Valid Causal Inference
with (Some) Invalid Instruments

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Abstract

Instrumental variable methods provide a powerful approach to estimating causal effects in the presence of unobserved confounding. But a key challenge when applying them is the reliance on untestable “exclusion” assumptions that rule out any relationship between the instrument variable and the response that is not mediated by the treatment. In this paper, we show how to perform consistent IV estimation despite violations of the exclusion assumption. In particular, we show that when one has multiple candidate instruments, only a majority of these candidates—or, more generally, the modal candidate–response relationship—needs to be valid to estimate the causal effect. Our approach uses an estimate of the modal prediction from an ensemble of instrumental variable estimators. The technique is simple to apply and is “black-box” in the sense that it may be used with any instrumental variable estimator as long as the treatment effect is identified for each valid instrument independently. As such, it is compatible with recent machine-learning based estimators that allow for the estimation of conditional average treatment effects (CATE) on complex, high dimensional data. Experimentally, we achieve accurate estimates of conditional average treatment effects using an ensemble of deep network-based estimators, including on a challenging simulated Mendelian Randomization problem.

1 Introduction

Instrumental variable (IV) methods are a powerful approach for estimating treatment effects: they are robust to unobserved confounders and they are compatible with a variety of flexible nonlinear function approximators [see e.g. Newey and Powell, 2003, Darolles et al., 2011, Hartford et al., 2017, Lewis and Syrgkanis, 2018, Singh et al., 2019, Bennett et al., 2019], thereby allowing nonlinear estimation of heterogeneous treatment effects.

In order to use an IV approach, one must make three assumptions. The first, relevance, asserts that the treatment is not independent of the instrument. This assumption is relatively unproblematic, because it can be verified with data. The second assumption, unconfounded instrument, asserts that the instrument and outcome do not share any common causes. This assumption cannot be verified directly, but in some cases it can be justified via knowledge of the system; e.g. the instrument may be explicitly randomized or may be the result of some well understood random process. The final assumption, exclusion, asserts that the instrument’s effect on the outcome is entirely mediated through
the treatment. This assumption is even more problematic; not only can it not be verified directly, but it can be very difficult to rule out the possibility of direct effects between the instrument and the outcome variable. Indeed, there are prominent cases where purported instruments have been called into question for this reason. For example, in economics, the widely used “judge fixed effects” research design [Kling, 2006] uses random assignment of trial judges as instruments and leverages differences between different judges’ propensities to incarcerate to infer the effect of incarceration on some economic outcome of interest [see Frandsen et al., 2019, for many recent examples]. Mueller-Smith [2015] points out that exclusion is violated if judges also hand out other forms of punishment (e.g. fines, a stern verbal warning etc.) that are not observed. Similarly, in genetic epidemiology “Mendelian randomization” [Davey Smith and Ebrahim, 2003] uses genetic variation to study the effects of some exposure on an outcome of interest. For example, given genetic markers that are known to be associated with a higher body mass index (BMI), we can estimate the effect of BMI on cardiovascular disease. However, this only holds if we are confident that the same genetic markers do not influence the risk of cardiovascular disease in any other ways. The possibility of such “direct effects”—referred to as “horizontal pleiotropy” in the genetic epidemiology literature—is regarded as a key challenge for Mendelian randomization [Hemani et al., 2018].

It is sometimes possible to identify many candidate instruments, each of which satisfies the relevance assumption; in such settings, demonstrating exclusion is usually the key challenge, though in principle unconfounded instrument could also be a challenge. For example, many such candidate instruments can be obtained in both the judge fixed effects and Mendelian randomization settings, where individual judges and genetic markers, respectively, are treated as different instruments. Rather than asking the modeler to gamble by choosing a single candidate about which to assert these untestable assumptions, this paper advocates making a weaker assumption about the whole set of candidates. Most intuitively, we can assume majority validity: that at least a majority of the candidate instruments satisfy all three assumptions, even if we do not know which candidates are valid and which are invalid. Or we can go further and make the still weaker assumption of modal validity: that the modal relationship between instruments and response is valid. Observe that modal validity is a weaker condition because if a majority of candidate instruments are valid, the modal candidate–response relationship must be characterized by these valid instruments. Modal validity is satisfied if, as Tolsoy might have said, “All happy instruments are alike; each unhappy instrument is unhappy in its own way.”

