV and \( h_4 \) is an NPI, the former term is
\[ n^{1/2} \sigma^{-1} \| T_1(\hat{h}_1 - h_1)\|_2 \| \hat{h}_4 - h_4\|_2 \] = \( O\left[ n^{1/2 - \gamma - \alpha(\text{WELL}(\beta_1 g) + \text{WELL}(\beta_4))} \right] \).
Meanwhile the latter term is
\[ n^{1/2} \sigma^{-1} \| \hat{h}_1 - h_1\|_2 \| T_4(\hat{h}_4 - h_4)\|_2 \] = \( O\left[ n^{1/2 - \gamma - \alpha(\text{WELL}(\beta_1 h) \text{WELL}(\beta_1 g) + 1)} \right] \).
In summary, the first product rate condition requires
\[ \left[ \frac{1}{2} - \gamma - \alpha \{ \text{WELL}(\beta_1 g) + \text{WELL}(\beta_4) \} \right] \wedge \left[ \frac{1}{2} - \gamma - \alpha \{ \text{WELL}(\beta_1 h) \text{WELL}(\beta_1 g) + 1 \} \right] < 0. \]
Rearranging, \( \frac{1}{2} < \gamma + \alpha \{ \text{WELL}(\beta_1 g) + \text{WELL}(\beta_4) \} \lor \{ \text{WELL}(\beta_1 h) \text{WELL}(\beta_1 g) + 1 \} \).
The latter branch of the maximum weakly dominates the former since \( \text{WELL}(\beta) \in [0, 1/2] \) and \( \text{WELL}(\beta_1 g) \) appears in both branches.

2. The second product rate condition is similar. Again, the latter branch weakly dominates the former.

3. For the third product rate condition, we require
\[ n^{1/2} \sigma^{-1} \{ \| T_2(\hat{h}_2 - h_2)\|_2 \| \hat{h}_4 - h_4\|_2 \wedge \| \hat{h}_2 - h_2\|_2 \| T_4(\hat{h}_4 - h_4)\|_2 \}. \]
Since \((h_2, h_4)\) are NPIVs, the former term is
\[ n^{1/2} \sigma^{-1} \| T_2(\hat{h}_2 - h_2)\|_2 \| \hat{h}_4 - h_4\|_2 = O\left[ n^{1/2 - \gamma - \alpha(1 \text{+ \text{WELL}(\beta_4))}} \right] \].
Meanwhile the latter term is
\[ n^{1/2} \sigma^{-1} \| \hat{h}_2 - h_2\|_2 \| T_4(\hat{h}_4 - h_4)\|_2 = O\left[ n^{1/2 - \gamma - \alpha(\text{WELL}(\beta_2) + 1)} \right] \].
In summary, the first product rate condition requires
\[ \left[ \frac{1}{2} - \gamma - \alpha \{ 1 + \text{WELL}(\beta_4) \} \right] \wedge \left[ \frac{1}{2} - \gamma - \alpha \{ \text{WELL}(\beta_2) + 1 \} \right] < 0. \]
Rearranging, \( \frac{1}{2} < \gamma + \alpha \{ 1 + \text{WELL}(\beta_4) \} \lor \{ \text{WELL}(\beta_2) + 1 \} \).
H.2 Simultaneous approach

Proof of Corollary 4. To lighten notation, let $\beta = \min(\beta_h, \beta_y, \beta_y')$ and $\|\bar{w}\|^2 = \max(\|w_h\|^2, \|w_y\|^2, \|w_y'\|^2)$. We minimize the mean square bound in Theorem 3:

$$\mathbb{E}(\hat{\beta} - \beta_h)^2 = \mathbb{E}(\hat{\beta} - \beta_y)^2 = O\left(\frac{\mu^{\min(\beta,1)}}{\delta_n} + \mu^{-1}\delta_n^2\right).$$

In the case $\beta \geq 1$, the first order condition is $\|\bar{w}\|^2 - \mu^{-2}\delta_n^2 = 0$, suggesting $\mu \asymp \delta_n$, $R_n \asymp \mu^2 + \delta_n^2$, and $\mu^{-1}R_n \asymp \delta_n$.

In the case $\beta < 1$, the first order condition is $\mu^{\beta - 1}\beta \|\bar{w}\|^2 - \mu^{-2}\delta_n^2 = 0$, suggesting $\mu \asymp \delta_n^{\frac{2}{\beta - 1}}$, $R_n \asymp \mu^{\beta + 1} + \delta_n^2$, and $\mu^{-1}R_n \asymp \delta_n^{2 - \frac{2}{\beta - 1}} = \delta_n^{\frac{2\beta}{\beta - 1}}$.

