OPTIMAL REGIMES FOR ALGORITHM-ASSISTED HUMAN DECISION-MAKING

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Abstract. We consider optimal regimes for algorithm-assisted human decision-making. Such regimes are decision functions of measured pre-treatment variables and, by leveraging natural treatment values, enjoy a “superoptimality” property whereby they are guaranteed to outperform conventional optimal regimes. When there is unmeasured confounding, the benefit of using superoptimal regimes can be considerable. When there is no unmeasured confounding, superoptimal regimes are identical to conventional optimal regimes. Furthermore, identification of the expected outcome under superoptimal regimes in nonexperimental studies requires the same assumptions as identification of value functions under conventional optimal regimes when the treatment is binary. To illustrate the utility of superoptimal regimes, we derive new identification and estimation results in a common instrumental variable setting. We use these derivations to analyze examples from the optimal regimes literature, including a case study of the effect of prompt intensive care treatment on survival.

1. Introduction

Foundational work on causal inference and dynamic treatment regimes presents a promising pathway towards precision medicine (Robins, 1986; Richardson and Robins, 2013; Murphy, 2003; Robins, 2004; Tsiatis et al., 2019; Kosorok et al., 2021). In a precision-medicine system, decision rules might be algorithmically individualized based on an optimal rule previously learned from non-experimental or experimental data (Topol, 2019). However, wide-scale implementation of such a system will almost certainly roll-out under...
the supervision of existing medical care providers (Matheny et al., 2019). Indeed, there is some resistance to the notion that implementation of an optimal regime, successfully learned from the data, will result in better expected outcomes on average, compared to existing human-decision rules. This resistance stems in part from the belief that existing care providers often will have access to relevant information for decision-making that is not recorded in the observed data (Verghese et al., 2018). While these beliefs do not prohibit identification of decision rules that are optimal with respect to a set of measured covariates (Cui and Tchetgen Tchetgen, 2021a; b; Qiu et al., 2021; Pu and Zhang, 2021; Han, 2021; Miao et al., 2018; Qi et al., 2021; Kallus and Zhou, 2021), care providers may be inclined to override the treatment recommendations provided by the identified optimal regimes, based on their privileged patient observations.

We present methodology for leveraging human intuition, given by the intended treatment values, by identifying a superoptimal regime using data generated by either nonexperimental or experimental studies, and clarify when a fusion of such data is beneficial. The superoptimal regime will indicate to a care provider – in an algorithm-assisted decision setting – precisely when expected outcomes would be maximized if the care provider would override the optimal regime recommendation and, importantly, when the optimal regime recommendation should be followed regardless of the care-provider’s assessment. This superoptimal regime will be guaranteed to yield as good or better expected outcomes compared to both the optimal regime and the implicit regime independently implemented by the care provider in the observed data, which have been studied in previous work (Cui and Tchetgen Tchetgen, 2021a; b; Han, 2021; Miao et al., 2018; Qi et al., 2021; Kallus and Zhou, 2021). In particular, the superoptimal regime is identical to the (conventional) optimal regime in settings with no unmeasured confounding. Furthermore, in many settings identification of the superoptimal regime requires no additional assumptions beyond those used to identify the optimal regime and its expected outcome, i.e.
value function, allowing us to identify superoptimal regimes by making small modifications of existing methods (Robins, 2004; Murphy, 2003; Cui and Tchetgen Tchetgen, 2021a; Qiu et al., 2021).

Our work builds on literatures arising from historical interest in the so-called average treatment on the treated (ATT) (Bloom, 1984; Heckman, 1990). One strand of literature expands on the ATT by defining, identifying and estimating a general class of causal parameters defined by the values of patient’s natural treatment choices or intentions in the absence of intervention (Robins et al., 2004, 2006; Hanusa and Rotnitzky, 2013; Richardson and Robins, 2013; Young et al., 2014; Díaz et al., 2021). While this strand of literature is ostensibly interested in the values of ATT-like parameters per se, a second strand of literature is especially concerned with heterogeneity among them and its implications for the transportability of clinical trial results. This second strand focuses on identification of ATT-like parameters using augmented experimental designs, historically referred to as patient preference trials (Rücker, 1989; King et al., 2005; Long et al., 2008; Knox et al., 2019). Finally, an independent set of contributions in the machine learning literature studies the optimal selection of treatment based on a patient’s treatment intentions in an online experimental learning setting (Bareinboim et al., 2015; Forney et al., 2017; Forney and Bareinboim, 2019).

Our contribution unifies and extends these related, but independently developed, literatures and our framing clarifies relations between optimal and superoptimal regimes that are obscured in the extant literature. Furthermore, like the literature characterized by Robins et al. (2004), Richardson and Robins (2013) and others, we do not focus on, or restrict ourselves to, experimental settings: we emphasize the non-experimental setting, and locate the results on experimental settings as special cases.
2. Preliminaries

2.1. Non-experimental data structure. Consider a treatment $A \in \{0, 1\}$, a pretreatment vector $L \in L$, and an outcome $Y \in \mathbb{R}$. Suppose that we have access to $n$ iid observations of $(L, A, Y)$ among patients who received treatment in a non-experimental setting. An unmeasured variable $U \in U$ can be a common cause of $A$ and $Y$. Some of our results, in particular those in our case study in Section 7 will further rely on observations of an instrumental variable (IV) $Z \in \{0, 1\}$, and we use $O = (Z, L, A, Y)$ to denote the observed non-experimental data in the IV setting.

2.2. Potential outcomes and the natural values of treatment. Let superscripts denote potential outcome variables. In particular, $Y^a$ is the potential outcome when treatment $A$ is fixed to the value $a \in \{0, 1\}$. More specifically will let $Y^g \equiv Y^g(V)$ be the potential outcome under an arbitrary regime $g$, where the treatment is assigned as a function of measured covariates $V \subset O$. Following Richardson and Robins (2013), we use the + symbol to distinguish between the assigned value of treatment under the regime $(A^g)^+$ and the natural value of the treatment under the regime $(A^g)$. The natural value will be important in our arguments, and we state its definition explicitly (Richardson and Robins, 2013).

Definition 1 (Natural value of treatment). The natural value of treatment $A^g$ is the value of treatment that an individual would choose in the absence of it being assigned by an intervention.

We have used counterfactuals to define the natural values of treatment, like previous authors (Haneuse and Rotnitzky, 2013; Young et al., 2014; Muñoz and Van Der Laan, 2012). However, we could alternatively give the natural values an interventionist interpretation, which does not require conceptualization of counterfactuals: following Robins et al.

\footnote{See also Robins et al. (2006); Geneletti and Dawid (2011a); Young et al. (2014) for interesting discussions on dynamic treatment regimes that depend on the natural value of treatment.}
(2006) and Geneletti and Dawid (2011a), the natural value of treatment is a variable that is temporally prior but deterministically equal to the active treatment in non-experimental data; that is, the natural treatment value and the active treatment value are equal with probability one.

The natural value of treatment under the regime $g$, $A^g$, is equal to $A$ in any non-experimental study that investigates the effect of a point treatment. Thus, if $A$ is observed, then $A^g$ is observed. In particular, this is true in non-experimental studies that identify causal effects in the presence of unmeasured confounding, e.g. using IVs or proxy variables (Miao et al., 2018; Tchetgen Tchetgen et al., 2020). Henceforth, we will simply denote the natural value of treatment with $A$ because we focus on a point treatment setting.

