In this paper we propose a method for nonparametric estimation and inference for heterogeneous bounds for causal effect parameters in general sample selection models where the initial treatment can affect whether a post-intervention outcome is observed or not. Treatment selection can be confounded by observable covariates while the outcome selection can be confounded by both observables and unobservables. The method provides conditional effect bounds as functions of policy relevant pre-treatment variables. It allows for conducting valid statistical inference on the unidentified conditional effect curves. We use a flexible semiparametric de-biased machine learning approach that can accommodate flexible functional forms and high-dimensional confounding variables between treatment, selection, and outcome processes. Easily verifiable high-level conditions for estimation and misspecification robust inference guarantees are provided as well.

**Keywords:** De-biased machine learning; Effect bounds; Partial identification; Treatment effect

**JEL classification:** C14, C21

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1. Introduction

In this paper, we propose a novel method for estimation and inference of heterogeneous bounds for causal effects when outcome data is only selectively observed and no exclusion restrictions are available. In particular, we are concerned with the case when the treatment of interest itself can affect the selection process and when effects are heterogeneous along both observable and unobservable dimensions. Heterogeneous bounds are derived from a \textit{conditional monotonicity} assumption in the selection equation. They can be used to study the effects of interventions on \textit{inframarginal} or \textit{always-taker} units, e.g. the effects of active labor market policies on earnings on the population that is working regardless of their whether they were subject to the intervention or not. They can also be applied to obtain credible bounds in experimental studies when the original treatment affects selection. This is common in (field-)experiments where the willingness of the participants to reply to e.g follow-up surveys can heavily depend on the initial treatment investment (Hjortskov et al., 2018). When applying established partial identification approaches for similar sample selection problems in practice, unconditional or subgroup specific effect bounds (Horowitz and Manski, 2000; Lee, 2009; Semenova, 2020) can sometimes be very wide and thus too uninformative to inform policy. Narrower bounds that exploit covariate information can be used for a better targeting of interventions under weaker, i.e. more credible, conditions compared to restrictive point-identified methods that require exclusion restrictions and/or distributional assumptions. The nonparametric heterogeneity based approach in this paper helps to substantially tighten bounds along policy relevant pre-treatment variables. This is due to the fact that the severity of the identification problem, i.e. the width of the identified set, can vary substantially along the total confounding dimensions most associated with the heterogeneity variables of interest. The method in this paper can incorporate a high-dimensional number of confounding variables building on de-biased machine learning.
methodology (Chernozhukov et al., 2018a; Semenova and Chernozhukov, 2021). We derive explicit high-level conditions regarding the quality of the nuisance quantity estimators that can be verified in a variety of settings for popular nonparametric or machine learning estimators such as high-dimensional sparse regression, deep neural networks, or random forests. We also provide an inference method for the heterogeneous effects that is robust against two different types of model misspecification exploiting recent advances in the literature on robust inference in partially identified models (Andrews and Kwon, 2019; Stoye, 2020).

Figure 1.1 contains an illustration of the proposed method for a one-dimensional heterogeneity analysis using simulated data. It plots the identified set and confidence intervals for the causal effect in dependence of a specified pre-treatment variable $z$\textsuperscript{1}. These could, for example, be bounds on the effect of a job training program on earnings as a function of the pre-training earnings of the participants. The black lines (left plot) correspond to state-of-the-art unconditional “generalized Lee-type bounds” (Semenova, 2020) with 95%-confidence intervals (dashed). The shaded red area is the identified region using the method from this paper. The blue area between the dashed blue lines is the 95%-confidence region for the heterogeneous effect. The black line (right plot) depicts the true conditional average treat-

\textsuperscript{1}Estimation of nuisance parameters is done using honest generalized random forests (first step). Heterogeneous bounds are estimated using basis splines (second step) with sample size $n = 5000$ and $d = 100$ regressors. For more details regarding the data-generating process consider Section 5.
ment effect of the design. We can see that a simple unconditional analysis cannot rule out a zero effect of the treatment while the 95%-confidence interval of the heterogeneous bounds clearly suggest a significant negative effect for units with \( z \) dimension between 0.4 to 0.8 and a positive effect for \( z > 0.9 \) leading to different policy recommendations. It is important to note that these conclusions are achieved not just by a different location of the heterogeneous bounds but also by narrower width for larger \( z \) values compared to the unconditional case. Thus, heterogeneous bounds can help to reduce the uncertainty stemming from weaker identification assumptions for certain sub-populations. Our Monte Carlo simulations suggest, that the associated confidence intervals also perform well in finite samples.

The paper is structured as follows: Section 2 discusses the related literature. Section 3 outlines the methodology and presents the estimator and confidence intervals. Section 4 introduces the technical assumptions and provides the large sample properties. Section 5 contains some Monte Carlo simulations analyzing the finite sample properties of the suggested confidence intervals. Section 6 contain additional remarks. Proofs and supplementary material can be found in the Appendix.

2. Related Literature

Estimating causal effects and sample selectivity is a long-standing problem in economic research (Heckman, 1979). Bounding causal effects under weak assumptions has been considered in a series of papers by Charles Manski and others, see Molinari (2020) for a comprehensive overview. In particular, Horowitz and Manski (2000) develop nonparametric bounds for treatment effects in selected samples. Zhang and Rubin (2003) consider bounds for “always-observed” or always-taker units under a monotonicity assumption regarding the effect of treatment on selection commonly imposed in generic sample selection models and/or stochastic dominance assumptions on the potential outcomes. Imai (2008) demonstrates
the sharpness of these bounds. Huber and Mellace (2015) consider similar sharp bounds for other principal strata. Lee (2009) provides asymptotic theory and an application to the evaluation of a large-scale job training program for bounds based on a (conditional) monotonicity assumption as in Zhang and Rubin (2003). These bounds are only applicable unconditionally or for low-dimensional discrete partitions of the covariate space and now commonly referred to as “Lee bounds”. Semenova (2020) provides “generalized Lee bounds” under the conditional monotonicity assumption. Our paper uses the same main identification assumptions. Semenova (2020) allows for high-dimensional and/or continuous confounders. It also generalizes to multiple outcomes and/or endogenous treatment receipt but does neither consider flexible heterogeneity analysis nor misspecification-robust inference. In a recent paper, Bartalotti et al. (2021) also propose identification of bounds for always-takers within a marginal treatment effect framework. Using monotonicity together with stochastic dominance assumptions, they are able tighten effect bounds based on the underlying treatment propensities. They are mostly focused on unconditional effect bounds and do not consider heterogeneity analysis beyond the propensity score. Bartalotti et al. (2021) also do not provide an inference procedure, analysis of the asymptotic properties of the proposed estimators, and do not address potential misspecification. Moreover, contrary to the approach taken in this paper, the method is not suitable for heterogeneous bounds under many confounding variables without imposing additional parametric assumptions.

Our work is also directly related to the literature on robust or (Neyman-)orthogonal moment functions and de-biased machine learning. Orthogonal moment functions are a key element to cope with flexible nonparametric or machine learning estimators for complex functional relationships and/or a large number of confounding variables. For estimation of point-identified parameters, there are now many approaches that use machine learning estimators in both experimental and observational studies, see e.g. Belloni et al. (2014), Farrell (2015), Chernozhukov et al. (2018a), and Wager and Athey (2018). Chernozhukov et al.
(2018a) develop a canonical framework for de-biased machine learning estimators that apply
to a wide range of orthogonal moment problems and can be used for asymptotically valid
inference on low-dimensional target parameters such as the average treatment effect. In
the context of heterogeneity analysis, orthogonal moment functions have been exploited in
point-identified problems by using them as pseudo-outcomes in (nonparametric) regression
models to obtain predictive causal summary parameters, see e.g. Lee et al. (2017), Fan et al.
(2020), Semenova and Chernozhukov (2021), and Heiler and Knaus (2021) or Knaus (2022)
for an overview. Our localization approach is closest to Semenova and Chernozhukov (2021)
who estimate heterogeneity parameters via nonparametric projections using least squares
series methods (Belloni et al., 2015).

Semenova (2020) also builds on the framework by Chernozhukov et al. (2018a) to construct
estimators for unconditional Lee-type bounds that can handle generic machine learning esti-
mators in the first stage. Semenova (2021) considers partially identified parameters for linear
moment functions with nuisance function estimated via machine learning. The crucial point
in both papers is that, while the effect of interest might not be point-identified, bounds them-
selves are characterized by well-understood convex moment problems or the corresponding
support function. The same applies to the heterogeneous bounds considered in this paper.
We derive the asymptotic distribution of the nonparametric heterogeneous double machine
learning based estimators for the identified set instead of a single parameter or functional as
considered by Semenova and Chernozhukov (2021). This nests the uni-variate generalized
Lee bounds by Semenova (2020) as a special case. In contrast to Semenova (2021), the
moment functions are nonlinear in the outcome and non-differentiable with respect to the
underlying nuisance functions. The use of machine learning (random forests) for Lee-type
bounds has also been heuristically discussed by Cornelisz et al. (2020). They do, however, not
provide any formal theory or methods for analyzing the uncertainty of the estimated bounds
or other statistical properties. Nareklishvili (2022) also considers heterogeneous partially
identified parameters using random forests under different identification assumptions.

Assessing uncertainty and providing confidence intervals for partially identified parameters in sample selection models is a non-trivial task. In this paper, we are concerned with construction two-sided confidence regions and associated tests for the heterogeneous causal effects. Relying on the quantiles of the large sample distributions of the bounds only is overly conservative for the actual effect of interest. The relevant uncertainty for the latter depends on the actual width of the identified set. If it is small, then deviations from a null value are likely to occur both in the positive and negative direction, i.e. the problem is effectively two-sided. For large intervals, however, uncertainty in one direction will likely dominate rendering the testing problem close to being one-sided. Imbens and Manski (2004) consider confidence intervals for partially identified parameter and provide a method for correction. Their method relies on a implicit superefficiency assumption that does not apply in many setups (Stoye, 2009). In these cases, the Imbens and Manski (2004) bounds are not uniformly valid with regards to the width of the underlying interval. As a remedy, Stoye (2009) suggests to artificially impose superefficiency via shrinkage methods. Andrews and Soares (2010) provide a more general approach for inference in moment inequality frameworks. However, when analyzing heterogeneous effect bounds, we are concerned with bounding effects at potentially many points and thus there is an additional risk of (local) misspecification compared to simple unconditional effect bounds. Under such misspecification the aforementioned methods can produce empty or very narrow confidence regions suggesting spuriously precise inference (Andrews and Kwon, 2019). Andrews and Kwon (2019) propose inference methods that extend the notion of coverage to pseudo-true parameter sets in general moment inequality frameworks, see also Stoye (2020) for a simpler method with adaptive critical values for generic regular parametric bound estimators. This paper adapts the inference method of Stoye (2020) to nonparametric heterogeneous bounds with machine learning in the first stage.
3. Methodology

In this section we introduce the sample selection model and the main identification assumptions followed by a brief review of the construction of effect bounds based on Lee (2009) and Semenova (2020). We then show how to exploit the latter to construct, estimate, and conduct inference on the heterogeneous partially identified effect parameters.