Proof of Corollary 7. By Corollary 4, the projected rates are $O(\delta_n)$ and the mean square rates are $O\left(\delta_n^{\text{WELL}(\beta_j)}\right)$ where $\beta_j = \min(\beta_j)$. The first product rate condition of Corollary 5 is satisfied when

$$n^{1/2}\sigma^{-1}\left\{\|T_1(\hat{h}_1 - h_1)\|_2\|\hat{h}_4 - h_4\|_2 \wedge \|\hat{h}_1 - h_1\|_2\|T_4(\hat{h}_4 - h_4)\|_2\right\} = o_p(1).$$

The former term is $n^{1/2}\sigma^{-1}\|T_1(\hat{h}_1 - h_1)\|_2\|\hat{h}_4 - h_4\|_2 = O\left[n^{\frac{1}{2} - \gamma - \alpha}\{1 + \text{WELL}(\beta_4)\}\right]$. Meanwhile the latter term is $n^{1/2}\sigma^{-1}\|\hat{h}_1 - h_1\|_2\|T_4(\hat{h}_4 - h_4)\|_2 = O\left[n^{\frac{1}{2} - \gamma - \alpha}\{\text{WELL}(\beta_4) + 1\}\right]$. In summary, the first product rate condition requires

$$\left[\frac{1}{2} - \gamma - \alpha\{1 + \text{WELL}(\beta_4)\}\right] \wedge \left[\frac{1}{2} - \gamma - \alpha\{\text{WELL}(\beta_4) + 1\}\right] < 0.$$

Rearranging, $\frac{1}{2} \leq \gamma + \alpha\left\{\text{WELL}(\beta_4) + 1\right\} \vee \left\{\text{WELL}(\beta_4) + 1\right\}$. The other product rate conditions are similar. \hfill \Box

I Simulation and application details

I.1 Nested NPIV

Let $g_0(A) = A^T_1$ and $h_0(B) = f(B_1)$, where $f : \mathbb{R} \to \mathbb{R}$ is one of four possible functions. For simplicity, we write $p = \text{dim}(A) = \text{dim}(B) = \text{dim}(C) = \text{dim}(C')$. We define $F : (x_1, \ldots, x_p) \mapsto (x_1^{1/3}, \ldots, x_p^{1/3})$ and $1_p = (1, \ldots, 1)^\top \in \mathbb{R}_p$.

Each observation is generated as follows. Independently draw the instruments $C \sim \mathcal{N}(0, \ldots 1_p)$ and $C' \sim \mathcal{N}(0, \ldots 1_p)$. Next draw the noise terms $U \sim \mathcal{N}(0, 1), U_A \sim \mathcal{N}_p(0, \ldots 1_p)$.
\[ \mathcal{N}\{0, \min(1, |C_1|)\}, \quad U_B \sim \mathcal{N}(0, 0.1), \quad \text{and} \quad U_Y \sim \mathcal{N}\{0, \min(1, |C'_1|)\}. \]

Finally, set \( B = C + 1_p \cdot U + 1_p \cdot U_B, \) \( A = F\{h_0(B) \cdot 1_p + U \cdot 1_p + C' + U_A \cdot 1_p\}, \) and \( Y = g_0(A) + U + U_Y. \)

**Proposition 1** (Nested NPIV simulation). The nested NPIV simulation design satisfies \( \mathbb{E}\{h_0(B)|C\} = \mathbb{E}\{g_0(A)|C\} \) and \( \mathbb{E}\{g_0(A)|C'\} = \mathbb{E}(Y|C'). \)

**Proof.** Clearly \( \mathbb{E}\{Y - g_0(A)|C'\} = \mathbb{E}\{U + U_Y|C'\} = 0. \) Moreover, \( \mathbb{E}\{g_0(A) - h_0(B)|C\} = \mathbb{E}\{A_1^3 - h_0(B)|C'\} = \mathbb{E}\{U + C_1 + U_A|C\} = 0. \)

\[ \square \]

### I.2 Coverage

To begin, we recap the linear design of [Dukes et al., 2023] in our notation. Each variable is a scalar except for \( X \in \mathbb{R}^2. \) Each observation is generated as follows:

1. \((X_1, X_2, U)^\top \sim \mathcal{N}\{(0.25, 0.25, 0)^\top, \Sigma\} \) where \( \Sigma = \begin{pmatrix} 0.25 & 0.00 & 0.05 \\ 0.00 & 0.25 & 0.05 \\ 0.05 & 0.05 & 1.00 \end{pmatrix}; \)

2. \( D|X, U \sim \text{Bernoulli}[1 + \exp\{(0.5, 0.5)^\top X + 0.4U\}]^{-1}; \)