To fix ideas about natural treatment values, consider a doctor who determines whether a patient will be transferred to an intensive care unit (ICU); let $A = 1$ denote ICU admission and $A = 0$ denote no ICU admission. In the observed data, the doctor determined the ICU admission and thus the natural value $A^g$ is equal to $A$ with probability 1. We could, however, conceive a regime where the assigned ICU admission, $A^{g+}$, is determined by some arbitrary function $g$ of patient characteristics such as the pretreatment covariates $L$. It is possible that the assignment $A^{g+}$ differs from the natural value $A$.

2.3. Definitions of treatment regimes. In this section we formally define $L$-optimal and $L$-superoptimal regimes in a point treatment setting, where we employ the prefix “$L$−” to emphasize their definitional dependence on the elements in the covariate vector $L$. Throughout, we suppose that larger values of $Y$ are desirable.

**Definition 2** ($L$-Optimal regimes). The $L$-optimal regime, $g_{opt}$, assigns treatment $A^{g_{opt}+} = a$ given a vector $L = l$ by

$$g_{opt}(l) \equiv \arg \max_{a \in \{0, 1\}} \mathbb{E}(Y^a \mid L = l).$$
Figure 1. A dynamic SWIG with instrumental variable $Z$ describing a regime that depends on $A$ and $L$, consistent with a superoptimal regime.

**Definition 3 ($L$-Superoptimal regimes).** The $L$-superoptimal regime, $g_{sup}$ assigns treatment $A^{g_{sup}+} = a$ given $A = a'$ and $L = l$ by

$$g_{sup}(a', l) \equiv \arg \max_{a \in \{0, 1\}} \mathbb{E}(Y^a | A = a', L = l).$$

We denote the counterfactual expectation $\mathbb{E}(Y^a | L = l)$ as a 'conditional value function'. In particular $\mathbb{E}(Y^{g_{opt}} | L = l)$ and $\mathbb{E}(Y^{g_{sup}} | A = a', L = l)$ are conditional value functions under the $L$-optimal and $L$-superoptimal regimes, respectively.

Treatment rules given by $L$-optimal and $L$-superoptimal regimes can be presented in Single World Interventions Graphs (SWIGs) (Richardson and Robins, 2013), as illustrated by the IV setting in Figure 1: the green arrow encodes regime-specific effects of the measured covariates $L$ on the assigned value of treatment under the regime, $A^{g+}$, a feature of both the $L$-optimal and the $L$-superoptimal regime. The blue arrow further encodes the effect of the natural value of treatment $A$ on $A^{g+}$, a feature of the $L$-superoptimal, but not the $L$-optimal, regime.

Consider again the setting where a patient might be transferred to an ICU. Suppose we have access to non-experimental data from a setting where physicians determined ICU admission, and thus $A = A^g$. Using these data, an investigator aims to find the dynamic regime for ICU admission that gives the highest 7 day survival in a future decision setting. To specify this regime, we could assign $A^{g+}$ as a function of measured covariates $L$,
describing the patient’s age, gender and a collection of clinical measurements. However, beyond using the values of $L$, we could also ask the treating physician the following question: “if you were to choose, would you transfer the patient to an ICU?” The answer to this question would encode the natural treatment value $A$, and we can indeed use both $L$ and $A$ as input to our decision rule; a superoptimal regime will precisely let $A^{g+}$ be a function of both $L$ and $A$.

This brief example suggests how the natural treatment value interventions feasibly can be implemented; just before intervening we ask the decision maker about the treatment they intend to provide, and then we record their response to this question as a covariate. Nearly identical measurement strategies for “patient preference” or ”intent” are leveraged in a literature interested in the so-called “preference effects” in clinical trials (see, for example, Rücker (1989); Long et al. (2008); Knox et al. (2019)).

We consider identification of superoptimal regimes from observational data, wherein unmeasured confounding between the treatment and the outcome is often expected. Such settings are increasingly studied in the optimal regimes literature (Cui and Tchetgen Tchetgen, 2021a,b; Han, 2021; Miao et al., 2018; Qi et al., 2021; Kallus and Zhou, 2021). For example, Cui and Tchetgen Tchetgen (2021b) studied the effect of having a third child on remaining in the labour market among mothers who already had at least two children, using data from Angrist and Evans (1996). The aim of Cui (2021) was to “provide a personalized recommendation”, based on baseline covariates $L$. Beyond using the baseline covariates $L$, however, the $L$-superoptimal regime would further rely on whether the mother intends to have three or more children. In the observed data, this intention is deterministically related to actually having three or more children at the census time. Yet, for a future women seeking advice, we could nevertheless imagine asking the question “do you intend to have a third child?”

\footnote{Under the assumption that the doctor’s response to the question actually agrees with the decision they had made if we did not intervene.}
3. SUPEROPTIMAL REGIMES AND THEIR PROPERTIES

Our first proposition states that $L$-superoptimal regimes are always better than, or as good as, $L$-optimal regimes.

**Proposition 1** (Superoptimality). The expected potential outcome under the $L$-superoptimal regime is better than or equal to that under the $L$-optimal regime,

$$\mathbb{E}(Y^{g_{\text{opt}}} \mid L = l) \leq \mathbb{E}(Y^{g_{\text{sup}}} \mid L = l) \text{ for all } l \in \mathcal{L}.$$ 

**Proof.** Using laws of probability and Definitions 2 and 3,

$$\mathbb{E}(Y^{g_{\text{opt}}} \mid L = l) = \sum_{a'} \mathbb{E}(Y^{g_{\text{opt}}} \mid A = a', L = l)P(A = a' \mid L = l)$$

$$\leq \sum_{a'} \mathbb{E}(Y^{g_{\text{sup}}} \mid A = a', L = l)P(A = a' \mid L = l)$$

$$= \mathbb{E}(Y^{g_{\text{sup}}} \mid L = l),$$  

where the inequality follows because, by definition of $g_{\text{opt}}$ and $g_{\text{sup}}$, we have that

$$\mathbb{E}(Y^{g_{\text{opt}}} \mid A = a', L = l) \leq \mathbb{E}(Y^{g_{\text{sup}}} \mid A = a', L = l),$$

for each $a'$. \hfill \square

Proposition 1 is not surprising, because the regime $g_{\text{sup}}$ uses more observed information compared to $g_{\text{opt}}$; that is, the $L$-superoptimal regime is optimized not only with respect to $L$ but also with respect to $A$. A similar argument has appeared in Bareinboim et al. (2015) for an online bandit setting with no additional covariates, proposing that rewards are maximized when an agent bases decisions on their natural treatment choice.

In the remainder of the manuscript, we will assume that interventions on the treatment variable $A$ are well-defined, such that the following causal consistency assumption holds.

**Assumption 1** (Consistency). If $A = a$ then $Y = Y^a$ for $a \in \{0, 1\}$. 

Remark 1. Consistency in Assumption 1 can equivalently be formulated as \( Y = Y^A \). This formulation highlights that the factual outcome is equivalent to a particular counterfactual outcome under a regime that assigns treatment \( A^g+ \) according to the trivial regime \( g(A, L) = A \) for all patients. Thus, the factual regime is a member of the class of regimes that depends on \( A \) and \( L \), among which \( g_{sup} \) is the one that maximizes the expected potential outcome. Thus, under consistency, we have that the expected potential outcome under the \( L \)-superoptimal regime is better than or equal to that under the factual regime.