Assume for \( i = 1, \ldots, n \) we observe iid data \((X'_i, D_i, S_i, Y_i S_i)\) where \( X_i \) is a vector of predetermined covariates supported on \( X \subseteq \mathbb{R}^d \), \( D_i \) is a treatment indicator, \( S_i \) indicates whether the outcome is observed, i.e. we only observe \( Y_i S_i \) and not \( Y_i \). We would like to evaluate the average causal effect of \( D_i \) on outcome \( Y_i \) for the units that are selected under both treatment or control condition. We focus on the case of known treatment propensities \( e(x) = P(D_i = 1|X_i = x) \) during the exposition, but the methodology also extends to observational studies where they are unknown and have to be estimated. The prototypical setup is given by the graph in Figure 3.1 derived from a nonparametric structural causal model.

![Figure 3.1: Causal Graph](image)

This is a graphical representation of the sample selection model. Nodes denote variables and edges are structural relationships. Unobserved variables are depicted in dashed nodes.

The edges depict structural relationships, i.e. a missing arrow from one node to another
is an exclusion restriction. The model nests the case of the classic sample selection model (Heckman, 1979) where the treatment of interest enters in selection step, see Lee (2009) for the more restrictive parametric sample selection model representation. It allows for the treatment \( D \) to affect the selection \( S \). The model does not restrict selection to not affect the partially unobserved outcome of interest. There can be unobservables related to both selection and potential outcomes indicated by the double headed arrow between \( S \) and \( Y \). In addition, there are no exclusion restrictions available for variables which only affect selection that could be used to identify causal effects on the partially unobserved outcome via instrumental variable based methods.

Based on this model, we can define unit potential outcomes \( Y_i(1) \) and \( Y_i(0) \) and potential selection indicators \( S_i(1) \) and \( S_i(0) \) for units \( i = 1, \ldots, n \). They correspond to a unit’s value in outcome or selection when the treatment is exogenously set to \( D_i = 1 \) or \( D_i = 0 \) respectively under the model in Figure 3.1. Note that potential selection and potential outcomes can still be dependent. This implies that, even conditional on \( X_i \), causal effects can differ for different sub-types defined by their respective \( S_i(1) \) and \( S_i(0) \) variables. The target is to evaluate the causal effect of \( D_i \) for the units that are selected under both control or treatment regime, i.e. units for which \( S_i(1) = S_i(0) = 1 \).

As \( D \) affects \( S \), a comparison of treated and control units for selected units does not yield a valid causal comparison for the sub-population \( S_i(1) = S_i(0) = 1 \). However, the model implies the following conditional independence relationship in Rubin-Neyman potential outcome notation:\(^2\)

\[
Y_i(1), Y_i(0), S_i(1), S_i(0) \perp\!
\!
\!
\perp D_i \mid X_i.
\]

\(^2\)Note that \( Y \) and \( S \) have the identical connections and parent nodes in the graph. Thus, when considering \( (Y, S) \) jointly as pair in one node, the Markov assumption for the corresponding stacked graph holds, i.e. it is a directed acyclical graph where variables are independent of all their non-descendants given their direct parental nodes (Tian and Pearl, 2002).
Condition (3.1) cannot be exploited in a standard selection on observables strategy for point identification as, even conditional on \( X_i \), we only observe the selected subset of potential outcomes for which \( S_i = 1 \). However, we can use the fact that, conditional on \( X_i \), the treatment is exogenous with respect to selection to obtain bounds for the causal effect in the \( S_i(1) = S_i(0) = 1 \) population, i.e. the effect is partially identified under the model. For that it is not necessary to impose any restriction of the direction of the effect of \( D \) on \( S \). In particular, treatment can affect selection positively or negatively. The sign, however, must be uniquely determined by the vector of covariates \( X_i \), i.e. we impose a weak or conditional monotonicity assumption:

**Assumption 3.1** There exists partitions of the covariate space \( \mathcal{X} = \mathcal{X}_+ \cup \mathcal{X}_- \) such that
\[
P(S_i(1) \geq S_i(0)|X_i \in \mathcal{X}_+) = P(S_i(1) \leq S_i(0)|X_i \in \mathcal{X}_-) = 1
\]

We also assume that there are comparable units between selected treated and selected non-treated units with positive probability and treated and non-treated overall (multiple overlap):

**Assumption 3.2** For all \( x \in \mathcal{X} \) and \( d \in \{0, 1\} \) we have that \( 0 < P(S_i = 1|X_i = x, D_i = d) < 1 \) and \( P(D_i = d|X_i = x) > 0 \).

Moreover, we rule out the case where treatment does not affect selection as in this case effects are point-identified:

**Assumption 3.3** There is a constant \( c > 0 \) and a set \( \bar{\mathcal{X}} \subset \mathcal{X} \) with \( P(\mathcal{X}\setminus \bar{\mathcal{X}}) = 0 \) such that
\[
\inf_{x \in \bar{\mathcal{X}}} |P(S_i = 1|X_i = x, D_i = 1) - P(S_i = 1|X_i = x, D_i = 0)| > c.
\]

For constructing the effect bounds, consider first a stronger version of Assumption 3.1: \( S_i(1) \geq S_i(0) \) with probability one, i.e. unconditional monotonicity. In this case, Zhang and Rubin (2003) and Lee (2009) show that selected units within the control group are always-takers or inframarginal in the sense of \( S_i(1) = S_i(0) = 1 \) while within the treated group
there is a mixture of always-takers and *marginal* units or *compliers* who are induced to be selected by the treatment.\(^3\) This allows us to define sharp bounds on the conditional causal effect of treatment on the outcome for the population of always-takers

\[
\theta(x) = E[Y_i(1) - Y_i(0)|S_i(1) = S_i(0) = 1, X_i = x].
\] (3.2)

This is the expected causal effect for a unit with covariates \(x\) whose outcome would be observed independently of its treatment status. Denote \(s(d, x) = P(S_i = 1|X_i = x, D_i = d)\).

For a given \(x \in \mathcal{X}\), the worst case under monotonicity is obtained when the smallest \(1 - p_0(x)\) values of \(Y_i\) are all marginal units and the remaining \(p_0(x)\) units are always-takers with

\[
p_0(x) = \frac{s(0, x)}{s(1, x)}
\] (3.3)

denoting the share of always-takers relative to always-takers and marginal units conditional on \(X_i = x\). Thus, trimming the outcome for the selected treated units from below by its corresponding \(1 - p_0(x)\) quantile allows us to obtain an upper bound for the effect. Trimming the observed treated selected outcome by the \(p_0(x)\) quantile from above yields the lower bound. Under the weaker conditional monotonicity Assumption 3.1 an equivalent argument holds separately for units with either \(p_0(x) < 1\) or \(p_0(x) > 1\) and inverted trimming shares.

Denote the conditional quantile \(q(u, x) = \inf\{q : u \leq P(Y_i \leq q|D_i = 1, S_i = 1, X_i = x)\}\). As \(p_0(x)\) is identified from the observed joint distribution of \((X'_i, D_i, S_i)\), we obtain the following sharp conditional bounds for any \(x \in \mathcal{X}\)

\[
\theta_L(x) \leq \theta(x) \leq \theta_U(x)
\] (3.4)

\(^3\)Note that in contrast to the typical setup and nomenclature in the IV literature, the latent sub-types here are defined with respect to the potential selection state caused by the treatment, not the potential treatment states caused by an excluded instrument.
where
\[ \theta_L(x) = E[Y_i|D_i = 1, S_i = 1, Y_i \leq q(p_0(x), x), X_i = x] - E[Y_i|D_i = 0, S_i = 1, X_i = x] \]
\[ \theta_U(x) = E[Y_i|D_i = 1, S_i = 1, Y_i \geq q(1 - p_0(x), x), X_i = x] - E[Y_i|D_i = 0, S_i = 1, X_i = x] \] (3.5)
if \( p_0(x) < 1 \) and
\[ \theta_L(x) = E[Y_i|D_i = 1, S_i = 1] - E[Y_i|D_i = 0, S_i = 1, Y_i \geq q(1 - 1/p_0(x), x), X_i = x] \]
\[ \theta_U(x) = E[Y_i|D_i = 1, S_i = 1] - E[Y_i|D_i = 0, S_i = 1, Y_i \leq q(1/p_0(x), x), X_i = x] \] (3.6)
if \( p_0(x) > 1 \). Assumption 3.3 rules out \( p_0(x) = 1 \) as in this case the treatment does not affect the response and thus causal effects for the always-takers are point-identified by comparing the outcome of the selected treated to the selected control units.

While the \( x \)-specific or “personalized bounds” (3.4) can provide some insights, they are not very useful in applications with continuous variables and/or many discrete cells to evaluate. Moreover, in such cases it is often no longer possible to consistently estimate the conditional bounds and to construct asymptotically valid confidence intervals without further restrictions. This is equivalent to estimation of personalized treatment effects under unconfoundedness in high dimensions (Chernozhukov et al., 2018b). Therefore, we propose to instead estimate heterogeneous effect bounds conditional on a smaller, pre-specified subset of (policy relevant) covariates \( Z_i \) supported on \( Z \subset X \). The true lower-dimensional heterogeneous effects are then defined as
\[ \theta(z) = E[\theta(X_i)|Z_i = z]. \] (3.7)
The goal is to estimate heterogeneous bounds
\[ \theta_L(z) \leq \theta(z) \leq \theta_U(z). \] (3.8)
for any $z \in \mathcal{Z}$. The bounds here are for the *predictive causal effect* $\theta(z)$. Such a functional parameter allows for evaluating effect heterogeneity along the pre-specified dimensions. This is conceptually equivalent to heterogeneity analysis of causal effects when dividing the sample into specific subgroups. However, it is more informative as it exploits the full variation in outcomes, selection, and treatment *before* conditioning on the subgroup variables. A special case are the *unconditional effect bounds* considered by Lee (2009) and Semenova (2020)

$$E[\theta_L(X_i)] \leq E[\theta(X_i)] \leq E[\theta_U(X_i)]. \quad (3.9)$$

Semenova (2020) derives moment functions/scores $\psi_L(W_i, \eta)$ and $\psi_U(W_i, \eta)$ for the upper and lower effect bounds under the conditional monotonicity assumption. They depend on the observed data and a nuisance quantity vector $\eta = \eta(W_i)$ that includes propensity scores, conditional selection probabilities, and conditional quantiles of the observed outcome distribution of the treated. For the formal definitions please consider Appendix A. The functions serve as approximately unbiased signals for the personalized bounds for the partially identified $\theta(x)$. Thus, they can be used for (nonparametric) projections onto lower dimensional sub-spaces such as $\mathcal{Z}$ to obtain the upper and lower bounds (3.4). As $\mathcal{Z}$ is of low dimension, this allows for conducting asymptotically valid inference for the heterogeneous causal effect even if the original confounding dimension of $\mathcal{X}$ is large. In particular, Semenova (2020) shows that $E[\psi_U(W_i, \eta_0)|X_i] = 0$ for both $B = L, U$ where $\eta_0$ denote the true nuisance vector. Thus, as $Z_i$ is known conditional on $X_i$, the heterogeneous bounds are nonparametrically identified as

$$\theta_B(z) = E[\theta_B(X_i)|Z_i = z] = E[E[\psi_B(W_i, \eta_0)|X_i]|Z_i = z] = E[\psi_B(W_i, \eta_0)|Z_i = z] \quad (3.10)$$