This paper introduces ModelIV, a robust instrumental variable technique that we show is asymptotically valid when modal validity holds. ModelIV allows the estimation of nonlinear causal effects and lets us estimate conditional average treatment effects that vary with observed covariates. ModelIV is a black-box method in the sense that it is compatible with any valid IV estimator, which allows it to leverage any of the recent machine learning-based IV estimators. We experimentally validated ModelIV using both a modified version of the Hartford et al. [2017] demand simulation and a more realistic Mendelian randomization example. In both settings—even when we generated data with a very low signal-to-noise ratio—we observed ModelIV to be robust to exclusion-restriction bias and to accurately recover conditional average treatment effects (CATE).

2 Background on Instrumental Variables

We are interested in estimating the causal effect of some treatment variable, t, on some outcome of interest, y. The treatment effect is confounded by a set of observed covariates, x, as well as unobserved confounding factors, ϵ, which affect both y and t. With unobserved confounding, we cannot rely on conditioning to remove the effect of confounders; instead we use an instrumental variable, z, to identify the causal effect.

Instrumental variable estimation can be thought of as an inverse problem: we can directly identify the causal effect of the instrument on both the treatment and the response before asking the inverse question, “what treatment–response mappings, f : t → y, could explain the difference between these two effects?” The problem is identified if this question has a unique answer. If the true structural relationship is of the form, y = f(t, x) + ϵ, one can show that, E[y|x, z] = \int f(t, x) dF(t|x, z), where E[y|x, z] gives the instrument–response relationship, F(t|x, z) captures the instrument–treatment relationship, and the goal is to solve the inverse problem to find f(·). In the linear case, f(t, x) =

1Strictly, non-causal instruments suffice but identification and interpretation of the estimates can be more subtle [see Swanson and Hernán, 2018].
\[ \beta t + \gamma x, \] so the integral on the right hand side of reduces to \( \beta E[t|x, z] + \gamma x \) and \( \beta \) can be estimated using linear regression of \( y \) on the predicted values of \( t \) given \( x \) and \( z \) from a first stage regression. This procedure is known as Two-Stage Least Squares [see Angrist and Pischke, 2008]. More generally, the causal effect is identified if the integral equation has a unique solution for \( f \) [for details, see Newey and Powell, 2003].

A number of recent approaches have leveraged this additive confounders assumption to extend IV analysis beyond the linear setting. Newey and Powell [2003] and Darolles et al. [2011] proposed the first nonparametric procedures for estimating these structural equations, based on polynomial basis expansion. These methods relax the linearity requirement, but scale poorly in both the number of data points and the dimensionality of the data. To overcome these limitations, recent approaches have adapted deep neural networks for nonlinear IV analyses. DeepIV [Hartford et al., 2017] fits a first-stage conditional density estimate of \( \hat{F}(t|x, z) \) and uses it to solve the above integral equation. Both Lewis and Syrgkanis [2018] and Bennett et al. [2019] adapt generalized method of moments [Hansen, 1982] to the nonlinear setting by leveraging adversarial losses, while Singh et al. [2019] proposed a kernel-based approach. Puli and Ranganath [2019] showed that constraints on the structural equation for the treatment also lead to identification.

3 Related work

Inference with invalid instruments in linear settings  Much of the work on valid inference with invalid instruments is in the Mendelian Randomization literature, where violations of the exclusion restriction are common. For a recent survey see Hemani et al. [2018]. There are two broad approaches to valid inference in the presence of bias introduced by invalid instruments: averaging over the bias, or eliminating the bias with ideas from robust statistics. In the first setting, valid inference is possible under the assumption that each instrument introduces a random bias, but that the mean of this process if zero (although this assumption can be relaxed, c.f. Bowden et al. [2015], Kolesár et al. [2015]). Then, the bias tends to zero as the number of instruments grow. Methods in this first broad class have the attractive property that they remain valid even if none of the instruments is valid, but they rely on strong assumptions that do not easily generalize to the nonlinear setting considered in this paper. The second class of approaches to valid inference assumes that some fraction of the instruments are valid. Then, biased instruments are outliers whose effect can be removed by leveraging the robustness of the median [Kang et al., 2016] and the mode [Hartwig et al., 2017]. In this paper, we use the same robust statistics insights, generalizing them to the nonlinear setting.

Ensemble models  Ensembles are widely used in machine learning as a technique for improving prediction performance by reducing variance [Breiman, 1996] and combining the predictions of weak learners trained on non-uniformly sampled data [Freund and Schapire, 1995]. These ensemble methods frequently use modal predictions via majority voting among classifiers, but they are designed to reduce variance. Both the median and mode of an ensemble of models have been explored as a way of improve robustness to outliers in the forecasting literature [Stock and Watson, 2004, Kourentzes et al., 2014], but we are not aware of any prior work that explicitly uses these aggregation techniques to eliminate bias from an ensemble.