3. \( Z|X, D, U \sim \mathcal{N}\{0.2 - 0.52D + (0.2, 0.2)^\top X - U, 1\}; \)

4. \( W|X, U \sim \mathcal{N}\{0.3 + (0.2, 0.2)^\top X - 0.6U, 1\}; \)

5. \( M|X, D, U \sim \mathcal{N}\{-0.3D - (0.5, 0.5)^\top X + 0.4U, 1\}; \)

6. \( Y|X, D, M, W, U = 2 + 2D + M + 2W - (1, 1)^\top X - U + 2\mathcal{N}(0, 1). \)

Recall that \( h_0 \) is an outcome confounding bridge that solves \( \mathbb{E}\{h(X, D, W)|X, Z, D = 0\} = \mathbb{E}\{g_0(X, 1, M, W)|X, Z, D = 0\}, \) where \( g_0 \) solves \( \mathbb{E}\{g(X, D, M, W)|X, Z, D = 1, M\} = \mathbb{E}(Y|X, Z, D = 1, M). \)

Recall that \( h'_0 \) is a treatment confounding bridge that solves \( \mathbb{E}\{h'(X, Z, D, M)|X, D = 1, M, W\} = \mathbb{E}\{g'_0(X, Z, 0) \frac{\mathbb{P}(D=0|X,M,W)}{\mathbb{P}(D=1|X,M,W)}|X, D = 1, M, W\}, \) where \( g'_0 \) solves \( \mathbb{E}\{g'(X, Z, D)|X, D = 0, W\} = \mathbb{E}\{\frac{1}{\mathbb{P}(D=0|X,W)}|X, D = 0, W\}. \)
We write the nuisances as \( h_1(X, W) = h_0(X, 0, W), h_2(X, M, W) = g_0(X, 1, M, W), h_3(X, Z, D, M) = 1_{D=1}h_0'(X, Z, 1, M), \) and \( h_4(X, Z, D) = 1_{D=0}g_0'(X, Z, 0). \)

Consider the notation \( \mathbb{E}(A|B, C) = \beta_A + \beta_{AB}B + \beta_{AC}C \) and \( \mathbb{V}(A|B, C) = v_{AB}^2. \)

Also define \( \mathbb{P}(D = 0|X, U) = [1 + \exp\{-(\pi_0 + \pi_X X + \pi_U U)\}]^{-1} \) and \( \log\left\{ \frac{\mathbb{P}(D = 0|X, M, U)}{\mathbb{P}(D = 1|X, M, U)} \right\} = \rho_0 + \rho_X X + \rho_M M + \rho_U U. \)

**Proposition 2** (Linear coverage simulation; c.f. Supplementary Material of [Dukes et al., 2023]). The linear design for coverage simulations satisfies

\[
\begin{align*}
    h_1(X, W) &= \nu_0 + \nu_X^T X + \nu_W W, \\
    h_2(X, M, W) &= \delta_0 + \delta_X^T X + \delta_M M + \delta_W W, \\
    h_3(X, Z, D, M) &= 1_{D=1}[1 + \exp\{-(\eta_0 + \eta_X^T X + \eta_Z Z)\}] \exp\left(\alpha_0 + \alpha_X^T X + \alpha_Z Z + \alpha_M M\right), \\
    h_4(X, Z, D) &= 1_{D=0}[1 + \exp\{-(\eta_0 + \eta_X^T X + \eta_Z Z)\}],
\end{align*}
\]

where \((\nu, \delta, \alpha, \eta)\) can be expressed in terms of \((\beta, v, \pi, \rho)\) as follows:

\[
(\nu_X, \nu_W^T, \nu_W) = \left(\delta_0 + \delta_M \beta_{M0} + \delta_W \beta_{W0} - \nu_W \beta_{W0}, \delta_M \beta_{MX} + \delta_W \beta_{WX} + \delta_X - \nu_W \beta_{WX}, \frac{\delta_M \beta_{MU} + \delta_W \beta_{WU}}{\beta_{WU}}\right)
\]

\[
(\delta_X, \delta_M, \delta_W) = \left(\beta_{Y0} + \beta_{YD} + \beta_{YW} \beta_{W0} - \delta_W \beta_{W0}, \beta_{YW} \beta_{WX} + \beta_X - \delta_W \beta_{WX}, \frac{\beta_{YW} \beta_{WU} + \beta_{YU}}{\beta_{WU}}\right);
\]

\[
(\alpha_0, \alpha_X^T, \alpha_Z, \alpha_M) = \left(\rho_0 - \alpha_Z \beta_{Z0} + \beta_{ZD} - \frac{\alpha_Z^2 \beta_{Z0}^2}{2}, \rho_X - \alpha_Z \beta_{ZX}, \frac{\rho_U}{\beta_{ZU}}, \rho_M\right);
\]

\[
(\eta_0, \eta_X^T, \eta_Z) = \left(\pi_0 - \eta_Z \beta_{Z0} + \frac{\pi_Z^2 \beta_{Z0}^2}{2}, \pi_X - \eta_Z \beta_{ZX}, \frac{\pi_U}{\beta_{ZU}}\right).
\]