4In principle, one could also be interested in bounds also conditional on the latent sub-type, i.e. $E[\theta(X_i)|S_i(1) = S_i(0) = 1, Z_i = z]$. These always-taker types, however, are usually not known or identified in practice and could therefore not be used e.g. for choosing an intervention population from a policy maker perspective. Thus, we focus explicitly on the expected bound given pre-treatment policy variables that could be used for treatment assignment on a population that potentially consists of all latent sub-types.
The very right hand sides can be estimated using flexible nonparametric methods. In particular, the heterogeneous bounds can be obtained by two separate regressions of each score function onto the spaces spanned by their respective $k_B$-dimensional transformations of $Z_i$, $b_B(Z_i)$ for each $B \in \{L, U\}$

$$\psi_B(W_i, \eta_0) = b_B(Z_i)' \beta_{B,0} + r_{\theta_B}(Z_i) + \varepsilon_{i,B}$$  \hspace{1cm} (3.11)

with conditional mean errors $E[\varepsilon_{i,B}|Z_i] = 0$ and approximation errors

$$r_{\theta_B}(Z_i) = E[\psi_B(W_i, \hat{\eta})|Z_i] - b_B(Z_i)' \beta_{B,0}.$$  \hspace{1cm} (3.12)

Replacing the unobserved true score by its sample counterpart yields the two estimators

$$\hat{\beta}_B = \left( \sum_{i=1}^{n} b_B(Z_i)b_B(Z_i) \right)^{-1} \sum_{i=1}^{n} b_B(Z_i)\psi_B(W_i, \hat{\eta})$$  \hspace{1cm} (3.13)

where the scores of the effect bounds with estimated nuisance quantities $\psi_B(W_i, \hat{\eta})$ serve as pseudo-outcomes in two separate least squares regression on their respective basis functions.\(^5\)

The heterogeneous effect bounds at policy variable value $Z_i = z$ can then calculated from the point predictions of the two models:

$$\hat{\theta}_B(z) = b_B(z)' \hat{\beta}_B$$  \hspace{1cm} (3.14)

When $b_B(Z_i)$ only contains a constant for $B = L, U$, the method collapses back to the unconditional generalized Lee bounds in Semenova (2020). Estimation of $\hat{\eta}$ can be done via modern machine learning such as random forests, deep neural networks, high-dimensional sparse likelihood and regression models, or other non- and semiparametric estimation methods with good approximation qualities for the nuisance functions at hand. The influence of their learning bias/approximation on the functional bound estimator is limited by the

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\(^5\)In principle, the two equations in (3.11) are only seemingly unrelated and could thus also be estimated using a system based approach that takes into account the correlation structure of the conditional mean errors to increase efficiency. While this is straightforward in the case of a finite-dimensional parametric mean functions, it introduces additional dependencies in the two-step estimation that might offset potential gains in efficiency in the nonparametric case. Thus, we leave an extension along this line for future work.
Neyman-orthogonality of the chosen moment functions (Chernozhukov et al., 2018a; Semenova, 2020). In particular, under suitable conditions, the estimation does not affect the large sample distribution if the RMSE-approximation rates for the nuisance quantities \( \hat{\eta} - \eta_0 \) are of order \( o((nk_B)^{-1/4}) \). This is similar to standard de-biased machine learning estimation of conditional average treatment effects using Neyman-orthogonal/doubly robust moment functions for nonparametric projection (Semenova and Chernozhukov, 2021). When \( z \) is one-dimensional, popular \( k_B \) choices for many bases under weak smoothness assumptions are of rate \( O(n^{1/5}) \) leading to an overall RMSE convergence requirement for the nuisances of \( o(n^{-3/10}) \). This is a rate achievable by many nonparametric and machine learning estimators such as forests, deep neural networks, or high-dimensional sparse models under moderate complexity and/or dimensionality restrictions, see Semenova (2020), Semenova and Chernozhukov (2021) and Heiler and Knaus (2021) for examples. More details regarding the technical assumptions can be found in Section 4. We also require that all components in \( \hat{\eta} \) are obtained via \( K \)-fold cross-fitting:

**Definition 1** **\( K \)-fold cross-fitting** (see Definition 3.1 in Chernozhukov et al. (2018a))

Take a \( K \)-fold random partition \( (I_f)_{f=1}^K \) of observation indices \( [K] = \{1, \ldots, n\} \) with each fold size \( n_f = n/K \). For each \( f \in [K] = \{1, \ldots, K\} \), define \( I_f^c := \{1, \ldots, n\} \setminus I_f \). Then for each \( f \in [K] \), the machine learning estimator of the nuisance function are given by

\[
\hat{\eta}_f = \hat{\eta}(W_i \in I_f^c).
\]

Thus for any observation \( i \in I_f \) the estimated score only uses the model for \( \eta \) learned from the complementary folds \( \psi_B(W_i, \hat{\eta}) = \psi_B(W_i, \hat{\eta}_f) \).

The use of cross-fitting controls potential bias arising from over-fitting using flexible machine learning methods without the need to evaluate complexity/entropy conditions for the function class that contains true and estimated nuisance quantities with high probability. If finite dimensional parametric models such as linear or logistic are assumed and estimated
for the nuisance quantities, the proposed methodology can be applied without the need for cross-fitting.

Under suitable assumptions, the heterogeneous bound estimators are jointly asymptotically normal

\[
\sqrt{n} \hat{\Omega}_n(z) \left( \begin{array}{c}
\hat{\theta}_L(z) - \theta_L(z) \\
\hat{\theta}_U(z) - \theta_U(z)
\end{array} \right) \overset{d}{\to} \mathcal{N} \left( \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \right),
\]

\[\hat{\Omega}_n(z) = \begin{pmatrix}
\hat{\sigma}_L^2(z) & \hat{\rho}(z)\hat{\sigma}_L(z)\hat{\sigma}_U(z) \\
\hat{\rho}(z)\hat{\sigma}_L(z)\hat{\sigma}_U(z) & \hat{\sigma}_U^2(z)
\end{pmatrix}\]

(3.15)

at each \(z \in \mathcal{Z}\). For the complete definitions of the variance terms consider Appendix B. The variances are allowed to depend on the sample size and are generally increasing in norm if we allow the basis functions \(b_B(z)\) to grow with the sample size. Thus, convergence is slower than the parametric rate equivalently to conventional nonparametric series regression (Belloni et al., 2015). If the approximation errors \(r_{\theta_B}(z)\) are rather large, then this distributional result is still valid if centered around the best linear predictors of the true bounds \(b_B(z)'\beta_{B,0}\) for \(B = L, U\) similar to classic quasi maximum likelihood estimation.

Inverting the quantiles of the distribution in (3.15) could in principle be used to construct confidence intervals for the upper and lower bounds. However, this would be overly conservative for the actual effect of interest \(\theta(z)\). Inference on this partially identified parameter should take into account the underlying true width of the interval, see Stoye (2009) and Andrews and Soares (2010) for a thorough treatment and adaptive confidence intervals. However, if we allow for (local) misspecification \(\theta_L(z) > \theta_U(z)\), corresponding confidence regions using such adaptive methods could be empty or narrow suggesting overly precise inference (Andrews and Kwon, 2019). Robustness to misspecification is important in our setup as, in contrast to unconditional bounds, the bound functions are estimated at potentially many points with different variances and varying strength of identification in the sense of
different widths of the underlying true intervals. A flexible estimator that is chosen e.g. by a
global goodness-of-fit criterion for the effect bound curves could well be locally misspecified
at some points. A limiting case of this type of misspecification would be to “overfit” the effect
of a treatment that is fully independent of selection for some units instead of imposing local
point identification. Corresponding confidence regions should be adaptive to such cases.

To do so, we introduce the notion of a pseudo-true parameter \( \theta^*(z) \) and its corresponding
standard deviation \( \sigma^*(z) \) that can be estimated as

\[
\hat{\theta}^*(z) = \frac{\hat{\sigma}_U(z)\hat{\theta}_L(z) + \hat{\sigma}_L(z)\hat{\theta}_U(z)}{\hat{\sigma}_L(z) + \hat{\sigma}_U(z)}, \quad \hat{\sigma}^*(z) = \frac{\hat{\sigma}_L(z)\hat{\sigma}_U(z)\sqrt{2(1 + \hat{\rho}(z))}}{\hat{\sigma}_L(z) + \hat{\sigma}_U(z)}.
\]

(3.16)

This is a variance weighted version of the upper and lower bound. The pointwise \((1 - \alpha)\%\)-
confidence intervals for the true always taker effect \( \theta(z) \) can then be obtained by the union
of two intervals

\[
CI_{\theta(z), 1-\alpha} = \left[ \hat{\theta}_L(z) - \frac{\hat{\sigma}_L(z)}{\sqrt{n}}\hat{c}(z), \hat{\theta}_U(z) + \frac{\hat{\sigma}_U(z)}{\sqrt{n}}\hat{c}(z) \right] \cup \left[ \hat{\theta}^*(z) \pm \frac{\hat{\sigma}^*(z)}{\sqrt{n}}\Phi^{-1}(1 - \alpha/2) \right],
\]

(3.17)

where the critical value \( \hat{c}(z) \) uniquely solves

\[
\inf_{\Delta \geq 0} P(u_1 - \Delta - c \leq 0 \leq u_2 \text{ or } |u_1 + u_2 - \Delta| \leq \sqrt{2(1 + \hat{\rho}(z))}\Phi^{-1}(1 - \alpha/2)) = 1 - \alpha,
\]

(3.18)

with \((u_1, u_2)\) being jointly normal with unit variances and covariance \( \hat{\rho}(z) \). This is an adap-
tation of the method by Stoye (2020) who considers simple parametric estimators for generic
bounds without two-stage estimation, data-splitting, and additional nuisance functions. In-
terval (3.17) is robust against misspecification of the form \( \theta_L(z) > \theta_U(z) \) as it is never empty
and guarantees at least nominal coverage over an extended parameters space. In particular,
it has at least \((1 - \alpha)\%\) asymptotic coverage uniformly for all widths \( \theta_U(z) - \theta_L(z) \) pointwise
at each \( z \in Z \). For more details consider Section 4.
4. Large Sample Properties

In this section we provide the assumptions for asymptotic normality, validity of the confidence intervals proposed in (3.17), and some more technical discussion. For simplicity, we present the case with known propensity scores.\(^6\) Denote \(\| \cdot \|_p\) as the \(L_p\) norm. Recall that \(E[\psi_B(W_i, \eta_0)|Z_i = z] = \theta_B(z), \theta_B \in G_B\) where \(G_B\) is a space of functions (possibly depending on \(n\)) that map from \(Z\) to the real line. Note that \(\theta_B(z) = b_B(z)'\beta_{B,0} + r\theta_B(z)\) with basis transformations \(b_B(z) \in S^{k_B} := \{ b \in \mathbb{R}^{k_B} : \|b\| = 1 \}\) and \(\beta_{B,0}\) being the parameter of the best linear predictor defined as root of equation \(E[b_B(Z_i)(\psi_B(W_i, \eta_0) - b_B(Z_i)'\beta_{B,0})] = 0\). Define bound \(\xi_{k,B} = \sup_{z \in Z} \|b_B(z)\|\). Denote the realization set \(\mathcal{T}_n = S_{0,n} \times S_{1,n} \times Q_n\) of nuisance quantities \(\eta = \{s(0,X), s(1,X), q(u,X)\}\). For corresponding estimators \(\hat{s}(0,X), \hat{s}(1,X),\) and \(\hat{q}(u,X)\) define their \(L_p\) error rates as

\[
\lambda_{s,n,p} = \sup_{d \in \{0,1\}} \sup_{\hat{s}(d) \in S_{d,n}} E[(\hat{s}(d, X_i) - s(d, X_i))^p]^{1/p}
\]

\[
\lambda_{q,n,p} = \sup_{u \in \tilde{U}} \sup_{\hat{q}(u) \in Q_n} E[(\hat{q}(u, X_i) - q(u, X_i))^p]^{1/p}
\]

where \(\tilde{U}\) is a compact subset of \((0,1)\) containing the relevant quantile trimming threshold support unions \(([\text{supp}(p_0(X_i)) \cup \text{supp}(1 - p_0(X_i))] \cap X_+) \cup ([\text{supp}(1/p_0(X_i)) \cup \text{supp}(1 - 1/p_0(X_i))] \cap X_-)\). All of the following assumptions are uniformly over \(n\) if not stated differently for both \(B = L, U\):

A.1) (Identification) \(Q_B = E[b_B(Z_i)b_B(Z_i)']\) has eigenvalues bounded above and away from zero.