Mode estimation  If a distribution admits a density, the mode is defined as the global maximum of the density function. More generally, the mode can be defined as the limit of a sequence of modal intervals—intervals of width \( h \) that contains the largest proportion of probability mass—such that \( x_{\text{mode}} = \lim_{h \to 0} \arg \max_x F((x - h/2, x + h/2)) \). These two definitions suggest two estimation methods for estimating the mode from samples: either one may try to estimate the density function and the maximize the estimated function [Parzen, 1962], or one might search for midpoints of modal intervals from the empirical distribution functions. To find modal intervals, one can either fix an interval width, \( h \), and choose \( x \) to maximize the number of samples within the modal interval [Chernoff, 1964], or one can solve the dual problem by fixing the target number of samples to fall into the modal interval and minimizing \( h \) [Dalenius, 1965, Venter, 1967]. We use this latter Dalenius–Venter approach as the target number of samples can be parameterized in terms of the number of valid instruments, thereby avoiding the need to select a kernel bandwidth \( h \).
4 ModeIV

In this paper, we assume we have access to a set of $k$ independent\(^2\) candidate instrumental variables, $\mathcal{Z} = \{z_1, \ldots, z_k\}$, which are ‘valid’ if they satisfy relevance, exclusion and unconfounded instrument, and ‘invalid’ otherwise. Denote the set of valid instruments, $\mathcal{V} := \{z_i : z_i \perp y|x, t, \epsilon\}$, and the set of invalid instruments, $\mathcal{I} := \mathcal{Z} \setminus \mathcal{V}$. We further assume that each valid instrument identifies the causal effect. This amounts to assuming that the unobserved confounder’s affect on $y$ is additive, $y = f(t, x, z_i; i \in \mathcal{Z}) + \epsilon$ for some function $f$ and $E[y|x, z_i; i \notin \mathcal{J}, z_j] = \int f(t, x, z_i; i \notin \mathcal{J}) dF(t|x, z_i; i \notin \mathcal{J}, z_j)$ has a unique solution for all $j \in \mathcal{Z}$.

The ModeIV procedure requires the analyst to specify a lower bound $V \geq 2$ on the number of valid instruments and then proceeds in three steps.

1. Fit an ensemble of $k$ estimates of the conditional outcome $\{\hat{f}_1, \ldots, \hat{f}_k\}$ using a non-linear IV procedure applied to each of the $k$ instruments. Each $\hat{f}$ is a function mapping treatment $t$ and covariates $x$ to an estimate of the effect of the treatment conditional on $x$.

2. For a given test point $(t, x)$, select $[\hat{l}, \hat{u}]$ as a smallest interval containing $V$ of the estimates $\{\hat{f}_1(t, x), \ldots, \hat{f}_k(t, x)\}$. Define $\hat{f}_{\text{mode}} = \{i : \hat{l} < \hat{f}_i(t, x) < \hat{u}\}$ to be the indices of the instruments corresponding to estimates falling in the interval.

3. Return $\hat{f}_{\text{mode}}(t, x) = \frac{1}{|\hat{f}_{\text{mode}}|} \sum_{i \in \hat{f}_{\text{mode}}} \hat{f}_i(t, x)$

The idea is that the estimates from the valid instruments will tend to cluster around the true value of the effect, $E[y|do(t), x]$. We assume that the most common effect instrument is a valid one; i.e., that the modal effect is valid. To estimate the mode, we look for the tightest cluster of points. These are the points contained in $\hat{f}_{\text{mode}}$. Intuitively, each estimate in this interval should be approximately valid and hence approximates the modal effect. We take the average of these estimates to gain statistical strength.

The next theorem formalizes this intuition and shows, in particular, that ModeIV asymptotically identifies and consistently estimates the causal effect.

**Theorem 1.** Fix a test point $(t, x)$ and let $\hat{\beta}_1, \ldots, \hat{\beta}_k$ be estimators of the causal effect of $t$ at $x$ corresponding to $k$ (possibly invalid) instruments. E.g., $\hat{\beta}_j = \hat{f}_j(t, x)$. Denote the true effect as $\beta = E[y|do(t), x]$. Suppose that

1. (consistent estimators) $\hat{\beta}_j \rightarrow \beta_j$ almost surely for each instrument. In particular, $\beta_j = \beta$ whenever the $j$th instrument is valid.

2. (modal validity) At least $p\%$ of the instruments are valid, and no more than $p\% - \epsilon$ of the invalid instruments agree on an effect. That is, $p\%$ of the instruments yield the same estimand if and only if all of those instruments are valid.