We will also invoke the usual positivity assumption.

**Assumption 2 (Positivity).** \( P(A = a \mid L) > 0 \) w.p.1 for \( a \in \{0, 1\} \).

The following lemma, which exploits positivity and consistency, is similar to arguments that have appeared in work on treatment effects on the treated (Robins et al., 2007; Dawid and Musio, 2022; Geneletti and Dawid, 2011b; Bareinboim et al., 2015), and will be used in our derivations of identification results.

**Lemma 1.** Under consistency and positivity, \( \mathbb{E}(Y^a \mid A = a', L = l) \) for \( a, a' \in \{0, 1\} \) and \( l \in \mathcal{L} \) can be expressed as

\[
\mathbb{E}(Y^a \mid A = a', L = l) = \begin{cases} 
\mathbb{E}(Y \mid A = a', L = l), & \text{if } a = a', \\
\frac{\mathbb{E}(Y^a \mid L = l) - \mathbb{E}(Y \mid A = a, L = l) P(A = a \mid L = l)}{P(A = a' \mid L = l)}, & \text{if } a \neq a'. 
\end{cases}
\]

**Proof.** When \( a = a' \), the equation holds by consistency. When \( a \neq a' \), the result follows from the law of total probability, positivity and consistency. \( \square \)

Based on Lemma 1, we can use simple algebra to derive the following result, also leveraged by Bareinboim et al. (2015) in a setting without covariates.
Corollary 1. Under consistency and positivity, the $L$-superoptimal regime $g_{\text{sup}}(a,l)$ for $a \in \{0,1\}$ and $l \in \mathcal{L}$ is equal to

$$g_{\text{sup}}(a,l) = \begin{cases} a & \text{if } \mathbb{E}(Y|L = l) \geq \mathbb{E}(Y^{1-a}|L = l), \\ 1 - a & \text{if } \mathbb{E}(Y|L = l) < \mathbb{E}(Y^{1-a}|L = l). \end{cases}$$

(3)

The next proposition states conditions for identification of $L$-superoptimal regimes from observed data.

Proposition 2 (Identification of superoptimal regimes). Under consistency and positivity, the $L$-superoptimal decision rule and its value function is identified by the joint distribution of $(L,A,Y)$ whenever

- $\mathbb{E}(Y^a | L = l)$ for all $a \in \{0,1\}$ and $l \in \mathcal{L}$ is identified.

Proof. The proposition follows from Lemma 1 and Corollary 1 because all the terms on the right hand side of (2) are identified under the two conditions in the proposition. \qed

Proposition 2 is useful because it justifies a two-step procedure for identification of $L$-superoptimal regimes using non-experimental data: first, we use (existing) approaches to identify conditional outcome means and the conditional densities of the natural treatment values. Second, we apply the result in Lemma 1 to compute counterfactual outcomes conditional on natural treatment values, which allow us to identify $L$-superoptimal regimes.

The next corollary concerns a setting where $L$-superoptimal regimes can be particularly relevant: it shows that the $L$-superoptimal regime $g_{\text{sup}}$ is identified whenever conditional potential outcomes means, $\mathbb{E}(Y^a | L = l)$, are identified in a non-experimental study, which covers studies using IVs or proxy variables as important special cases.

Corollary 2. If $\mathbb{E}(Y^a | L = l)$ for $a \in \{0,1\}$, $l \in \mathcal{L}$ is identified by the joint distribution of $(L,A,Y)$, then the superoptimal regime is identified.
Remark 2 (Instrumental variables). Corollary 2 implies that $L$-superoptimal regimes are identified under assumptions suggested in two recent contributions by Qiu et al. (2021) and Cui and Tchetgen Tchetgen (2021b), who developed theory for identification and estimation of optimal regimes in the presence of unmeasured confounding. That is, under Assumptions 8-11 in Appendix A the expected outcomes under the regimes given by Qiu et al. (2021) and Cui and Tchetgen Tchetgen (2021b) will be worse than, or equal to those under the $L$-superoptimal regimes, and, in both cases, the $L$-superoptimal regimes require no extra assumptions for identification of value functions.

Remark 3 (Proximal inference). Corollary 2 is also valid in proximal learning settings (Miao et al., 2018). Interestingly, heuristic arguments have been used to justify the inclusion of other covariates, but not the natural value $A$, in the decision function in proximal inference settings. For example, Qi et al. (2021) write that “This may be reasonable since $Z$ may contain some useful information of $U$, which can help improve the value function.”

We emphasize that the results presented thus far have been agnostic to the absence of unmeasured confounding, which is often equated with the following assumption.

Assumption 3 ($L$-Exchangeability). $Y^a \perp \perp A \mid L$ for $a \in \{0, 1\}$.

The following results describe different properties of the $L$-superoptimal regime that depend on the truth-value of $L$-Exchangeability.

Corollary 3. $L$-Exchangeability implies that $g_{\text{sup}}(A, L) = g_{\text{opt}}(L)$ w.p.1.

Proof. Let $a^* = \arg \max_{a \in \{0, 1\}} \mathbb{E}(Y^a \mid L = l)$. If $L$-Exchangeability holds, then

$$\mathbb{E}(Y^{a^*} \mid L = l) = \mathbb{E}(Y^{a^*} \mid A = a, L = l)$$

3There also exist alternative conditions for identifying optimal treatment rules in IV settings, which only require identification of (the sign of) the causal effect conditional on $L$, and not $\mathbb{E}(Y^a \mid L = l)$ itself, as thoroughly discussed by Cui and Tchetgen Tchetgen (2021a), see also Han (2021).
for all \( a \in \{0, 1\} \) and \( l \in \mathcal{L} \). Thus, \( a^* = \arg \max_{a \in \{0, 1\}} \mathbb{E}(Y^a | A = a', L = l) \) for all \( a' \in \{0, 1\} \).

\[ \square \]

**Remark 4.** Suppose that an \( L \)-superoptimal regime yields better outcomes than an \( L \)-optimal regime in a given study. Then, it follows from Corollary 3 that \( L \)-Exchangeability fails. When \( L \)-Exchangeability fails, an investigator will often assume that there exists a variable \( U \), often called an ‘unmeasured confounder’, that exerts effects on \( A \) and \( Y \). Then, measuring \( U \) in the future will further improve decision making. Because \( A \) often represents a decision made by a human in the course of natural practice, then the investigation and measurement of causes of \( A \) (e.g., \( U \)) may be feasible.

**Corollary 4.** Consistency implies that \( \mathbb{E}[Y^{g_{\text{sup}}}] \geq \mathbb{E}[Y] \). When \( L \)-Exchangeability additionally holds, then \( \mathbb{E}[Y^{g_{\text{opt}}}] \geq \mathbb{E}[Y] \).

**Proof.** As in Remark 1, \( Y = Y^A \) is generated under a special case of a regime that depends on the natural value of treatment, where \( A^{g^+} = g(A, L) = A \) w.p.1. Since \( g_{\text{sup}} \) is the optimal such regime, then \( \mathbb{E}[Y^{g_{\text{sup}}}] \geq \mathbb{E}[Y] \). When \( L \)-Exchangeability holds, application of Corollary 3 completes the proof.

\[ \square \]

**Remark 5.** Given an identified optimal regime, suppose that a human care provider insists that their own intuition about treatment decisions is superior, due to their own access to privileged observations not used by the regime. Corollary 3 highlights that this insistence is contradicted when the optimal regime is identified under assumptions of no-unmeasured confounding. Their claim might be depicted by paths in the SWIG of Figure 1: if this privileged information was truly useful for decision-making \( (U \rightarrow Y^g) \) and was leveraged by the clinician in the observed data \( (U \rightarrow A) \), then \( Y^a \not\perp \perp A | L \).