A.2) (Regular outcome) The outcome has bounded conditional moments \(E[Y_i^m|X_i = x, D_i = d, S_i = s] \lesssim 1\) for some \(m > 2\) and a continuous density \(f(y|X = x, D = d, S_i = s)\) that is uniformly bounded from above and away from zero with bounded first derivative

\(^6\)With propensity scores estimated, one has to augment the bias-correction in the moment functions and the nuisance parameter space as in Semenova (2020) as well as the Assumption A.5 by additional terms that equivalently depend on the (squared) \(L_p\) error rate of the propensity score estimator.
for any \( x \in X \) and \( s, d \in \{0, 1\} \).

A.3) (Strong multiple overlap) There exist constants \( \varepsilon, \delta \in (0, 1/2) \) such that
\[
\varepsilon < \inf_{x \in X} e(x) \leq \sup_{x \in X} e(x) < 1 - \varepsilon \\
\delta < \inf_{x \in X, d \in \{0, 1\}} s(d, x) \leq \sup_{x \in X, d \in \{0, 1\}} s(d, x) < 1 - \delta
\]

A.4) (Approximation) For any \( n \) and \( k_B \), there are finite constants \( c_{k,B} \) and \( l_{k,B} \) such that for each \( \theta_B \in G_B \)
\[
||r_{\theta_B}||_{P,2} := \left( \int_{z \in Z} r_{\theta_B}^2(z) dP(z) \right) ^{1/2} \leq c_{k,B}.
\]
\[
||r_{\theta_B}||_{P,\infty} := \sup_{z \in Z} |r_{\theta_B}(z)| \leq l_{k,B}c_{k,B}.
\]

A.5) (Basis growth) Let \( \sqrt{n/\xi_{k,B}} - l_{k,B}c_{k,B} \to \infty \) such that
\[
\frac{\xi_{k,B}^2 \log k_B}{n} \left( 1 + \sqrt{k_Bl_{k,B}c_{k,B}} \right) = o(1).
\]

A.6) (Machine learning bias) Let \( e_n = o(1) \). For all \( f \in [K] \), \( \hat{\eta}_f \) obtained via cross-fitting belongs to a shrinking neighborhood \( T_n \) around \( \eta_0 \) with probability of at least \( 1 - e_n \), such that
\[
\xi_{k,B}(\lambda_{q,n,2} + \lambda_{s,n,2}) = o(1)
\]
and (i) either
\[
\sqrt{nk_B(\lambda_{q,n,4}^2 + \lambda_{s,n,4}^2)} = o(1)
\]
or (ii) the basis is bounded \( \sup_{z \in Z} \|b(z)\|_\infty < C \) and
\[
\sqrt{nk_B(\lambda_{q,n,2}^2 + \lambda_{s,n,2}^2)} = o(1).
\]

A.7) (Lipschitz quantile) On the realization set with probability of at least \( 1 - e_n \), the condi-
The quantile estimator is Lipschitz continuous over \( \tilde{U} \), i.e. for some \( C > 0 \)

\[
\sup_{u, u' \in \tilde{U}} \sup_{\hat{q}(u), \hat{q}(u') \in Q_n} |\hat{q}(u, x) - \hat{q}(u', x)| < C|u - u'|.
\]

almost surely in \( X \).

Assumption A.1 excludes collinearity of the basis transformations of the heterogeneity variables. A.2 puts restrictions on the tails and the smoothness of the distribution for the observed outcome distribution in different selection and treatment states. A.3 assures that there are comparable units between units of different selection and/or treatment status. A.2 and A.3 together imply a continuously differentiable conditional quantile function for the selected observed units that is almost surely bounded. This, together with the strong overlap for the treatment and selection probabilities assures that the effect bounds are regularly identified (Khan and Tamer, 2010; Heiler and Kazak, 2021).

A.4 defines \( L_2 \) and uniform approximation error bounds for function class \( G_B \). This is a typical characterization in the literature on nonparametric series regression without nuisance functions (Belloni et al., 2015). We say the model is correctly specified if the basis is sufficiently rich to span \( G_B \), i.e. \( c_{k,B} \to 0 \) as \( k_B \to \infty \). However, the distributional theory also allows for the case of misspecification, i.e. \( c_k \not\to 0 \). A.5 controls the approximation error from linearization of the estimator with unknown design matrix \( Q_B \). This is equivalent to the condition required for localization in general least squares series regression (Belloni et al., 2015). For more specific series methods such as splines (Huang, 2003) or local partitioning estimators (Cattaneo et al., 2020), this rate can be improved to \( \sqrt{\xi_{k,B}^2 \log k_B/n(1+\sqrt{\log k_B l_{k,B} c_{k,B}})} \), see also (Belloni et al., 2015), Section 4 and Cattaneo et al. (2020), Supplemental Appendix Remark SA-4 for a related discussion.

A.6 is crucial: It says that the machine learning estimators for the conditional quantiles and selection probabilities have sufficiently good approximation qualities in an \( L_p \) sense. In the case of a bounded finite basis, the conditions reduce to the well-known requirement in
the semiparametric/double machine learning literature that the nuisance functions have tooot have mean squared error rates of order $o(n^{-1/4})$ (Chernozhukov et al., 2018a). In the more general case, they are comparable to the conditions in Semenova and Chernozhukov (2021) required for nonparametric estimation of conditional average treatment effects.

A.7 imposes some regularity on the conditional quantile function estimator. It says that the estimator is not changing too much in the underlying quantile on $\tilde{U}$. This assures that we can bound the expected differences in estimated quantiles at estimated versus true levels at the rate of the trimming levels. This is a weak assumption if the continuity Assumption A.2 for the true conditional distribution applies. In particular because the boundaries of $\tilde{U}$ are bounded away from zero and one due to Assumption A.3 assuring that the true quantile thresholds are bounded.

For the estimation of the asymptotic variance, we also assume that A.V holds:

A.V) (Asymptotic variance) The conditions in Appendix C.8, Assumption C.1 hold, i.e.

$$||\hat{\Omega}_n(z) - \Omega(z)|| = o_p(1) \text{ pointwise at each } z \in Z.$$  

A.V can require somewhat stronger outcome moment/tail and basis growth conditions. The corresponding primitive assumptions and discussion can be found in Appendix C.8. We obtain the following Theorem:

**Theorem 4.1** Suppose Assumptions 3.1 - 3.3 and A.1 - A.6 hold and $\hat{\theta}_B(z_0)$ for $B = L, U$ and $\hat{\Omega}_n(z_0)$ are estimators according to (3.14) and (B.2) respectively. Then, for any $z_0 = z_{0,n}$,

$$\sqrt{n}\hat{\Omega}_n^{-\frac{1}{2}}(z_0) \left( \begin{array}{c} \hat{\theta}_L(z) - b_L(z)'\beta_{L,0} \\ \hat{\theta}_U(z) - b_U(z)'\beta_{U,0} \end{array} \right) \xrightarrow{d} \mathcal{N}\left( \left( \begin{array}{c} 0 \\ 0 \end{array} \right), \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \right).$$

Moreover if $\sup_B n^{1/2}k_B^{-1/2}l_{k,B}c_{k,B} = o(1)$, then

$$\sqrt{n}\hat{\Omega}_n^{-\frac{1}{2}}(z_0) \left( \begin{array}{c} \hat{\theta}_L(z) - \theta_L(z_0) \\ \hat{\theta}_U(z) - \theta_U(z_0) \end{array} \right) \xrightarrow{d} \mathcal{N}\left( \left( \begin{array}{c} 0 \\ 0 \end{array} \right), \left( \begin{array}{cc} 1 & 0 \\ 0 & 1 \end{array} \right) \right).$$
Theorem 4.1 shows that nonparametric heterogeneous bounds using double machine learning are jointly asymptotically normal. It allows for the case of misspecification when centered around the best linear predictor. It is most useful under the additional slight undersmoothing condition that makes any misspecification bias vanish sufficiently fast.\(^7\)

Theorem 4.1 would in principle be sufficient to construct confidence intervals for the heterogeneous effect bounds. They are, however, too wide for the actual effect parameter of interest \(\theta(z)\) depending on the width of \(\theta_U(z) - \theta_L(z)\). This is a well-known phenomenon in the partial identification literature, see e.g Imbens and Manski (2004). If the difference between upper and lower bound is large, the testing problem is essentially one-sided compared to the case of only having a small difference. This raises the question of how to conduct inference that is uniformly valid with respect to the underlying difference between upper and lower effect bound and has more power compared to using naive two-sided critical values. Imbens and Manski (2004) propose a method construct confidence intervals for the partially identified parameter under a local super-efficiency assumption which cannot be guaranteed in many applications. Stoye (2009) showed that this assumption can also be imposed artificially to conduct uniformly valid inference using shrinkage methods, see also Andrews and Soares (2010) for a more general framework. The corresponding confidence intervals, however, are sometimes found to be narrow or empty. This can arise due to finite sample variation but is more often conceived as a sign of misspecification. Then, these approaches can suggest spuriously precise inference for the target parameter (Andrews and Kwon, 2019). This is particularly relevant for heterogeneous bounds as here we estimate two functions at potentially many points which makes (local) potential misspecification a much larger concern compared to the single partially identified parameter in Lee (2009) or