Let $[\hat{l}, \hat{u}]$ be the smallest interval containing $p\%$ of the instruments and let $\hat{f}_{\text{mode}} = \{i : \hat{l} < \hat{\beta}_i < \hat{u}\}$. Then,

$$\sum_{i \in \hat{f}_{\text{mode}}} \hat{w}_i \hat{\beta}_i \rightarrow \beta$$

almost surely, where $\hat{w}_i, w_i$ are any non-negative set of weights such that each $\hat{w}_i \rightarrow w_i$ a.s. and $\sum_{i \in \hat{f}_{\text{mode}}} w_i = 1$. Further suppose that the individual estimators are also asymptotically normal,

$$\sqrt{n} \hat{\beta}_j \rightarrow N(\beta_j, \sigma_j^2)$$

for each instrument. Then it also holds that the modal estimator is asymptotically normal:

$$\sqrt{n} \sum_{i \in \hat{f}_{\text{mode}}} \hat{w}_i \hat{\beta}_i \rightarrow N(\beta, \sum_i w_i^2 \sigma_i^2).$$

\(^2\)This independence requirement can be weakened to conditionally independent, conditional on some variable $c$. See appendix A.2 for details.
We defer the proof to the supplementary material.

Of course, the ModeIV procedure can be generalized to allow different estimators of the mode than the one used in Steps 2 and 3. The particular choice we make here has the advantage of being straightforward, statistically stable, computationally inexpensive, and relatively insensitive to the choice of $V$. The procedure as a whole is, however, $k$ times more computationally expensive than running single estimation procedure at both training and test time.

5 Experiments

We studied ModeIV empirically in two simulation settings. First, we investigated the performance of ModeIV for non-linear effect estimation as the proportion of invalid instruments increased for various amounts of direct effect bias. Second, we applied ModeIV to a realistic Mendelian randomization simulation to estimate heterogeneous treatment effects. For all experiments, we use DeepIV [Hartford et al., 2017] as the nonlinear estimator. Full experimental details are given in the appendix.

5.1 Biased demand simulation

We evaluated the effect of invalid instruments on estimation by modifying the low dimensional demand simulation from Hartford et al. [2017] to include multiple candidate instruments. The Hartford et al. demand simulation models a scenario where the treatment effect varies as a nonlinear function of time $\psi(t)$, and observed covariates $x$.

$$
\begin{align*}
  z_{1:k}, \nu &\sim \mathcal{N}(0, 1) \\
  t &\sim \text{unif}(0, 10) \\
  e &\sim \mathcal{N}(\rho \nu, 1 - \rho^2), \\
  p & = 25 + (z^T \beta(z \nu) + 3) \psi(t) + \nu \\
  y & = 100 + 10x^T \beta(x) \psi(t) + (x^T \beta(x) \psi(t) - 2)p + \gamma \sin(z^T \beta(z \nu)) + e
\end{align*}
$$

We highlight the differences between our data generating process and the Hartford et al. data generating process in red: we have $k$ instruments whose effect on the treatment is parameterized by $\beta(z \nu)$; instead of a single instrument in the original; we include an exclusion violation term which introduces bias into standard IV approaches whenever $\gamma$ is non-zero. The vector $\beta(z \nu)$ controls the direct effect of each instrument: invalid instruments have nonzero $\beta_i(z \nu)$ coefficients, while valid instrument coefficients are zero.

We fitted an ensemble of $k$ different DeepIV models that were each trained with a different instrument $z_i$. In Figure 1, we compare the performance of ModeIV with three baselines: DeepIV with oracle access to the set of valid instruments (DeepIV-opt); the ensemble mean (Mean); and a naive approach that fit a single instance of DeepIV treating all instruments as valid (DeepIV-all). The $x$-axis of the

\[ \psi(t) = \frac{2}{600} \left[ (t - 5)^4 + 4(t - 5)^2 + t/10 - 2 \right] \]

See the appendix for a plot of the function.
plots indicates the scaling factor $\gamma$, which scales the amount of bias introduced via violations of the exclusion restriction.

All methods performed well when all the instruments were valid. Once the methods had to contend with invalid instruments, Mean and DeepIV-all performed significantly worse than ModeIV because of both methods’ sensitivity to the biased instruments. ModeIV’s mean squared error closely tracked that of the oracle method as the number of biased instruments increased, and the raw mean squared errors of both methods also increased as the number of valid instruments in the respective ensembles correspondingly fell.