Moreover, \(\rho\) can be expressed in terms of \((\beta, v, \pi)\) as

\[
(\rho_0, \rho_X^T, \rho_M, \rho_U) = \left\{\frac{\beta_{MD}}{v_{M[D,X,U]}}(\beta_{M0} + \beta_{MD}/2) + \pi_0, \frac{\beta_{MD}}{v_{M[D,X,U]}} \beta_{MX} + \pi_X, \frac{\beta_{MD}}{v_{M[D,X,U]}} + \pi_U, \frac{\beta_{MD}}{v_{M[D,X,U]}} + \pi_U\right\}.
\]

Finally, in this design, \(\theta_0 = 4.05\).

Next, we extend the linear design to a nonlinear design. Instead of observing \((X_1, X_2, Z, D, M, Y, W)\), we observe

\[
(\tilde{X}_1, \tilde{X}_2, \tilde{Z}, \tilde{D}, \tilde{M}, \tilde{Y}, \tilde{W}) = \{f(X_1), f(X_2), f(Z), D, f(M), Y, f(W)\}
\]

where \(f : \mathbb{R} \rightarrow \mathbb{R}\) is one of four possible functions. Let \(\tilde{\theta}_0\) be the causal parameter in the nonlinear design, and let \((\tilde{h}_1, \tilde{h}_2, \tilde{h}_3, \tilde{h}_4)\) be the nuisances.

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Proposition 3 (Nonlinear coverage simulation). The nonlinear design for coverage simulations satisfies

\[
\tilde{h}_1(\tilde{X}_1, \tilde{X}_2, \tilde{W}) = h_1\{f^{-1}(\tilde{X}_1), f^{-1}(\tilde{X}_2), f^{-1}(\tilde{W})\},
\]

\[
\tilde{h}_2(\tilde{X}_1, \tilde{X}_2, \tilde{M}, \tilde{W}) = h_2\{f^{-1}(\tilde{X}_1), f^{-1}(\tilde{X}_2), f^{-1}(\tilde{M}), f^{-1}(\tilde{W})\},
\]

\[
\tilde{h}_3(\tilde{X}_1, \tilde{X}_2, \tilde{Z}, \tilde{D}, \tilde{M}) = h_3\{f^{-1}(\tilde{X}_1), f^{-1}(\tilde{X}_2), f^{-1}(\tilde{Z}), \tilde{D}, f^{-1}(\tilde{M})\},
\]

\[
\tilde{h}_4(\tilde{X}_1, \tilde{X}_2, \tilde{Z}, \tilde{D}) = h_4\{f^{-1}(\tilde{X}_1), f^{-1}(\tilde{X}_2), f^{-1}(\tilde{Z}), \tilde{D}\},
\]

where \((h_1, h_2, h_3, h_4)\) are characterized in Proposition 2. Hence \(\tilde{h}_1\) is linear in \(f^{-1}(\tilde{X})\) yet nonlinear in \(\tilde{X}\), and so on. In this design, \(\tilde{\theta}_0 = 4.05\).

Proof. By Proposition 2

\[
0 = \mathbb{E}\{Y - h_2(X, M, W)|X, Z, D = 1, M\}
\]

\[
= \mathbb{E}\{Y - h_2\{f^{-1}(\tilde{X}_1), f^{-1}(\tilde{X}_2), f^{-1}(\tilde{M}), f^{-1}(\tilde{W})\}|f^{-1}(\tilde{X}_1), f^{-1}(\tilde{X}_2), f^{-1}(\tilde{Z}), \tilde{D}, f^{-1}(\tilde{M})\}
\]

\[
= \mathbb{E}\{Y - \tilde{h}_2(\tilde{X}_1, \tilde{X}_2, \tilde{Z}, \tilde{D})|\tilde{X}_1, \tilde{X}_2, \tilde{Z}, \tilde{D} = 1, \tilde{M}\}
\]

and similarly for the other bridge functions. \(\square\)

I.3 Real world application

The Project STAR application directly extends [Athey et al., 2020]. The Job Corps application directly extends [Dukes et al., 2023].