\(^7\)For example, when \(G_B\) is in a \(s\)-dimensional ball on \(Z\) of finite diameter, then the condition simplifies to \(n^{1/2} k_B^{-\left(\frac{1}{2} + \frac{s}{2}\right)} \log(k_B) \rightarrow 0\). See Belloni et al. (2015), Comment 4.3 for additional details. Note that undersmoothing does in general not admit mean-squared error optimal \(k_B\) choices, see e.g. Cattaneo et al. (2020) for multiple bias-correction alternatives methods for local partitioning estimators.
Semenova (2020). We relax the notion of coverage to include an artificial pseudo-true target parameter that guarantees non-empty confidence intervals. Our method is based on Stoye (2020) who demonstrates that in the simple case of two regular, jointly asymptotically normally distributed parameters, uniformly valid intervals with good power properties can be obtained by concentrating out the unobserved true difference in effect bounds. We adapt his framework to the nonparametric heterogeneous effect bounds with estimated nuisances. For any \( z \in Z \) let the identified set be

\[
\Theta_z = [\theta_L(z), \theta_U(z)]
\]

which contains the true causal effect \( \theta(z) \). Now denote the pseudo-true parameter \( \theta^*(z) \) and its variance as

\[
\begin{align*}
\theta^*(z) &= \frac{\sigma_U(z)\theta_L(z) + \sigma_L(z)\theta_U(z)}{\sigma_L(z) + \sigma_U(z)}, \\
\sigma^*(z) &= \frac{\sigma_L(z)\sigma_U(z)\sqrt{2(1 + \rho(z))}}{\sigma_L(z) + \sigma_U(z)}.
\end{align*}
\]

The pseudo-true identified set is then given by

\[
\Theta^*_z = \Theta_z \cup \{\theta^*(z)\}.
\]

This set is implicitly defined by an estimand corresponding to setting a test statistic for the heterogeneous effect at \( z \) to (i) zero (meaning no rejection of the null) if the interval is nonempty and the null value is inside the estimated intervals and to (ii) the larger of the two \( t \)-statistics for upper and lower bound for the null of the bound being equal to the hypothesized value. In particular, it chooses the test statistic under the null as

\[
\max\left\{ \frac{(\theta(z) - \hat{\theta}_U(z))}{\hat{\sigma}_U(z)}, \frac{(\hat{\theta}_L(z) - \theta(z))}{\hat{\sigma}_L(z)} \right\}. 
\]

Case (ii) collapses to a standard test for the parameter

\[8\]

Note also that we allow for the use of different basis functions across when estimating upper and lower effect bounds. This seems reasonable as it could well be that lower and upper effect bounds are curves of e.g. different smoothness and not equally difficult to approximate. Alternatively one could impose the largest complexity of any bound for both models, i.e. paying the price of a potentially higher estimation variance in the effect bound with a higher degree of smoothness. While this will generally yield a better approximation for each separate bound, it could contribute to a reverse ordering in the sense that \( \hat{\theta}_L(z) \geq \hat{\theta}_U(z) \) for at some \( z \) which requires an adaptive inference solution similar to partial identification problems resulting from misspecification (Andrews and Kwon, 2019; Stoye, 2020).
lying in $\Theta_z$ in the case of a well-defined interval with $\theta_U > \theta_L$ and to a test on the pseudo-true parameter under misspecification $\theta_U < \theta_L$. This extended inference procedure can also be interpreted as resulting from a moment inequality problem that allows for misspecification by adding slacks/deviations to equations defining upper and lower effect bounds (Andrews and Kwon, 2019). If such slacks are large, $\theta_U < \theta_L$, can be admitted as solution. In principle, alternative definitions for the pseudo-true set $\Theta_z^*$ that use different weighting compared to (4.2) could be considered as well. This would change the definition of the pseudo-true parameter. Not all choices of such pseudo-true parameter are of equal use. This is equivalent to e.g. GMM models under misspecification where the pseudo-true parameter is defined implicitly as the maximizer of a GMM population criterion using a particular weighting matrix. Therefore, the choice of the pseudo-true parameter and its usefulness should be balanced versus the robustness against spurious precision under misspecification (Andrews and Kwon, 2019). The particular choice in (4.2) leads to a convenient solution in terms of critical value adjustment due to the asymptotic bi-variate normal distribution (Stoye, 2020). We obtain the following Theorem:

**Theorem 4.2** Suppose Assumptions 3.1 - 3.3 and A.1 - A.6 hold and $\hat{\theta}_B(z_0)$ for $B = L, U$ and $\hat{\Omega}_n(z_0)$ are estimated according to (3.14) and (B.2) respectively. Let the confidence interval be constructed according to 3.17 and assume that $\sup_B n^{1/2}k_B^{-1/2}l_{k_B}c_{k_B} = o(1)$. Then, for any $z_0 = z_{0,n}$,

$$\liminf_{n \to \infty} \inf_{\theta(z_0) \in \Theta_{z_0}^*} P(\theta(z_0) \in CI_{\theta(z_0),1-\alpha}) \geq 1 - \alpha.$$  

Theorem 4.2 demonstrates the asymptotic validity of the confidence intervals proposed in (3.17): We achieve at least nominal coverage independently of the actual width of the true identified region for the heterogeneous effect bound. Coverage is uniform with respect to the width of the true identified region $\theta_U(z) - \theta_L(z)$ pointwise at each $z \in \mathcal{Z}$ or along sequences therein. The coverage notion over the augmented parameter set $\Theta_z^*$ assures non-emptiness.
of the interval and avoids spuriously precise inference in regions where the estimated lower bound might be too large relative to the estimated upper bound. Coverage will be closer to the nominal level when correlations between the conditional mean errors are small. In particular, near one-sided critical values apply for the usual levels of confidence when \( \rho(z) = 0 \) (up to minor simulation inaccuracies of solving for \( \hat{c}(z) \) in (3.18), see Stoye (2020)). Note that the residual correlation \( \rho(z) \) can generally vary between different values of \( z \). Thus, power and size properties of the corresponding tests depend on the location of the local effect bound. In particular, they are driven by the share of missing outcome data at the given \( z \). In the case of point identification (meaning no missing outcomes), upper and lower bounds and pseudo true parameter are equivalent and \( \rho(z) = 1 \), and thus the confidence interval collapses to one using standard two-sided critical values at the point \( z \).

5. Monte Carlo Simulation

In this section we analyze the size and power properties of the proposed confidence intervals in finite samples. In particular we look at the size along a grid of \( z \)-values that vary with respect to the share of always-takers and thus the width of the identified set in the population. We consider a generalized Roy model with a random binary treatment and missing responses.

Similar designs have been considered for simulation for point-identified effects under exclusion restrictions, see e.g. Heckman and Vytlacil (2005) or Heiler (2021). Note that the true model here assumes one-sided/strong monotonicity of the effect of the treatment on response. This knowledge, however, is not imposed onto the estimation procedures, i.e. they are agnostic with respect to the type of monotonicity. We chose \( Z_i = X_{i,1} \). Thus, the true

---

\(^9\)Alternatively, one could employ an additional data splitting step for estimating the two bounds on different subsamples to assure that \( \rho(z) \) is equal to zero. We refrain from this approach to avoid inaccuracies in finite samples as the first estimation step already includes cross-fitting and potential data splitting for tuning of the machine learning methods within folds.
Table 5.1.: Monte Carlo Study: Generalized Roy Model

\[ S_i = \mathbb{I}(X_i' \gamma + D_i - v_i \geq 0) \]
\[ Y_i(0) = \epsilon_i(0) \]
\[ Y_i(1) = \mu_1(X_i, 1) + \epsilon_i(1) \]
\[ Y_i^* = D_i Y_i(1) + (1 - D_i) Y_i(0) \]
\[ Y_i = S_i Y_i^* \]
\[ D_i \sim \text{binomial}(0.5) \]
\[ X_i,d \sim \text{uniform}(0, 1) \]
\[ \epsilon_i(1), \epsilon_i(0) \sim \mathcal{N}(0, \sigma_1^2) \]
\[ v_i \sim \mathcal{N}(0, \rho \sigma_1) \]

with \( X_i = (X_{i,1}, \ldots, X_{i,d})' \), \( \gamma = (\Phi^{-1}(0.99) - 1, 0, 0, \ldots, 0)' \), \( \mu_1(x) = 0.35 - 4x^2 + 4x^3 \), \( \sigma_1 = \sigma_0 = 0.2 \), and \( \rho = 0.5 \). \( \Phi^{-1}(\cdot) \) denotes the quantile function of the standard normal distribution.

response function for the always-takers is given by

\[ \theta(z) = E[E[Y_i(1) - Y_i(0)|X_i, S_i(1) = S_i(0) = 1]|Z_i = z] \]
\[ = \mu_1(z) - \rho \frac{\phi(z \gamma)}{\Phi(z \gamma)}. \tag{5.1} \]

The parameters are chosen such that non-response rates vary from 84.13% to 99.00% and are monotonically increasing in \( z \). This will allow us to discover potential differences in coverage rates for varying setups. We consider both the continuous case, i.e. the size of confidence intervals for the continuous \( \theta(z) \) as well as power curves for a simple discretized version where \( z \) is integrated from 0 to 0.5 and 0.5 to 1 respectively. The nuisance quantities are estimated using honest generalized random forest and honest quantile regression forests (Athey et al., 2019) with default tuning parameters and two-fold cross-fitting. The design is sufficiently sparse for the forest to achieve the required convergence rates for estimating (5.1) according to Assumption A.5. For the heterogeneity analysis, we use b-splines with nodes and order selected via leave-one-out cross-validation for the continuous case and indicator functions for the discrete case. We analyze the size and power of the misspecification robust confidence intervals (3.17) at a 95% confidence level.

Figure 5.1 depict the simulated coverage rates in the case of \( p = 10 \) and \( p = 100 \) regressors
for total sample sizes of $n = 400$ and $n = 2000$. The rates for $n = 400$ can sometimes drop to around 90% but overall coverage is still decent. For $n = 2000$, the confidence intervals have at least nominal size with coverage ranging from 95% to 100% depending on $z$. Thus, the theoretical large sample guarantee in Theorem 4.2 seems to approximate the finite sample behavior reasonably well in these designs.

Figure 5.3 depict the power curves for two different heterogeneous effect parameters $\theta(z_0)$ and $\theta(z_1)$ for $p = 10$ and $p = 100$ at sample sizes $n = 400$ and $n = 2000$. $\theta(z_0)$ corresponds to an area with larger uncertainty regarding the partially identified parameter, i.e. it is integrated over the range of the heterogeneity with the largest share of unobserved outcome while $\theta(z_1)$ integrates over the range with the largest share of observed outcome. The difference in uncertainty can also be seen in Figure 1.1. The results show that the power curves are close to zero around the null for all sample size and designs reflecting the conservativeness of the inferential method. However, power converges quickly to 100% when moving away from the null. Power is lower for smaller sample sizes and a larger amount of possible confounding variables as expected. Moreover, in the $z = z_0$ case for which the share of missing outcome
Figure 5.3.: Coverage rates for $\hat{\theta}(z)$

(a) Design: $z_0$, $p = 10$
(b) Design: $z_0$, $p = 100$
(c) Design: $z_1$, $p = 10$
(d) Design: $z_1$, $p = 100$

Designs with $z = z_0$ depict the power curves as a function of the deviation from the null hypothesis for parameter $\theta(z_0) = \int_0^{1/2} \theta(z) dF(z)$. Designs with $z = z_1$ depict the power curves as a function of the deviation from the null hypothesis for parameter $\theta(z_1) = \int_{1/2}^1 \theta(z) dF(z)$. Results are based on 1000 Monte Carlo replications.

is larger, confidence intervals have lower power compared to the $z = z_1$ case that is closer to the case of point identification. Overall, intervals seems to perform reasonably well for different degrees of identification in the overall heterogeneous effect but being closer to point identification tends to yield more power in finite samples.
6. Concluding Remarks

This paper provides a method for estimation and inference for heterogeneous bounds for treatment effects under sample selection. There are multiple extensions possible: For example, in many applications where the method could be useful, the iid assumption is overly restrictive. In particular, in social experiments units are often clustered within groups such as schools or regions. In this case, the cross-fitting requires adaptation to the dependence structure and standard errors should be based on cluster-robust or jackknife type estimators. It would also be interesting to see under which conditions the methodology in this paper can be extended to more general non-smooth moment inequality problems.