**Sensitivity**  When using ModeIV, one key practical question that an analyst faces is choosing $V$, the lower bound on the number of valid instruments. We evaluated the importance of this choice in figure 2 (left) by testing the performance of ModeIV across the full range of choices for $V$ with different numbers of biased instruments. We found that, as expected, the best performance was achieved when $V$ equaled the true number of valid instruments, but also that similar levels of performance could be achieved with more conservative choices of $V$. That said, with only 5 valid instruments, ModeIV tended to perform worse when $V$ was set too small. To see why this is the case, notice that in figure 2 (right), there are a number of regions of the input space where the invalid instruments agreed by chance (e.g. $t \in [-1, 0]$), so these regions bias ModeIV for small mode set sizes. Overall, we observed that setting $V$ to half the number of instruments tended to work well in practice.

Asymptotically, ModeIV remains consistent when fewer than half of the instruments are valid, but when this is the case there are far more ways that Assumption 2 of Theorem 1 can be violated. This is illustrated in Figure 2 (right) which shows that there are a number of regions where the bias instruments agree by chance. Because of this, we recommend only using ModeIV when one can assume that the majority of instruments are valid, unless one has prior knowledge to justify modal validity without assuming the majority of instruments are valid.

**Selecting instruments?**  ModeIV constitutes a consistent method for making unbiased predictions but, somewhat counter-intuitively, it does not directly offer a way of inferring the set of valid instruments. For example, one might imagine identifying the set of candidates that most often form part of the modal interval $\hat{I}_{\text{mode}}$. The problem is that while candidates that fall within the modal

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4For example, if direct effects are strictly monotone and disagree, chance agreements among invalid instruments can only occur in a finite number of locations.
We evaluate our approach on the simulated data adapted from Hartwig et al. [2017], which is designed which tend to perform best on low-noise regimes. To address this, we leveraged the inductive bias that while making it easier to visually show the differences between the fitted functions and their true targets.

We make the treatment effect vary as a function of observable characteristics to model a scenario where treatments may affect different sub-populations differently. We simulate this by making the instrument’s effect on the treatment, $\alpha_i$, and direct effect on the response, $\delta_i$, are both drawn from Uniform($0_{10}, 0.2$) distributions for all $i$. For all experiments we used 100 candidate instruments and varied the number of valid instruments from 50 to 100 in increments of 10; we set $\delta_i$ to 0 for all valid instruments. More formally,

$$z_i \sim \text{Binomial}(2, p_i) \quad \text{for } i \in [1 \ldots K], \quad \beta(x) := \text{round}(x^T \gamma(x), 0.1).$$

$$t := \sum_{j=1}^K \alpha_j z_j + \rho u + \epsilon_x \quad y := \beta(x)t + \sum_{j=1}^K \delta_j z_j + u + \epsilon_y$$

In the original Hartwig et al. simulation, the treatment effect $\beta$ was fixed for all individuals. Here, we make the treatment effect vary as a function of observable characteristics to model a scenario where treatments may affect different sub-populations differently. We simulate this by making the treatment effect, $\beta(x)$, a sparse linear function of observable characteristics, $x \in R^10$, where 3 of the 10 coefficients, $\gamma_i(x)$, were sampled from $U(0.2, 0.5)$ and the remaining $\gamma_i(x)$ were set to 0. We introduce non-linearity by rounding to the nearest 0.1, which makes the learning problem harder, while making it easier to visually show the differences between the fitted functions and their true targets.

Mendelian randomization problems tend to have low signal-to-noise ratios, where the treatment explains only 1-3% of the response variance. This makes the setting challenging for neural networks, which tend to perform best on low-noise regimes. To address this, we leveraged the inductive bias that the data is conditionally linear in the treatment effect, using a neural network to parameterize the...
The LATE for instrument $i$ can be thought of as the average treatment effect for the sub-population that change their behavior in response to a change in the value of instrument $i$; if the LATEs differ across instruments, this implies that each instrument will result in a different estimate of $\hat{f}(t, x)$ regardless of whether any of the instruments are invalid. In such settings, ModeIV will return the closest $f_i(t, x)$’s, but one would need additional assumptions on how these estimates cluster relative to biased estimates to apply any causal interpretation to this quantity. The alternative is the approach that we take here: assume that a common function $f(t, x)$ is shared across all units and allow for heterogeneous treatment effects by allowing the treatment effect to vary as a function of observed covariates $x$. This shared heterogeneous effect assumption is weaker than prior work.
on robust IV, which requires a “constant effect” effect assumption that every individual responds in exactly the same way to the treatment via a linear parameter, \( \beta \).