4. **On Experimental Data**

We have thus far only considered observed data \( (L, A, Y) \) generated in a non-experimental setting. As anticipated in Definition 1 we do so because we leverage the natural value
of treatment, that is, the treatment an individual would choose in the absence of it being assigned by an intervention. In a non-experimental setting, no intervention is made and the treatment a patient actually receives is indeed this natural value. We let $A^*$ denote the treatment a patient actually receives. Formally, we define a setting to be non-experimental when $A = A^*$ w.p.1. Conversely, $A$ may not equal $A^*$ in an experimental setting, because the patient’s natural treatment intentions will be subverted by the experimental design. Here we discuss several consequences of this distinction, including strategies for identifying the $L$-superoptimal regime with experimental data that differ from those for the non-experimental setting.

A first consequence of the experimental setting is that Assumption 1 (Consistency) will almost certainly be violated; in an experiment, a patient actually receives the treatment value corresponding to $A^*$. Thus an investigator who would justify Assumption 1 (Consistency) in a non-experimental setting might alternatively conclude that $Y = Y^{A^*}$ in an experimental setting. But if $A \neq A^*$ for some individuals then $Y = Y^{A^*} \neq Y^A$ for those individuals, thus contradicting Assumption 1 (Consistency). Instead the following assumption is more reasonable:

**Assumption 4** (Consistency in an experiment). If $A^* = a$ then $Y = Y^a$ for $a \in \{0, 1\}$.

The results in Section 3 all suppose Assumption 1 and not Assumption 4. Thus, they will not in general apply to experimental data. Similar reasoning has historically motivated alternative trial designs, in which investigators would attempt to measure $A$ and $A^*$ concurrently, see for example Rücker (1989); Knox et al. (2019); Forney and Bareinboim (2019).

A second consequence of the experimental setting is that $A^*$ is (usually) allocated such that $Y^a \perp A^*$ by design, and so covariates $L$ will be measured for reasons other than confounding control. Therefore, it is unlikely that $L$-Exchangeability (Assumption 3) will hold in experimental data. Instead the following assumption is more reasonable:
**Assumption 5** (\(L\)-Exchangeability in an experiment). \(Y^a \perp \perp A^* \mid L\) for \(a \in \{0, 1\}\).

Despite the irrelevance of the results in Section 3, the experimental setting may seem especially appealing for \(L\)-superoptimal regime identification: because \(A^*\) is randomized by design, we might adopt an even more elaborate exchangeability assumption that includes \(A\) as a covariate.

**Assumption 6** ((\(L, A\))-Exchangeability in an experiment). \(Y^a \perp \perp A^* \mid L, A\) for \(a \in \{0, 1\}\).

Furthermore, we do not have \(A = A^*\) by definition, and so we might adopt the following positivity condition:

**Assumption 7** (Positivity in an experiment). \(P(A^* = a \mid L, A) > 0\) w.p.1 for \(a \in \{0, 1\}\).

Lemma 1 permitted identification of the \(L\)-superoptimal regime even when Assumption 7 is contradicted, as it is in a non-experimental setting. With assumptions 4, 6, and 7 and experimental data, for example as in patient preference trial designs \cite{Forney and Bareinboim, 2019} we might trivially identify the \(L\)-superoptimal regime without appealing to Lemma 1. In this second approach, the natural treatment value \(A\) is simply considered as an additional covariate (and thus effectively subsumed into \(L\)).

**Lemma 2.** Under consistency, positivity, and \((A, L)\)-Exchangeability in an experiment (Assumptions 4, 6, and 7), we have that

\[
\mathbb{E}(Y^a \mid A = a', L = l) = \mathbb{E}(Y \mid A^* = a, A = a', L = l).
\] (4)

*Proof.* The equality holds through sequential application of Assumptions 4 and 6, where Assumption 7 ensures that the functional remains well-defined for all values of \(a, a'\). □

Unfortunately, the natural treatment value \(A\) is not measured in most experimental settings. Therefore, when only experimental data are available and \(A\) is unmeasured,
then Lemma 2 cannot be used to identify the $L$-superoptimal regime. Alternatively, the $L$-optimal regime can be learned with such data via identification of $\mathbb{E}[Y^a | L = l]$. The claim and proof is trivial, by considering Lemma 2 without $A$ in the conditioning set and replacing Assumption 6 by Assumption 5.

**Remark 6.** While not useful on its own for learning the $L$-superoptimal regime, knowledge of the parameters $\mathbb{E}[Y^a | L = l]$ from an experiment will be instrumental as a supplement to non-experimental data, even if $L$-Exchangeability (Assumption 3) does not hold for those non-experimental data. If the conditions of Lemma 1 are met for the non-experimental data, then its identification functional can be evaluated using the combination of the parameters $\mathbb{E}[Y^a | L = l]$ learned in the experiment, and those parameters of $(L, A, Y)$ directly observed in the non-experimental setting. This heuristic for combining experimental and non-experimental data has been suggested by Bareinboim et al. (2015) for the identification of a $\emptyset$-superoptimal regime. Augmented 2-stage experimental designs, in which patients are first randomized to either a free-choice or a random treatment assignment paradigm (Rücker, 1989; Knox et al., 2019) would ensure the availability of such data, even when the natural treatment values $A$ are not measured in the assigned treatment arms.

5. **On algorithm-assisted human decision making**

One vision for optimal regimes is to use them in an algorithmic treatment-assignment paradigm, wherein treatments are assigned completely according to learned algorithms without human intervention. This algorithmic paradigm would replace current paradigms centered on consensus standards-of-care guidelines and human care-providers’ (possibly fallible) intuition. However, the medical community may be resistant to ceding control to such algorithms in the absence of guarantees that expected outcomes will be better under the novel optimal regime. We have showed in Corollary 4 that the superiority of the $L$-optimal regime is indeed guaranteed whenever $L$-Exchangeability
holds. However, the medical community has historically expressed a deep skepticism to 
$L$-Exchangeability or any of identification strategy that depends on independence condi-
tions in non-experimental data; see for example the Journal of the American Medical
Association’s prohibition on causal language for the results of non-experimental studies
(AMA Manual of Style, 2020). When an $L$-optimal regime is learned in the absence of $L$-
Exchangeability – for example, when the $L$-optimal regime is learned using experimental
data – clinician skepticism may be justified: we cannot guarantee that
\[ \mathbb{E}[Y^{\text{opt}}] \geq \mathbb{E}[Y^A]. \]

A primary benefit of the super-optimal regime $g_{\text{sup}}$ is to provide an algorithm with
 guarantees that
\[ \mathbb{E}[Y^{g_{\text{sup}}}] \geq \mathbb{E}[Y^A]. \]

We illustrate in Section 4 that the super-optimal regime is estimable from a combination
of experimental and non-experimental data whereby all relevant assumptions are enforced
by design; thus such results may be acceptable to a skeptical medical community.