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Appendix A  Moment Functions

Assume propensity scores are known, i.e. $P(D_i = 1|X_i = x) = e(x)$ known. For the correction terms for the unknown case consider Semenova (2020). The nuisance vector is given by $\eta_0 = \{s(0,x), s(1,x), q(u,x)\}$ where

\[
\begin{align*}
    s(d, x) &= P(S_i = 1|X_i, D_i = d) \\
    q(u, x) &= \inf\{q : u \leq P(Y_i \leq q|D_i = 1, S_i = 1, X_i = x)\}
\end{align*}
\] (A.1) (A.2)

for all $u \in [0, 1]$, $x \in \mathcal{X}$, $d \in \{0, 1\}$. Moreover define

\[
\begin{align*}
p_0(x) &= \frac{s(0,x)}{s(1,x)} \\
\mathbb{1}_i^+ &= \mathbb{1}(p_0(X_i) < 1) \\
\mathbb{1}_i^- &= \mathbb{1}(p_0(X_i) > 1) \\
\mu_{i0}^+ &= E[s(0, X_i) | \mathbb{1}_i^+ = 1] \\
\mu_{i1}^- &= E[s(1, X_i) | \mathbb{1}_i^- = 1]
\end{align*}
\]
The Neyman orthogonal moment functions are given by
\[
\psi_L(W_i, \eta) = \psi^*_L(W_i, \eta) + \frac{1^+}{\mu_{10}} \alpha^+_L(W_i, \eta) + \frac{1^-}{\mu_{11}} \alpha^-_L(W_i, \eta)
\]
\[
\psi_U(W_i, \eta) = \psi^*_U(W_i, \eta) + \frac{1^+}{\mu_{10}} \alpha^+_U(W_i, \eta) + \frac{1^-}{\mu_{11}} \alpha^-_U(W_i, \eta)
\]
with nonrobust moment functions
\[
\psi^*_L(W_i, \eta) = \frac{1^+}{\mu_{10}} \left( \frac{D_i}{e(X_i)} S_i Y_i \mathbb{1}(Y_i \leq q(p_0(X_i), X_i)) - \frac{1 - D_i}{1 - e(X_i)} S_i Y_i \right)
\]
\[
\psi^*_U(W_i, \eta) = \frac{1^+}{\mu_{10}} \left( \frac{D_i}{e(X_i)} S_i Y_i \mathbb{1}(Y_i \geq q(1 - p_0(X_i), X_i)) - \frac{1 - D_i}{1 - e(X_i)} S_i Y_i \right)
\]
and bias-corrections
\[
\alpha^+_L(W_i, \eta) = q(p_0(X_i), X_i) \left( \frac{1 - D_i}{e(X_i)} S_i - s(0, X_i) \right)
\]
\[
- q(p_0(X_i), X_i) p_0(X_i) \left( \frac{D_i S_i}{e(X_i)} - s_1(X_i) \right)
\]
\[
- q(p_0(X_i), X_i) s(1, X_i) \left( \frac{D_i S_i \mathbb{1}(Y_i \leq q(p_0(X_i), X_i))}{s(1, X_i) e(X_i)} - p_0(X_i) \right)
\]
\[
\alpha^-_L(W_i, \eta) = -q(1 - 1/p_0(X_i), X_i) p_0(X_i) \left( \frac{1 - D_i}{e(X_i)} S_i - s(0, X_i) \right)
\]
\[
+ q(1 - 1/p_0(X_i), X_i) \left( \frac{D_i S_i}{e(X_i)} - s_1(X_i) \right)
\]
\[
- q(1 - 1/p_0(X_i), X_i) s(0, X_i) \left( \frac{D_i S_i \mathbb{1}(Y_i \leq q(1 - 1/p_0(X_i), X_i))}{s(0, X_i) e(X_i)} - (1 - p_0(X_i)) \right)
\]
\[ \alpha^+_U(W_i, \eta) = q(1 - p_0(X_i), X_i) \left( \frac{1 - D_i S_i}{e(X_i)} - s(0, X_i) \right) \\
- q(1 - p_0(X_i), X_i)p_0(X_i) \left( \frac{D_i S_i}{e(X_i)} - s_1(X_i) \right) \\
+ q(1 - p_0(X_i), X_i)s(1, X_i) \left( \frac{D_i S_i 1(Y_i \leq q(1 - p_0(X_i), X_i))}{s(1, X_i)e(X_i)} - (1 - p_0(X_i)) \right) \]

\[ \alpha^-_U(W_i, \eta) = q(1/p_0(X_i), X_i)p_0(X_i) \left( \frac{1 - D_i S_i}{e(X_i)} - s(0, X_i) \right) \\
+ q(1/p_0(X_i), X_i)s(1, X_i) \left( \frac{D_i S_i}{e(X_i)} - s_1(X_i) \right) \\
+ q(1/p_0(X_i), X_i)s(0, X_i) \left( \frac{D_i S_i 1(Y_i \leq q(1/p_0(X_i), X_i))}{s(0, X_i)e(X_i)} - p_0(X_i) \right) \]

**Appendix B  Definition of Variances**

The true variance is given by

\[ \Omega(z) = B(z)' E[B(Z_i)(\varepsilon_i + r_i)(\varepsilon_i + r_i)' B(Z_i)] B(z). \quad (B.1) \]

Its consistent estimator is

\[ \hat{\Omega}_n(z) = B(z)' \frac{1}{n} \sum_{i=1}^{n} [B(Z_i)e_i e_i' B(Z_i)'] B(z), \quad (B.2) \]

where

\[ e_i = \begin{pmatrix} e_i,L(Z_i) \\ e_i,U(Z_i) \end{pmatrix} \]

with \( e_{i,B} = \psi_B(W_i, \hat{\eta}) - b_B(Z_i)' \hat{\beta}_B \) being the residuals of the nonparametric regression for \( B = L, U \).
Appendix C  Proof of Theorem 4.1 and 4.2

C.1  Notation

First we introduce notation and establish some important auxiliary results. We then show the small machine learning bias and linearization result, followed by asymptotic. This serves as the input for the main assumption for adaptation of the method by Stoye (2020) that provides the coverage result. We use $x \leq y$ whenever $x = O(y)$ and $x \lesssim_P y$ when $x = O_p(y)$. Statements about random variables are almost surely if not stated differently. We refer to Semenova and Chernozhukov (2021) as SC.

C.2  Auxiliary Results

(a.i) $p$ and $s$ rates  By definition $p_0(x) = s(0, x)/s(1, x)$ and equivalently for $\hat{p}(x)$, thus
\[
\hat{p}(x) - p_0(x) = \frac{\hat{s}(0, x) - s(0, x)}{\hat{s}(1, x) - s(1, x)} = \frac{\hat{s}(0, x) - s(0, x)}{s(1, x)} \frac{s(1, x)}{\hat{s}(1, x) - s(1, x)} \leq \sup_d |\hat{s}(d, x) - s(d, x)|
\]
almost surely in $\mathcal{X}$ due to Assumption A.3.

(a.ii) Quantile function and level bounds  By Assumption A.2, we have that on $\mathcal{T}_n$ that
\[
|q(\hat{p}(X), X) - q(p_0(X), X)| = \frac{1}{f(q(\hat{p}(X), X))}|\hat{p}(X) - p_0(X)| \lesssim |\hat{p}(X) - p_0(X)|
\]
\[
\Rightarrow E[|q(\hat{p}(X), X) - q(p_0(X), X)|^2]^{1/2} \lesssim \lambda_{s,n,2}
\]
using a mean-value expansion and exploiting that \( \hat{p} \) is almost surely bounded away from 0 and 1. Now we bound the expectation of estimated versus true truncation thresholds
\[
E[|\mathbb{1}_{\{Y < \hat{q}(\hat{p}(X), X)\}} - \mathbb{1}_{\{Y < \hat{q}(p_0(X), X)\}}| |D_i = 1, S_i = 1] \\
\lesssim E[|F_{y|x,d=1,s=1}(\hat{q}(\hat{p}(X), X)) - F_{y|x,d=1,s=1}(\hat{q}(p_0(X), X))| |D_i = 1, S_i = 1] \\
\lesssim \sup_y f_{y|x,d=1,s=1}(y) E[|\hat{q}(\hat{p}(X), X) - \hat{q}(p_0(X), X)|] \\
\lesssim E[|\hat{p}(X) - p_0(X)|^2] \\
\lesssim \lambda_{s,n,2}^2
\]
by a mean-value expansion and (a.i) together with Assumption A.2 and A.7. Similarly,
\[
E[|\mathbb{1}_{\{Y < \hat{q}(p_0(X), X)\}} - \mathbb{1}_{\{Y < \hat{q}(p_0(X), X)\}}| |D_i = 1, S_i = 1] \\
\lesssim E[|F_{y|x,d=1,s=1}(\hat{q}(p_0(X), X)) - F_{y|x,d=1,s=1}(q(p_0(X), X))| |D_i = 1, S_i = 1] \\
\lesssim \sup_y f_{y|x,d=1,s=1}(y) E[|\hat{q}(p_0(X), X) - q(p_0(X), X)|] \\
\lesssim \lambda_{q,n,2}^2
\]

\section*{C.3 Machine Learning Bias and Linearization}

We know verify that our assumptions are sufficient for SC, Assumption 3.5 and provide the linearization result first. For simplicity, we consider the moment function for the lower bound under positive monotonicity. The full bounds under conditional monotonicity follows analogously. SC Assumption 3.5 requires that
\[
B_n := \sqrt{n} \sup_{\eta \in T_n} \|E[b_i(\psi(W_i, \eta) - \psi(W_i, \eta_0))]| = o(1)
\]
\[
\Lambda_n := \sup_{\eta \in T_n} E[\|b_i(\psi(W_i, \eta) - \psi(W_i, \eta_0))|^2]^{1/2} = o(1).
\]
Unit subscripts \( i \) of random variables are omitted in the remainder of this subsection. Define the moment function for the lower bound with bias correction as
\[
\psi(W, \eta) = \sum_{j=1}^4 \psi^{[j]}(W, \eta)
\]
with
\[
\psi^{[1]}(W, \eta) := \frac{D}{e(X) SY} \mathbb{1}_{\{Y < q(p_0(X), X)\}} - \frac{1 - D}{1 - e(X) SY}SY
\]
\[
\psi^{[2]}(W, \eta) := q(p_0(X), X) \left( \frac{1 - D}{1 - e(X)} S - s(0, X) \right)
\]
\[
\psi^{[3]}(W, \eta) := -q(p_0(X), X)p_0(X) \left( \frac{D}{e(X)} S - s(1, X) \right)
\]
\[
\psi^{[4]}(W, \eta) := -q(p_0(X), X)s(1, X) \left( \frac{DS}{e(X) s(1, X)} \mathbb{1}_{\{Y < q(p_0(X), X)\}} - p_0(X) \right).
\]