Second, we have focused on settings where each instrument is independent. In principle ModeIV extends to settings where some instruments are confounded or all the instruments share a common cause, but the conditions for valid inference are more delicate because one has to ensure all backdoor paths between the instruments and response are blocked (see appendix A.2).

**Broader Impact**

IV methods are important tools in the causal inference toolbox. These methods have been applied to study causal effects across a wide range of settings, spanning economic policies, phenotypes that may cause disease, and recommendation algorithms. Typically, analysts use their best expert judgment to assess whether various candidate instruments satisfy the exclusion restriction and then proceed with effect estimation. However, this judgement is both difficult to make and highly consequential: biased instruments can invalidate the analyst’s conclusions.

This paper offers the analyst a potentially easier alternative: assuming that some fixed proportion of instruments are valid. With this, the paper provides a method for estimating causal effects in the presence of invalid instruments, backed by theoretical guarantees. Because ModeIV captures nonlinear effects, it may be better suited to applications in genetics and economics than previous methods.

Of course, caveats still apply. As with all causal inference methods, ModeIV still requires an analyst to make assumptions and to assess potentially delicate, mathematical statements. Although we have striven to make the limitations of our method explicit and to provide guidelines where possible, negative impacts could arise if analysts apply our method without prudence and thus obtain invalid causal conclusions, particularly if these are offered as policy suggestions. To mitigate the potential for such negative impacts, we have clearly noted when ModeIV should not be applied. Beyond that, we recommend that analysts considering applying this or any other causal estimation procedure conduct as much sensitivity analysis and external validation as possible.

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A Appendix

A.1 Proof of Theorem 1

The next theorem formalizes this intuition and shows, in particular, that MODE-IV asymptotically identifies and consistently estimates the causal effect.

**Theorem 2.** Fix a test point \((t, x)\) and let \(\hat{\beta}_1, \ldots, \hat{\beta}_k\) be estimators of the causal effect of \(t\) at \(x\) corresponding to \(k\) (possibly invalid) instruments. E.g., \(\hat{\beta}_j = \hat{f}_j(t, x)\). Denote the true effect as \(\beta = E[y|do(t, x)]\). Suppose that

1. (consistent estimators) \(\hat{\beta}_j \to \beta\) almost surely for each instrument. In particular, \(\beta_j = \beta\) whenever the \(j\)th instrument is valid.
2. (valid mode) At least \(p\%\) of the instruments are valid, and no more than \(p\% - \epsilon\) of the invalid instruments agree on an effect. That is, \(p\%\) of the instruments yield the same estimand if and only if all of those instruments are valid.

Let \([\hat{l}, \hat{u}]\) be the smallest interval containing \(p\%\) of the instruments and let \(\hat{I}_{\text{mode}} = \{i : \hat{l} < \hat{\beta}_i < \hat{u}\}\). Then,

\[
\sum_{i \in \hat{I}_{\text{mode}}} \hat{w}_i \hat{\beta}_i \to \beta
\]

almost surely, where \(\hat{w}_i, w_i\) are any non-negative set of weights such that each \(\hat{w}_i \to w_i\) a.s. and \(\sum_{i \in \hat{I}_{\text{mode}}} w_i = 1\). Further suppose that the individual estimators are also asymptotically normal,

\[
\sqrt{n} \hat{\beta}_j \to N(\beta_j, \sigma_j^2)
\]

for each instrument. Then it also holds that the modal estimator is asymptotically normal:

\[
\sqrt{n} \sum_{i \in \hat{I}_{\text{mode}}} \hat{w}_i \hat{\beta}_i \to N(\beta, \sum_i w_i^2 \sigma_i^2).
\]

**Proof.** First we argue that \(\hat{I}_{\text{mode}}\) converges to a set that contains only valid instruments. All valid instruments converge to a common value \(\beta\). The distance between any two valid instruments is at most twice the distance between \(\beta\) and the furthest valid instrument. Since at least \(p\%\) of the instruments are valid, this means that there is an interval (containing the mode) with distance going to \(0\) that contains \(p\%\) of the instruments. Eventually this must be the smallest interval containing \(p\%\) of the instruments, because the limiting \(\beta_j\) of the invalid instruments are spaced out by assumption.

The result follows by continuous mapping.

A.2 Relaxing independence of instrumental variables

For simplicity, we presented ModelIV in the context of independent candidate instruments. This setting is shown in Figure 4 (left) where we have \(k\) candidates, \(\{z_i : i \in 1, \ldots, k\}\), some of which are valid (shown in blue), and some of which are invalid (e.g. \(z_k\) shown in pink has a direct effect on the response). This independent candidates setting is most common where the instruments are explicitly randomized: e.g. in judge fixed effects where the selection of judges is random.