Nevertheless, current formulations of the $L$-superoptimal regime $g_{\text{sup}}$ consider treat-
ment intentions $A$ as simply an additional covariate. Thus, this formulation suggests a
paradigm in which the algorithm is rhetorically centered. This radical departure from
existing treatment assignment paradigms may result in the persistence of skepticism and
resistance, despite the guarantees of the $L$-superoptimal regime. Therefore, we provide
the following equivalent formulation of $g_{\text{sup}}$ that suggests a paradigm in which the human
care provider remains centered.
Proposition 3. There exists a function $\gamma : \mathcal{L} \rightarrow \{0, 1, 2\}$ such that the following equality holds w.p.1,

$$g_{\text{sup}}(A, L) = \begin{cases} g_{\text{opt}}(L) & \text{if } \gamma(L) = 0 \\ A & \text{if } \gamma(L) = 1 \\ 1 - A & \text{if } \gamma(L) = 2. \end{cases}$$

Proposition 3 formulates an algorithm that directly negotiates between the $L$-optimal decision rule $g_{\text{opt}}$, and a human care provider’s own privileged intuition, captured by their natural treatment intention $A$: when a provider encounters a patient, they are given the value of the random variable $\gamma(L)$; if $\gamma(L) = 0$, then the provider is instructed to follow the $L$-optimal regime’s recommendation, $g_{\text{opt}}(L)$; if $\gamma(L) = 1$ then the provider is instructed to override the $L$-optimal regime’s recommendation and provide the treatment according to their natural intention, $A$. Finally, if $\gamma(L) = 2$ then the provider is instructed to override the $L$-optimal regime’s recommendation and provide the treatment opposite to their natural intention, $1 - A$. With this formulation, superoptimal regime methodology can be described as a strategy for optimally negotiating between a typical $L$-optimal regime and a provider’s privileged intuition: when the $L$-optimal regime is already known, the function $\gamma$ can be learned to indicate to a care provider when the $L$-optimal regime should be followed, or else should be overridden as a function of their natural treatment intention $A$. Because this formulation is equivalent to the $L$-superoptimal regime $g_{\text{sup}}$, then the provider has guarantees that this algorithm will outperform the status quo. Thus, the use of $L$-superoptimal regimes is accurately described as “algorithm-assisted human decision making”.

Remark 7. The treatment assignment paradigm suggested by Proposition 3 is nearly analogous to current operationalizations of self-driving cars. Therein, the default is “self-driving mode” where the vehicle makes the optimal decision according to measured covariates $L$. However, the vehicle may encounter an environment $\gamma(L) = 1$ (e.g. a complex
traffic pattern) in which the human passenger is indicated to take control and make decisions according to their natural intentions \(A\).

6. **ON THE NON-PRESCRIPTIVE USE OF SUPEROPTIMAL REGIMES**

The formulation of \(g_{sup}\) in Proposition 3 highlights a counterintuitive possibility of an \(L\)-superoptimal regime: when \(P(\gamma(L) = 2) > 0\), the \(L\)-superoptimal regime will indicate that a decision maker should assign precisely the treatment value that is the **opposite** of their natural intentions, \(1 - A\), for some patients. This could be the case when humans currently use outcome-predicting variables in precisely the **opposite** way from that which would optimize outcomes.

An algorithm-driven health care system might dismiss this occurrence as an ancillary curiosity; if \(\gamma(L) = 2\), then providing treatment \(1 - A\) would simply be the optimal choice, given covariates \(A\) and \(L\). However, \(g_{sup}\) is more than simply a prescriptive treatment policy; a positive probability of \(\gamma(L) = 2\) might indicate an opportunity to radically adjust existing theories or systems for patient care for some groups, which were apparently grossly misformulated. The history of the study of human behavior offers many examples of fallacies where humans systematically (but unintentionally) undermine their own objectives, and iatrogenic harm is one well-documented subclass of this phenomenon. Detecting these occurrences is surely an important scientific aim, as major paradigm shifts in medical history have been portended by the scientific communities attention to such paradoxes (Kuhn, 1970).

**Example 1 (Semmelweis).** Consider the case of Ignaz Semmelweis, a 19th-century Hungarian physician. Semmelweis famously observed that it was precisely the women who were admitted to elite teaching hospital wards in anticipation of obstetric complications \((A = 1)\) who were experiencing increased mortality from puerperal fever. This was an ostensibly paradoxical observation: the elite venues \((A = 1)\) purported to offer the best possible care. If Semmelweis had used data to learn the \(L\)-superoptimal regime, he would
have observed that $P(\gamma(L) = 2) > 0$; that is, there exist subgroups where the best thing to do is to not admit to the elite teaching hospital ($A^{sup+} = 0$) precisely those patients who would otherwise be admitted to such a ward ($A = 1$), and admit those patients ($A^{sup+} = 1$) who would otherwise be treated in a less prestigious venue ($A = 0$). Semmelweis ultimately uncovered an explanation: women sent to the prestigious hospitals were the most likely to need surgical intervention, which was then often provided by physicians returning from autopsy procedures with hands unwashed (Semmelweis, 1983). Semmelweis’s observations helped initiate a hygiene and hand-washing revolution in medicine.

Semmelweis did not need the formalisms of super-optimal regimes to make his discovery. Instead, he relied on savvy intuition and large effect sizes. Superoptimal regime methodology provides a tool for systematic surveillance of (iatrogenic) harm, even when effect sizes are modest, or human intuition would otherwise fail.

7. CASE STUDY: INSTRUMENTAL VARIABLES

The results we have derived so far are general. They can be used in any setting where value functions and the joint distribution of the factals ($L, A, Y$) are identified. Thus, these results could be of interest in a range of settings where investigators would otherwise aim to find $L$-optimal regimes in the presence of unmeasured confounding. In each particular setting, an investigator can derive explicit identification formulae, which in turn motivate estimators.

In our first case study, we re-visit an example from the seminal paper by Balke and Pearl (1997), illustrating that $L$-superoptimal regimes for certain values of $A$ can be point identified even if $L$-optimal regimes are not.

Example 2 (Vitamin A supplementation and mortality). Balke and Pearl (1997) derived bounds for average causal effects in instrumental variable settings. In particular, these bounds are sharp under an individual level exclusion restriction and a randomized
instrument assumption,

\[ Y^{a,z} = Y^{a,z} \text{ for all } a, z, \]

\[ Z \perp \perp \{Y^{a=1}, Y^{a=0}, A^{z=0}, A^{z=1}\}, \]

and also under weaker assumptions (Swanson et al., 2018).