For \(B_n\) note that, conditional on the cross-fitted model, the following expansion applies for any \(\eta \in \mathcal{T}_n\)
\[
\frac{1}{\sqrt{k}} E[|b\psi(W, \eta)| | X = x] \leq \left| \frac{1}{\bar{c}} E[|Y(1)| | X = x] \right| + \left| \frac{1}{1 - \bar{c}} E[|Y(1)| | X = x] \right| + \left| \tilde{Q} \right| + \left| \bar{Q} \right|
\]
\[
+ \left| \frac{\bar{Q} \left( \frac{1}{\bar{c}} + \frac{1}{2} \right)}{2} \right| + \left| \bar{Q} \left( \frac{1}{\bar{c}} + \frac{1}{2} \right) \right|
\]
\[
\leq E[|Y(1)| | X = x]
\]
almost surely in \(\mathcal{X}\) due to Assumption A.3. Now note that \(b\) is \(\mathcal{X}\)-measurable and thus we can apply the following bound using the Cauchy-Schwarz inequality:
\[
\frac{1}{\sqrt{k}} E[|b\psi(W, \eta)|] \leq \frac{1}{\sqrt{k}} E[||b|| | E[|Y| | X]]
\]
\[
\leq \frac{E[|b||b|]^{1/2}}{\sqrt{k}} E[E[Y^2 | X]]^{1/2}
\]
\[
\leq 1
\]
where the last inequality come from Assumptions A.1 and A.2. This bounds allows us to apply dominated convergence
\[
\frac{1}{\sqrt{k}} \partial_r E[b\psi(W, \eta_0 + r(\eta - \eta_0))] = \frac{1}{\sqrt{k}} E[b\partial_r E[\psi(W, \eta_0 + r(\eta - \eta_0))|X]]
\]
where the last step follows from Neyman-orthogonality of \(\psi(W, \eta)\) around \(\eta_0\) (Semenova, 2020). A uniform bound for the second derivative of \(E[\psi(W, \eta)|X = x]\) has been provided in SC, Proof of Lemma C.1. Thus, we obtain
\[
||\frac{1}{\sqrt{k}} E[b\psi(W, \eta)] - \frac{1}{\sqrt{k}} E[b\psi(W, \eta_0)]|| \lesssim \frac{1}{\sqrt{k}} E[||b|| ||\eta - \eta_0||^2].
\]
Together this implies that, as \(E[||b(z)||] = k_B\)
\[
\sqrt{n} \sup_{\eta \in T_n} ||E[b_i(\psi(W_i, \eta) - \psi(W_i, \eta_0))] \lesssim \sqrt{n}k_L(\lambda_{s,n,2}^2 + \lambda_{q,n,2}^2) = o(1)
\]
by the Cauchy-Schwarz and triangle inequality. In the case of a bounded basis similarly
\[
\sqrt{n} \sup_{\eta \in T_n} ||E[b_i(\psi(W_i, \eta) - \psi(W_i, \eta_0))] \lesssim \sqrt{n}k(\lambda_{s,n,2}^2 + \lambda_{q,n,2}^2) = o(1)
\]
by Assumption A.6 and Lemma 6.1 by Chernozhukov et al. (2018a). Now consider the variance term \(\Lambda_n\). We first bound the differences for each component \(\psi^{[1]}, \ldots, \psi^{[4]}\) separately:

\(\psi^{[1]}:\) For any \(\hat{\eta} \in T_n\), note that
\[
\psi^{[1]}(W, \hat{\eta}) - \psi^{[1]}(W, \eta_0)
= \frac{D}{e(X)} SY \{Y < q(\hat{p}(X), X)\} - \frac{D}{e(X)} SY \{Y < q(p(X), X)\}
= \frac{D}{e(X)} SY \left( \{Y < q(\hat{p}(X), X)\} - \{Y < q(p(X), X)\} + \{Y < q(p(X), X)\} - \{Y < q(p(X), X)\} \right)
\]
and thus, by \((a.ii)\) and Assumption A.2, we obtain
\[
\sup_{\eta \in T_n} E[(\psi^{[1]}(W, \hat{\eta}) - \psi^{[1]}(W, \eta_0))^2] \lesssim \lambda_{q,n,2}^2 + \lambda_{s,n,2}^2
\]
\(\psi^{[2]}: \)

\[
\psi^{[2]}(W, \hat{\eta}) - \psi^{[2]}(W, \eta_0) = \hat{q}(\hat{p}(X), X) \left( \frac{(1 - D)S}{1 - e(X)} - \hat{s}(0, X) \right) - q(p_0(X), X) \left( \frac{(1 - D)S}{1 - e(X)} - s(0, X) \right)
\]

\[
= [\hat{q}(\hat{p}(X), X) - q(p(X), X)] \left( \frac{(1 - D)S}{1 - e(X)} \right) + (\hat{q}(\hat{p}(X), X) - q(p_0(X), X))\hat{s}(0, X)
\]

\[
+ \hat{q}(p_0(X), X)(\hat{s}(0, X) - s(0, X)) + (\hat{q}(p_0(X), X) - q(p_0(X), X))s(0, X)
\]

\[
\lesssim |\hat{q}(\hat{p}(X), X) - q(p_0(X), X)| + |\hat{q}(p_0(X), X) - q(p_0(X), X)|
\]

almost surely by Assumption A.2 and A.7. (a.i) then implies that

\[
\sup_{\eta \in \mathcal{T}_n} E[(\psi^{[2]}(W, \hat{\eta}) - \psi^{[2]}(W, \eta_0))^2] \lesssim \lambda_{q,n,2}^2 + \lambda_{s,n,2}^2.
\]

\(\psi^{[3]}: \)

\[
\psi^{[3]}(W, \hat{\eta}) - \psi^{[3]}(W, \eta_0) = -\hat{q}(\hat{p}(X), X)\hat{p}(X) \frac{DS}{e(X)} + q(p_0(X), X)\hat{p}(X)\hat{s}(0, X)
\]

\[
+ q(p_0(X), X)p_0(X) \frac{DS}{e(X)} - q(p_0(X), X)s(0, X)
\]

\[
\lesssim |\hat{p}(X) - p_0(X)| + |\hat{q}(p_0(X), X) - q(p_0(X), X)| + |\hat{s}(0, X) - s(0, X)|
\]

almost surely by the same logic as for the previous components. Thus, we again obtain by (a.i) that

\[
\sup_{\eta \in \mathcal{T}_n} E[(\psi^{[3]}(W, \hat{\eta}) - \psi^{[3]}(W, \eta_0))^2] \lesssim \lambda_{q,n,2}^2 + \lambda_{s,n,2}^2.
\]
\(\psi[4]:\)

\[
\psi^{[4]}(W, \hat{\eta}) - \psi^{[4]}(W, \eta_0) = -\hat{q}(\hat{p}(X), X) \left( \frac{DS}{e(X)} \mathbb{1}_{\{Y < \hat{q}(\hat{p}(X), X)\}} \right) + \hat{q}(\hat{p}(X), X)s(0, X) - q(p_0(X), X)s(0, X)
\]

\[
\lesssim |\hat{q}(\hat{p}(X), X)\mathbb{1}_{\{Y < \hat{q}(\hat{p}(X), X)\}} - q(p_0(X), X)\mathbb{1}_{\{Y < q(p_0(X), X)\}}| + |\hat{s}(0, X) - s(0, X)|
\]

almost surely. Thus, using (a.i), (a.ii), and Assumption A.7, we obtain

\[
\sup_{\eta \in T_n} E[|\psi^{[4]}(W, \hat{\eta}) - \psi^{[4]}(W, \eta_0)|^2] \lesssim \lambda_{q,n,2}^2 + \lambda_{s,n,2}^2.
\]

Putting everything together we then obtain the required

\[
\sup_{\eta \in T_n} E[|\psi^{[4]}(W, \hat{\eta}) - \psi^{[4]}(W, \eta_0)|^2]^{1/2} \leq \xi_{k,L} E[|\psi^{[4]}(W, \hat{\eta}) - \psi^{[4]}(W, \eta_0)|^2]^{1/2}
\]

\[
\lesssim \xi_{k,L} (\lambda_{q,n,2} + \lambda_{s,n,2}) = o(1)
\]

by the triangle inequality and Assumption A.6. Therefore Assumption 3.5 from SC applies. This together with Assumptions A.1, A.2, A.4, and A.5 then covers all conditions required for SC, Lemma 3.1(b). Thus, we have that, for any \(z \in Z\) and \(B \in \{L, U\}\), the estimators are asymptotically linear:

\[
\sqrt{n}b_B(z)'(\hat{\beta}_B - \beta_{B,0}) = b(z)' E[b_B(Z_i)b_B(Z_i)']^{-1} \frac{1}{\sqrt{n}} \sum_{i=1}^{n} [b_b(Z_i)(\varepsilon_i + r_{\theta_B}(Z_i))] + o_p(1),
\]

where the remainder convergence follows from Assumption A.5.

C.4 Proof of Theorem 4.1

C.5 Preliminaries

Without loss of generality, instead of Assumption A.1, we assume that the basis functions are orthogonalized, i.e. \(E[b_B(Z_i)b_B(Z_i)'] = I_{b_B}\). Stacking the linearizations from the previous
section yields
\[ \sqrt{n} \left( \frac{b_L(z)'(\hat{\beta}_L - \beta_{L,0})}{b_U(z)'(\hat{\beta}_U - \beta_{U,0})} \right) = B(z)' \frac{1}{\sqrt{n}} \sum_{i=1}^{n} [B(Z_i)(\varepsilon_i + r_i)] \]
where
\[ B(z) = \begin{pmatrix} b_L(z) & 0 \\ 0 & b_U(z) \end{pmatrix}_{(k_L+k_U)\times 2} \]

Define
\[ \Omega(z) = B(z)'E[B(Z_i)(\varepsilon_i + r_i)(\varepsilon_i + r_i)'B(Z_i)]B(z) \]

Thus we have
\[ \sqrt{n}\Omega(z)^{-1/2}B(z) \frac{1}{\sqrt{n}} \sum_{i=1}^{n} [B(Z_i)(\varepsilon_i + r_i)] = \sum_{i=1}^{n} w_{i,n}(z)(\varepsilon_i + r_i) \]
with
\[ w_{i,n}(z) = \frac{\Omega(z)^{-1/2}}{\sqrt{n}} B(z)'B(Z_i). \]

Note that invertibility of \( \Omega(z) \) is guaranteed by Assumption 3.3 as this excludes the case of perfectly correlated conditional mean errors between upper and lower bound.