A more complex setting is shown in Figure 4 (right). Here, the candidates share a common cause, \(u\). In this scenario, if \(u\) is not observed, each of the previously valid instruments (e.g. \(z_1, z_2\) and \(z_{k-1}\) in the figure) are no longer valid because they fail the unconfounded instrument assumption via the backdoor path \(z_1 \leftarrow u \rightarrow z_k \rightarrow y\). However, if we condition on all the candidates that have a direct effect on \(y\) and treat them as observed confounders, we block this path which allows for valid inference. Of course we do not know which of the candidates have a direct effect, so when building an ensemble, for each candidate \(z_i\), we treat all \(z_j \neq i\) as observed confounders to block these potential backdoor paths. This addresses the issue as long as there is not some \(z_{k+1}\) which is not part of our candidate set, but nevertheless opens up a backdoor path \(z_1 \leftarrow u \rightarrow z_{k+1} \rightarrow y\).

If \(u\) is observed, we can simply control for it. This suggests a natural alternative approach would be to try to estimate \(u\) and control for its effect, using an approach analogous to Wang and Blei [2019]. We plan to investigate this in future work.
Figure 4: We primarily focus on the setting on the left where each candidate, $z_i$, is independent. It is also possible to apply the method in the setting on the right where the candidates share a common cause, more care is needed. See the discussion in section A.2.

Table 2: Average absolute bias in estimation of the conditional average treatment effect. The ensemble methods tended to have slightly larger bias than the optimal model, but far less than the naive approach which uses all instruments. The mean aggregation function performs relatively well on this task, but this approach comes with no guarantees, so it degrades in settings with more bias.

A.3 Additional experimental details

Network architectures and experimental setup All experiments used the same neural network architectures to build up hidden representations for both the treatment and response networks used in DeepIV, and differed only in their final layers. Given the number of experiments that needed to be run, hyper-parameter tuning would have been too expensive, so the hyper-parameters were simply those used in the original DeepIV paper. In particular, we used three hidden layers with 128, 64, and 32 units respectively and ReLU activation functions. The treatment networks all used mixture density networks with 10 mixture components and the response networks were trained using the two sample unbiased gradient loss [see Hartford et al., 2017, equation 10]. We used our own PyTorch [Paszke et al., 2019] re-implementation of DeepIV to run the experiments.

For all experiments, 10% of the original training set was kept aside as a validation set. The demand simulations had 90 000 training examples, 10 000 validation examples and 50 000 test examples. The Mendelian randomization simulations had 360 000 training examples, 40 000 validation examples and 50 000 test examples. All mean squared error numbers reported in the paper are calculated with respect to the true $y$ (with no confounding noise added) on a uniform grid of 50 000 treatment points between the 2.5\% and 97.5\% percentiles of the training distribution. 95\% confidence intervals around mean performance were computed using Student’s $t$ distribution.

The networks were trained on a large shared compute cluster that has around 100 000 CPU cores. Because each individual network was relatively quick to train (less than 10 minutes on a CPU), we used CPUs to train the networks. This allowed us to fit the large number of networks needed for the experiments. Each experiment was run across 30 different random seeds, each of which required 10 (demand simulation) and 102 (Mendelian randomization) network fits. In total, across
all experimental setups, random seeds, ensembles, etc. approximately 100 000 networks were fit to run all the experiments.

### Biased demand simulation

The biased demand simulation code was modified from the public DeepIV implementation. In the original DeepIV implementation, both the treatment and response are transformed to make them approximately mean zero and standard deviation 1; we left these constants unchanged ($p_{sd} = 3.7$, $p_{y} = 17.779$, $y_{sd} = 158$, $y_{y} = -292.1$). The observed features include a time feature, $t \sim \text{unif}(0,10)$, and $x \sim \text{Categorical}([\frac{1}{2}, \ldots, \frac{1}{2}])$, a one-hot encoding of 7 different equally likely “customer types”; each type modifies the treatment via the coefficient $\beta^x = [1, 2, \ldots, 7]^T$. These values are unchanged from the original Hartwig et al. data generating process. We introduce multiple instruments, $z_{1:k}$, whose effect on the treatment, $p$, and response, $y$, is via two different linear maps $\beta^{zp} \in \mathbb{R}^k$ and $\beta^{zy} \in \mathbb{R}^k$; each of the coefficients in these vectors are sampled independently so $\beta_i^{zp} \sim \text{unif}(0,5, 1.5)$, with the exception of the valid instruments where $\beta_i^{zy} = 0$ for all $i \in \mathcal{V}$. The $\gamma$ parameter scales the amount of bias introduced via exclusion violations; note that because the $\sin$ varies between $[-1, 1]$, we scale up this bias by a factor of 60 so that the effect it introduces is of the same order of magnitude as the variation in the original Hartwig et al. data generating process (where std. dev$(y) \approx y_{sd} = 158$). The full data generating process is as follows,