To illustrate the practical relevance of these bounds, Balke and Pearl (1997) analyzed data from a randomized experiment in Northern Sumatra, where 450 villages were randomly offered oral doses of Vitamin A supplementation \((Z = 1)\) or no treatment \((Z = 0)\). Villages receiving Vitamin A supplementation were encouraged to provide them to preschool children \((12-71\text{ months})\). The dataset contained 10231 individuals from villages assigned to Vitamin A \((Z = 1)\) and 10919 untreated individuals \((Z = 0)\). Balke and Pearl (1997) studied the effect of consuming Vitamin A supplementation \((A = 1)\) vs no treatment \((A = 0)\) on survival \((Y = 1)\) after 12 months. Leveraging that \(Z\) is an instrument, Balke and Pearl (1997) reported bounds on the average treatment effect,

\[ -0.1946 \leq \mathbb{E}(Y^{a=1} - Y^{a=0}) \leq 0.0054. \]

They concluded that “Vitamin A supplement, if uniformly administered, is seen as capable of increasing mortality rate by much as 19.46% and is incapable of reducing mortality rate by more than 5.4%”. Balke and Pearl (1997) did not consider further covariates, and thus we define \(L = \emptyset\). It follows that the \(L\)-optimal regime,

\[ g_{\text{opt}} = \arg \max_{a \in \{0,1\}} \mathbb{E}(Y^a), \]

nor the value function \(\mathbb{E}(Y^a)\) are point identified, but both functionals are non-trivially bounded. However, consider now the regime

\[ g_{\text{sup}}(a') = \arg \max_{a \in \{0,1\}} \mathbb{E}(Y^a | A = a'), \]
which uses the intended value of Vitamin A consumption as input to the decision function. Using Lemma 1 in this particular example, we have point identification of the superoptimal regimes for the treated, which is an analogous parameter to the ATT,

$$\mathbb{E}(Y_{a=1} - Y_{a=0} \mid A = 1) = 0.0032.$$  

This example illustrates the point that, under conditions that only allow partial identification of $L$-optimal regimes, the $L$-superoptimal regimes for a particular value of $A$ can still be point identified. Indeed, we conclude that among children who would consume Vitamin A supplementation when offered, the Vitamin A supplementation does have a beneficial effect.\(^4\)

Whereas the $L$-superoptimal regime given $A = 1$ is point identified, the $L$-superoptimal given $A = 0$ is not, that is,

$$-0.33 \leq \mathbb{E}(Y_{a=1} - Y_{a=0} \mid A = 0) \leq 0.0069.$$  

7.1. **Point identification of value functions.** To illustrate how explicit identification formulae and estimators can be derived, we further build on recent work on optimal regimes (Qiu et al., 2021; Cui, 2021; Cui and Tchetgen Tchetgen, 2021a). These results are given in detail in the online appendices, and we provide an overview in this section. Specifically, we give new identification results for $L$-superoptimal regimes (Appendix A) and derive the non-parametric influence function (Appendix B), which motivates new estimators (Appendix C and D). Furthermore, we suggest a strategy to further improve efficiency of these estimators, if the investigator only aims to identify the sign of the value function, and not the value function itself, which indeed is sufficient to identify the $L$-superoptimal regime (based on Corollary 1). We apply these new methods to study the effects of ICU admission on survival in Section 8.

\(^4\)In this example, the point identification of the superoptimal CATE follows because Vitamin A treatment was inaccessible to those randomly assigned to no treatment ($Z = 0$), see Balke and Pearl (1997)[Table 1], that is, there is one-sided compliance.
The results in IV settings might have practical consequences, in the sense that the superoptimal regime can deviate from the optimal regime. To illustrate this point, we revisit an example from Qiu et al. (2021, Remark 5), who emphasized that these \( L \)-optimal regimes can be worse than the regime that was implemented in the observed data, in Appendix A (See Example 3). Indeed, we show that the \( L \)-superoptimal regime is strictly better than the \( L \)-optimal regime in their example. We further give another example (See Example 4), with a minor change to the setting in Qiu et al. (2021), where the \( L \)-superoptimal regime outperforms both the \( L \)-optimal and the observed regime.

Furthermore, there is an important role of instruments in superoptimal regimes, which differ from their role in \( L \)-optimal regimes. Let a \((L, Z)\)-optimal regime be defined as

\[
g_{\text{opt}}(l, z) \equiv \arg \max_{a \in \{0, 1\}} \mathbb{E}(Y^a \mid L = l, Z = z),
\]

which is isomorphic to an \( L \)-optimal regime but further uses the instrument \( Z \). An instrument \( Z \) satisfies \( Y^a \perp \perp Z \mid L \), which can be read off of the SWIG in Figure 1. Using arguments isomorphic to those of Corollary 3, the \((L, Z)\)-optimal regime is always equal to the \( L \)-optimal regime. However, interestingly, an \((L, Z)\)-superoptimal regime is not necessarily equal to an \( L \)-superoptimal regime. This follows because in many cases

\[
Y^a \not\perp \perp Z \mid L, A,
\]

see the SWIG in Figure 1 as an example. The practical implication is that using the instrument \( Z \) can further improve superoptimal, but not optimal, regimes, see Appendix E for more details. We give intuition to this result in our ICU example in Section 8.

8. APPLICATION: INTENSIVE CARE UNIT ADMISSIONS

Following Keele et al. (2020), we study the effect of prompt ICU admission on 7-day survival. We use resampled data from a cohort study of patients with deteriorating health
who were referred for assessment for ICU admission in 48 UK National Health Service (NHS) hospitals in 2010-2011 (Harris et al., 2015).

Our treatment of interest, $A = 1$, is ICU admission within 4 hours upon arrival in the hospital (‘prompt ICU admission’). An individual is untreated, $A = 0$, if they were not admitted within 4 hours. Our sample consists of 13011 patients, of whom 10478 were treated. One reason for being untreated could be resource constraints, e.g., the lack of available ICU beds or insufficient staffing. Like Keele et al. (2020), we use an indicator of the ICU bed occupancy being below or above the median (4 beds) as our instrument, $Z$, which should only affect the outcome $Y$ through its effect on $A$ (Figure 1). We further considered an individual’s age, recorded sex and sequential organ failure assessment score as baseline variables ($L$).

In these non-experimental data, the individual’s natural value of treatment is directly recorded. In a future decision setting, we could measure the natural treatment variable by asking the following question to a doctor treating a patient: “Would you promptly admit this patient to an ICU?” A “yes” to this answer would correspond to $A = 1$ and a “no” would correspond to $A = 0$. Intuitively, the doctor’s response, $A$, serves as a proxy for factors $U$ which might indicate the risk of 7-day mortality. Furthermore, using the current bed occupancy $Z$ jointly with the doctor’s response $A$ could give a better proxy for factors $U$ not recorded in the observed data, even when ICU bed occupancy $Z$ is independent of $U$ marginally (but might be violated in some settings, e.g., a natural disaster or large-scale accident). For example, suppose $U$ represents a physician’s judgement of a patient’s underlying mortality risk based on unrecorded injury features or other implicit judgments of patient frailty (“moderate” or “severe”) and that a doctor will admit all patients on low-occupancy days but will only admit “severe”-risk patients on high-occupancy days. Occupancy has little predictive capacity for a patient’s underlying mortality risk

\footnote{We suppose a deterministic relation between the doctor’s response to this question and what they actually would have done.}
Parameter | Estimate (95 % confidence interval)
--- | ---
$E(Y_{g_{sup}})$ | 0.911 (0.817, 0.954)
$E(Y_{g_{sup}})$ | 0.911 (0.815, 0.955)
$E(Y_{opt})$ | 0.894 (0.549, 1.000)
$E(Y)$ | 0.860 (0.846, 0.864)

Table 1. Marginal value functions under different regimes, where the percentile 95%-confidence intervals are estimated by non-parametric Bootstrap in 500 samples.

marginally, but if it is known that a patient was admitted on a high occupancy day, then we can deduce that the patient must have been at “severe”-risk.