C.6 Auxiliary Results

For simplification we use notation \( B = B(z) \) and \( B_i = B(Z_i) \) whenever it does not cause confusion. We make use of the fact that for block matrices the induced \( L_2 \) norm \(||\cdot|||\) is given by
\[ M = \begin{pmatrix} M_1 & 0 \\ 0 & M_2 \end{pmatrix} \Rightarrow ||M|| = \max\{||M_1||, ||M_2||\}. \]

\((an.i)\) Expected norm of weights \( w_{i,n}(z) \) Note that Assumption 3.3 implies that the conditional mean have (absolute) correlation bounded away from one. Thus, their conditional variance-covariance matrix is strictly positive definite with \( \inf_{z \in Z} ||E[(\varepsilon_i + r_i)(\varepsilon_i + r_i)'|Z_i =
\[ \|\mathbf{z}\| > \lambda_{\text{min}} > 0. \text{ and consequently } \|E[B_i(\varepsilon_i + r_i)(\varepsilon_i + r_i)']B'_i]\| \geq \|\lambda_{\text{min}}^{-1}E[B_iB'_i]\|. \text{ This implies that} \\

\[
n\mathbb{E}[\|w_{i,n}(z)\|^2] \leq \|E[B_i(\varepsilon_i + r_i)(\varepsilon_i + r_i)']B'_i]\|^2 \mathbb{E}[\|B'_i\|^2] \\
= \|E[B_i(\varepsilon_i + r_i)(\varepsilon_i + r_i)']B'_i\|^2 \mathbb{E}[\|E[B'_i]\|^2] \\
\leq \frac{1}{\lambda_{\text{min}}} \|E[B_iB'_i]B'_i\| \mathbb{E}[\|(b_B(z)b_B(Z_i))^2\|] \\
= \frac{1}{\lambda_{\text{min}}} \|E[B'_i]\| \mathbb{E}[\sup_B b_B(z)b_B(z)] \\
\lesssim 1
\]
as \|b_B(z)\| = 1 \text{ and } \mathbb{E}[b_B(Z_i)b_B(Z_i)'|B = L, U].

\textbf{(an.ii) Norm of weights } w_{i,n}(z) \\
\|w_{i,n}\| = \frac{1}{\sqrt{n}} \|E[B_i(\varepsilon_i + r_i)(\varepsilon_i + r_i)']B'_i}\| \\
\leq \frac{1}{\sqrt{n}} \|E[B_i(\varepsilon_i + r_i)(\varepsilon_i + r_i)']B'_i\| \mathbb{E}[\|B'_i\|] \\
\leq \frac{1}{\sqrt{n}\lambda_{\text{min}}} \|E[B_iB'_i]\|^2 \mathbb{E}[\sup_z \|B(z)\|] \\
\leq \sup_B \sup_z \frac{\|b_B(z)\|}{\sqrt{n}} \\
\leq \sup_B \frac{\xi_{k,B}}{\sqrt{n}} \\
= o(1)
by Assumption A.5.
C.7 Multivariate Lindeberg Condition

In the following denote \( \bar{\xi} = \sup_B \xi_{k,B} \) and \( \bar{c} = \sup_B c_{k,B}(1 + \xi_{k,B}) \) and note that by Assumption A.5 we have that for any constant \( C_1, C_2 > 0 \)

\[
\frac{C_1 \sqrt{n}}{\bar{\xi}} - C_2 \bar{c} \to \infty.
\]

Now consider the weighted sum of the asymptotically linear representation. First note that by definition of the variance we have that

\[
V\left[ \sum_{i=1}^{n} w_{i,n}(z)(\varepsilon_i + r_i) \right] = I_2.
\]

Now we verify the Lindeberg condition. Note that for any \( \delta > 0 \),

\[
\sum_{i=1}^{n} E[||w_{i,n}(z)(\varepsilon_i + r_i)||^2 1(||w_{i,n}(\varepsilon_i + r_i)|| > \delta)]
\]

\[
= nE[||w_{i,n}(z)||^2 ||\varepsilon_i + r_i||^2 1(||\varepsilon_i + r_i|| > \delta/||w_{i,n}(z)||)]
\]

\[
\leq 2nE[||w_{i,n}(z)||^2 ||\varepsilon_i||^2 1(||\varepsilon_i|| + ||r_i|| > \delta/||w_{i,n}(z)||)]
\]

\[
+ 2nE[||w_{i,n}(z)||^2 ||r_i||^2 1(||r_i|| > \delta/||w_{i,n}(z)||)]
\]

\[
= (E.1) + (E.2)
\]

Now note that by the law of iterated expectations for some \( C > 0 \)

\[
(E.1) \lesssim 2nE[||w_{i,n}(z)||^2 E[||\varepsilon_i||^2 1(||\varepsilon_i|| + ||r_i|| > \delta/||w_{i,n}(z)||)]]
\]

\[
\leq 2nE[||w_{i,n}(z)||^2 \sup_{z \in \mathbb{Z}} E[||\varepsilon_i||^2 1(||\varepsilon_i|| + ||r_i|| > \delta/||w_{i,n}(z)||)|Z_i = z]]
\]

\[
\leq 2nE[||w_{i,n}(z)||^2 \sup_{z \in \mathbb{Z}} E[||\varepsilon_i||^2 1(||\varepsilon_i|| + 2\bar{\xi} > C\delta/\bar{c})|Z_i = z]]
\]

\[
= o(1)
\]

by auxiliary result \((an.i)\) and Assumption A.5 implying \( C\delta\sqrt{n}/\bar{\xi} - 2\bar{c} \to \infty \) together with the fact that the higher moment in Assumption A.2 implies uniform integrability of \( ||\varepsilon_i||^2 \)
as the moment function error tails are driven only by the (conditional) distribution of \(Y_i\).

\[
(E.2) \leq E[||w_{i,n}(z)||^2] \sup_B \sup_{z \in Z} |r_B(z)||^2 E[|\varepsilon_i| + |r_i| > \delta/||w_{i,n}(z)||]Z_i]
\]

\[
\leq nE[||w_{i,n}(z)||^2]2\bar{c}^2 \sup_{z \in Z} P(||\varepsilon_i|| > C\delta/\xi - 2\bar{c} |Z_i = z)
\]

\[
\lesssim \bar{c}^2 \sup_B \sup_{z \in Z} E[\varepsilon_{i,B}^2 |Z_i = z] \frac{C\delta \sqrt{n/\xi - 2\bar{c}}}{[C\delta \sqrt{n/\xi - 2\bar{c}}]^2}
\]

\[
= o(1)
\]

where the second to last step follows from Chebyshev’s inequality and the divergence of the denominator in the last step from Assumption A.5. The enumerator is again bounded due to Assumption A.2. Thus, overall we have that

\[
\lim_{n \to \infty} \sum_{i=1}^{n} E[||w_{i,n}(z)(\varepsilon_i + r_i)||^2]1(||w_{i,n}(\varepsilon_i + r_i)|| > \delta] = 0.
\]

which implies asymptotic normality around the best linear predictor. For the case with small approximation error, note that

\[
\sqrt{n}\Omega(z)^{-1/2} \begin{pmatrix} b_L(z)'(\hat{\beta}_L - \beta_{L,0}) \\ b_U(z)'(\hat{\beta}_U - \beta_{U,0}) \end{pmatrix}
\]

\[
= \sqrt{n}\Omega(z)^{-1/2} \begin{pmatrix} b_L(z)'\hat{\beta}_L - \theta_L(z) \\ b_U(z)'\hat{\beta}_U - \theta_U(z) \end{pmatrix} + \sqrt{n}\Omega(z)^{-1/2} \begin{pmatrix} \theta_L(z) - b_L(z)'\beta_{L,0} \\ \theta_U(z) - b_U(z)'\beta_{U,0} \end{pmatrix}
\]

\[
= \sqrt{n}\Omega(z)^{-1/2} \begin{pmatrix} b_L(z)'\hat{\beta}_L - \theta_L(z) \\ b_U(z)'\hat{\beta}_U - \theta_U(z) \end{pmatrix} + \sqrt{n}\Omega(z)^{-1/2} \begin{pmatrix} r_{\theta_L}(z) \\ r_{\theta_U}(z) \end{pmatrix}
\]

\[
= \sqrt{n}\Omega(z)^{-1/2} \begin{pmatrix} b_L(z)'\hat{\beta}_L - \theta_L(z) \\ b_U(z)'\hat{\beta}_U - \theta_U(z) \end{pmatrix} + o(1)
\]

where the last step follows from

\[
||\sqrt{n}\Omega(z)^{-1/2}(r_L(z) + r_u(z))|| \leq \sqrt{n}||\Omega(z)^{-1/2}|| \sup_{B,z \in Z} |r_B(z)| \lesssim \sqrt{n} \sup_B k_B^{-1/2}l_{k,B}c_{k,B}
\]

and the additional assumption in Theorem 4.1, Part 2.
C.8 Matrix Estimation

Now we consider difference between $\Omega(z)$ and $\hat{\Omega}_n(z)$. Denote

$$\xi_{k,B}^L := \sup_{z,z' \in \mathcal{Z}, z \neq z'} \frac{||a(z) - a(z')||}{||z - z'||}$$

where $a(z) := b(z)/||b(z)||$. Assume the following conditions hold for $B = L, U$:

Assumption C.1 There exists an $m_B > 2$ such that (i) $\sup_{x \in \mathcal{X}} E[|Y|^{m_B}|X = x] \lesssim 1$, (ii) $(\xi_{k,B}^L)^{2m/(m-2)} \log k_B/n \lesssim 1$, and (iii) $\xi_{k,B}^L \lesssim \log k$. Moreover assume that uniformly over $\mathcal{T}_n$

$$\kappa_n^1 := \sup_{\eta \in \mathcal{T}_n} E[\max_{1 \leq i \leq n} |\psi_B(W_i, \eta) - \psi_B(W_i, \eta_0)|] = o(n^{-\frac{1}{m_B}})$$

$$\kappa_n := \sup_{\eta \in \mathcal{T}_n} E[\max_{1 \leq i \leq n} (\psi_B(W_i, \eta) - \psi_B(W_i, \eta_0))^2]^{1/2} = o(1)$$

These assumptions are identical to or imply Assumptions 3.6 - 3.8 in Semenova and Chernozhukov (2021) and the additional conditions (i) and (ii) in their Theorem 3.3. Thus, pointwise consistency of $\hat{\Omega}_n(z)$ follows directly for any $z \in \mathcal{Z}$.

Note that in their Assumption 3.8 they first assume the weaker $\kappa_n^1 = o(1)$ for the asymptotic normality with true covariance matrix. For estimating the latter consistently, however, they also require that $n^{1/m} \kappa_n^1 = o(1)$, see Assumption (ii) in their Theorem 3.3. Thus there is no qualitative difference to the assumptions imposed here, see also Heiler and Knaus (2021) for a similar argument in a modified setup.

C.9 Inference

For the proof of Theorem 4.2 assume for simplicity that $k_L = k_U = k$, i.e. the rate of convergence of both nonparametric estimators is identical. Under A.V the estimators of $\sigma_L(z)$, $\sigma_U(z)$ and $\rho(z)$ are consistent. Thus, for each $z$, the asymptotic distribution in Theorem 4.1 matches the assumptions behind Stoye (2020), Theorem 1 (his Assumption 1). As Theorem 4.2 is pointwise at each $z$ it follows directly.