$$
\begin{align*}
    z_{1:k}, \nu & \sim \mathcal{N}(0,1) \quad t \sim \text{unif}(0,10) \quad e \sim \mathcal{N}(\rho \nu, 1-\rho^2) \\
    p' &= 25 + (z^T \beta^{zp} + 3) \psi(t) + \nu \\
    y' &= 100 + 10x^T \beta^{zx} \psi(t) + \left( x^T \beta^{zx} \psi(t) - 2 \right) p' + \gamma 60 \sin(z^T \beta^{zy}) + e \\
    p &= (p' - p_{sd})/p_{\mu} \quad y = (y' - y_{sd})/y_{\mu}
\end{align*}
$$

**Mendelian randomization simulation** This data generating process closely follows that of Simulation 1 of Hartwig et al. [2017], but was modified to include heterogeneous treatment effects. This description is an abridged version of that given in Hartwig et al.; we refer the reader to Hartwig et al. [2017] for more detail on the choice of parameters, etc.. The instruments are the genetic variables, $z_i$, which were generated by sampling from a Binomial $(2, p_i)$ distribution, with $p_i$ draw from a Uniform$(0.1, 0.9)$ distribution, to mimic bi-allelic SNPs in Hardy-Weinberg equilibrium. The parameters that modulate the genetic variable effect on the treatment are given by, $\alpha_i = \frac{\nu_i}{\sigma_{xx}}$, where $\nu_i \sim \text{unif}(0.01, 0.2)$ and $\sigma_{xx} = \text{std}(\sqrt{0.1 \sum_i \nu_i z_i})$. Similarly, the exclusion violation parameters, $\delta_i = \frac{|z_i \psi(t)|}{\sum_i \nu_i z_i}$, where again $\nu_i \sim \text{unif}(0.01, 0.2)$ and $\sigma_{zy} = \text{std}(\sqrt{0.1 \sum_i \nu_i z_i})$.

Note that $\delta_i$ is scaled by $\frac{|z_i \psi(t)|}{\sum_i \nu_i z_i}$ (the proportion of invalid instruments), which ensures that the average amount of bias introduced is constant as the number of invalid instruments vary. Error terms $u, \epsilon_x, \epsilon_y$ were independently generated from a normal distribution, with mean 0 and variances $\sigma_u^2, \sigma_x^2$ and $\sigma_y^2$, respectively, whose values were chosen to set the variances of $u, x$ and $y$ to one. These scaling parameters are chosen to enable an easy interpretation of the average treatment effect, $\beta$: with this scaling, $\beta = 0.1$ implies that one standard deviation of $t$ causes a 0.1 standard deviation of $y$ and hence the causal effect of $t$ on $y$ explains $0.1^2 = 0.01 = 1\%$ of the variance of $y$. The only place our simulation differs from Hartwig et al., is the treatment effect is a function of observed coefficients, $x \in \mathbb{R}^{10}$, with each $x_i \sim \text{uniform}(-0.5, 0.5)$, and the treatment effect is defined as, $\beta(x) := \text{round}(x^T \gamma^{(xt)}, 0.1)$, with $\gamma^{(xt)}$ a sparse vector of length 10, with three non-zeros $\gamma^{(xt)} \sim \text{uniform}(0.2, 0.5)$. The resulting true $\beta(x)$, takes on values in $\{-0.3, -0.2, \ldots, 0, 0.2, 0.3\}$. We also use 100 genetic variants instead of the 30 used in Hartwig et al., so that we could test ModelIV in a larger scale scenario. The resulting data generating process is given by,

$$
\begin{align*}
    z_i & \sim \text{Binomial}(2, p_i) \quad \text{for } i \in [1 \ldots K], \quad \beta(x) := \text{round}(x^T \gamma^{(xt)}, 0.1). \\
    t & := \sum_{j=1}^{K} \alpha_j z_j + \rho u + \epsilon_x \quad y := \beta(x) t + \sum_{j=1}^{K} \delta_j z_j + u + \epsilon_y
\end{align*}
$$