We estimated observed, $L$-optimal, $L$-superoptimal and $(L, Z)$-superoptimal regimes based on the estimation algorithm in Appendix D, where we also used 60-40 sample splitting to avoid the (positive) bias that might result from estimating and evaluating a (super)optimal decision rule in the same sample (Zhang et al., 2012; Qiu et al., 2021). The point estimates of the marginal value functions suggest that the $L$-superoptimal and $(L, Z)$-superoptimal regimes outperform the alternatives (Table 1). The fact that the confidence intervals are wide is not surprising, despite the large sample size, because of the reliance on an instrumental variable.

9. Future directions

An interesting problem is generalizing the results to longitudinal settings with time-varying treatments. A complicating factor is that the non-baseline natural treatment values will not in general correspond with a patient’s observed treatment values, even when the data arise from a non-experimental setting. Nevertheless, their distributions may be identified under assumptions commonly invoked to identify dynamic regimes that depend on the natural value of treatment in time-varying treatment settings, as described in Richardson and Robins (2013) and Young et al. (2014). Generalizations to non-binary treatments will also be of interest in some settings.
Our identification results motivate estimators of $L$-superoptimal regimes. We specifically gave semi-parametric estimators in an IV setting. However, alternative estimators of superoptimal regimes may also be developed, and the properties of these estimators must be evaluated on a case-by-case basis.

Finally, there exist results on $L$-optimal regime identification when conditional outcome means are only partially identified [Pu and Zhang, 2021; Cui and Tchetgen, 2021; Cui, 2021]. Using $L$-superoptimal regimes under partial identification conditions is a topic for future investigations.

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Online Appendix

Appendix A. Identification of the value function in IV settings

Here we review sufficient assumptions for identification of $E(Y^a \mid L = l)$ in instrumental variable settings (Cui and Tchetgen Tchetgen, 2021a). These conditions are invoked in Sections 7 and 8 of the main text. To simplify notation, define $f(z \mid l) := P(Z = z \mid L = l)$.

Assumption 8. (Latent unconfoundedness) $Y^{z,a} \perp \perp (Z,A) \mid L,U$ for $z,a \in \{0,1\}$.

Assumption 8 states that using $U$ and $L$ would, in principle, be sufficient to adjust for confounding between $A$ and $Y$. We further impose the following four IV assumptions, which are standard in the literature, see e.g. (Cui and Tchetgen Tchetgen, 2021a; Angrist et al., 1996):

Assumption 9. (IV relevance) $Z \not\perp \perp A \mid L$.

Assumption 10. (Exclusion restriction) $Y^{z,a} = Y^a$ for $z,a \in \{0,1\}$ w.p.1.

Assumption 11. (IV independence) $Z \perp \perp U \mid L$.

Assumption 12. (IV positivity) $0 < f(Z = 1 \mid L) < 1$ w.p.1.

Finally, we impose the independent compliance type assumption (Cui and Tchetgen Tchetgen, 2021b).

Assumption 13. (Treatment homogeneity)

$$
\delta(L) := P(A = 1 \mid Z = 1, L) - P(A = 1 \mid Z = 0, L) = \tilde{\delta}(L,U) \text{ w.p.1},
$$

where $\tilde{\delta}(L,U) := P(A = 1 \mid Z = 1, L,U) - P(A = 1 \mid Z = 0, L,U)$.

Identification assumptions [8][13][14] do not preclude $U$ from being a qualitative modifier of the effect of $A$ on $Y$ given $L$, as illustrated by the numerical Example 5 in Section F. This
is important because otherwise such a preclusion would imply that the $L$-superoptimal regime is identical to the $L$-optimal regime. Indeed, another common homogeneity assumption, $\mathbb{E}(Y^{a=1} - Y^{a=0} \mid L, U) = \mathbb{E}(Y^{a=1} - Y^{a=0} \mid L)$ w.p.1, which has been used frequently in instrumental variable settings, also based on seminal work on structural nested models (Robins, 1994), would – by assumption – lead to such an equality between $g_{\text{opt}}$ and $g_{\text{sup}}$.

Now we provide specific identification results for $g_{\text{sup}}$ in the IV setting under assumptions 8-13. First, define the new random variable $W(a)$ as

$$W(a) := \frac{(2Z - 1)I(A = a)Y(2a - 1)}{\delta(L)f(Z \mid L)}.$$  

(6)

Furthermore, let $\psi_1(a, l)$ denote the conditional expectation of $W(a)$ given $L = l$,

$$\psi_1(a, l) := \mathbb{E}\left[W(a) \mid L = l\right].$$  

(7)

Under positivity, consistency and assumptions 8-13, we have the following identification result,

$$\psi_1(a, l) = \mathbb{E}(Y^a \mid L = l).$$  

(8)

Applying (8) of Corollary 1 to Lemma 1 gives a specific identification functional for $\mathbb{E}(Y^a \mid A = 1 - a, L = l)$, as stated in the following Proposition.

**Proposition 4.** Under positivity, consistency and identification assumptions, 8-13,

$$\mathbb{E}(Y^a \mid A = a', L = l) = \begin{cases} \mathbb{E}(Y \mid A = a', L = l), & \text{if } a = a', \\ \Psi(a, l), & \text{if } a \neq a' \end{cases}$$  

(9)
for all $a, a'$ and $l$, where

$$
\Psi(a, l) = \frac{\psi_1(a, l) - \mathbb{E}(Y \mid A = a, L = l)P(A = a \mid L = l)}{P(A = a' \mid L = l)}.
$$

Furthermore, the $L$-superoptimal regime for all $a$ and $l$ is identified by

$$
g_{\text{sup}}(a, l) = \arg \max_g \left[ I[g(a, l) = a]\mathbb{E}(Y \mid L = l) + I[g(a, l) \neq a]\psi_1(1 - a, l) \right].
$$

**Proof.** We use that

$$
\psi_1(a, l) := \mathbb{E}\left[ \frac{(2Z - 1)Y(2A - 1)I(A = a)}{\delta(L)f(Z \mid L)} \mid L = l \right]
$$

and

$$
t(a, l, z) := \mathbb{E}\left[ Y(2A - 1)I(A = a) \mid L = l, Z = z \right].
$$

Then,

$$
g_{\text{sup}}
$$

$$
= \arg \max_g \mathbb{E}(Yg(A, L))
$$

$$
= \arg \max_g \mathbb{E}\left\{ \mathbb{E}\left[ I[g(A, L) = A]\mathbb{E}(Y \mid A, L) \right.ight.

$$

$$
+ I[g(A, L) \neq A]\psi_1(g(A, L), L) - \mathbb{E}(Y \mid 1 - A, L)p(1 - A \mid L) \left. \left. \mathbb{E}\left[ I[g(A, L) = A]\mathbb{E}(Y \mid L) + I[g(A, L) \neq A]\psi_1(g(A, L), L) \mid A, L \right) \right\}
$$

$$
= \arg \max_g \mathbb{E}\left\{ \mathbb{E}\left[ I[g(A, L) = A]\mathbb{E}(Y \mid L) + I[g(A, L) \neq A]\psi_1(g(A, L), L) \mid A, L \right) \right\}
$$

$$
= \arg \max_g \mathbb{E}\left\{ \mathbb{E}\left[ I[g(A, L) = A]\mathbb{E}(Y \mid L) + I[g(A, L) \neq A]\sum_z \frac{(2z - 1)}{\delta(L)}t(g(A, L), L, z) \mid A, L \right) \right\},
$$

$$
and it follows from simple algebra that

\[ g_{\text{sup}}(a, l) = \arg \max_g \left[ I[g(a, l) = a] \mathbb{E}(Y \mid L = l) + I[g(a, l) \neq a] \psi_1(1 - a, l) \right]. \]

\[ \square \]

**Appendix B. Semi-parametric influence functions**

Consider the observed data \( \mathcal{O} \) in our IV setting of Appendix A, and suppose that \( \mathcal{O} \) is described by the law \( P \) that belongs to the model \( \mathcal{M} = \{ P_\theta : \theta \in \Theta \} \), where \( \Theta \) is the parameter space. We will study the efficient influence function \( \varphi_{\text{eff}}(\mathcal{O}) \) for a parameter \( \Psi \equiv \Psi(\theta) \) in a non-parametric model \( \mathcal{M}_{np} \) that imposes no restrictions on \( P \) except positivity, such that \( \varphi_{\text{eff}}(\mathcal{O}) \) is given by

\[ \frac{d\Psi(\theta_t)}{dt}|_{t=0} = \mathbb{E}\{\varphi_{\text{eff}}(\mathcal{O})S(\mathcal{O})\}, \]

where \( d\Psi(\theta_t)/dt|_{t=0} \) is the pathwise derivative of \( \Psi \) along any parametric submodel of \( P \) indexed by \( t \), and \( S(\mathcal{O}) \) is the score function of the parametric submodel evaluated at \( t = 0 \), see more details in, for example, Newey (1994) and Van Der Vaart (2000). Indeed, Cui (2021) derived the efficient influence function for \( \psi_1(a, l) \), which we denote by \( \psi_{1\text{eff}}(a, l) \) in the following proposition.

**Proposition 5.** The efficient influence function of \( \Psi(a, l) \) in \( \mathcal{M}_{np} \) is given by

\[ \Psi_{\text{eff}}(a, l) = \frac{1}{P(A = 1 - a \mid L = l)} \left( \psi_{1\text{eff}}(a, l) P(A = 1 - a \mid L = l) - \psi_1(a, l) \frac{I[L = l]}{P(L = l)} (I[A = 1 - a] - P(A = 1 - a) \right) \]

\[ - \left( \frac{I[A = a, L = l]}{P(A = a, L = l)}(Y - \mathbb{E}[Y \mid A = a, L = l]) P(A = a \mid L = l) \right) \]

\[ + \mathbb{E}[Y \mid A = a, L = l] \frac{I[L = l]}{P(L = l)} (I[A = a] - P(A = a \mid L = l)) \right) P(A = 1 - a \mid L = l) \]

\[ + \mathbb{E}[Y \mid A = a, L = l] P(A = a \mid L = l) \frac{I[L = l]}{P(L = l)} (I[A = 1 - a] - P(A = 1 - a \mid L = l)) \right), \]
where

\[
\psi_{1\text{eff}}(a,l) = \frac{(2Z - 1)(2A - 1)YI[A = a]}{\delta(l)f(Z \mid L = l)P(L = l)} - \frac{Z\mathbb{E}[(2A - 1)YI[A = a] \mid Z, L = l]}{\delta(l)f(Z \mid L = l)P(L = l)} - \sum_z \frac{z\mathbb{E}[(2A - 1)YI[A = a] \mid Z = z, L = l]}{\delta(l)P(L = l)} + \frac{(2Z - 1)(2A - 1) - \mathbb{E}[2A - 1 \mid Z, L = l]}{2f(Z \mid L = l)\delta(l)P(L = l)} \sum_z \frac{z\mathbb{E}[(2A - 1)YI[A = a] \mid Z = z, L = l]}{\delta(l)} \tag{11}
\]

and

\[
\psi_{1\text{eff}}(a,l) = \mathbb{E} \left[ \frac{(2Z - 1)(2A - 1)YI[A = a]}{\delta(l)f(Z \mid L = l)P(L = l)} \mid L = l \right],
\]

that is, \(\psi_{1\text{eff}}(a,l)\) is the nonparametric influence function for \(\psi_1(a,l)\).

of Proposition 5. To express the efficient influence function of \(\Psi(a,l)\), we find the efficient influence function of (1) \(\psi_1(a,l) = \mathbb{E}(Y^a \mid L = l)\), (2) \(\psi_2(a,l) = \mathbb{E}(Y \mid A = a, L = l)\) and (3) \(\psi_3(a,l) = P(A = a \mid L = l)\). Using differentiation rules, the efficient influence function is

\[
\psi_{1\text{eff}}(a)\psi_3(a') - \psi_{3\text{eff}}(a')\psi_1(a) - \left\{ \psi_{2\text{eff}}(a)\psi_3(a) + \psi_2(a)\psi_{3\text{eff}}(a) \right\}\psi_3(a') + \psi_2(a)\psi_3(a)\psi_3^{\text{eff}}(a')
\]

\[
\psi_3^{\text{eff}}(a')
\]

where we have slightly abused notation by omitting \(l\) from all the arguments to make the expression less cluttered; that is, we e.g. wrote \(\psi_3(a')\) instead of \(\psi_3(a',l)\). However,

\[
\frac{d\psi_1(a,l; \theta_t)}{dt} \bigg|_{t=0}
\]

was also derived previously in Cui (2021); indeed, the nonparametric influence function for \(\psi_1(a,l)\) is
\[
\psi_1^{\text{eff}}(a,l) = \frac{(2Z - 1)(2A - 1)YI[A = a]I[L = l]}{\delta(l)f(Z \mid L = l)P(L = l)} - \left( \frac{Z\mathbb{E}[(2A - 1)YI[A = a] \mid Z, L = l]}{\delta(l)f(Z \mid L = l)P(L = l)} - \sum_z \frac{z\mathbb{E}[(2A - 1)YI[A = a] \mid Z = z, L = l]}{\delta(l)P(L = l)} + \frac{2f(Z \mid L = l)\delta(l)P(L = l)}{2f(Z \mid L = l)\delta(l)P(L = l)} \sum_z \frac{z\mathbb{E}[(2A - 1)YI[A = a] \mid Z = z, L = l]}{\delta(l)} \right).
\]

Furthermore,
\[
\frac{d\psi_2(a,l; \theta_t)}{dt}_{t=0} = \mathbb{E}\{YS(Y \mid A = a, L = l) \mid A = a, L = l\} = \mathbb{E}\{Y - \mathbb{E}(Y \mid A = a, L = l)\} S(Y \mid A = a, L = l) \mid A = a, L = l\} = \mathbb{E}\left[ \frac{I(A = a, L = l)}{P(A = a, L = l)} \left\{ Y - \psi_2(a,l) \right\} S(O) \right].
\]

and, similarly,
\[
\frac{d\psi_3(a,l; \theta_t)}{dt}_{t=0} = \mathbb{E}\left[ \frac{I(L = l)}{P(L = l)} \left\{ Y - \psi_3(a,l) \right\} S(O) \right].
\]

By plugging in these derivatives into (12), and after some steps of simple algebra, we obtain the formula given in the statement.
The influence function in Proposition 5 motivates a one-step estimator of $\Psi(a, l)$, that is,

$$\hat{\psi}_1(a, l) - \hat{\mathbb{E}}[Y \mid A = a, L = l] \hat{P}(A = a \mid L = l)$$

$$+ \mathbb{P}_n \left( \frac{1}{\hat{P}(A = 1 - a \mid L = l)} \left( \hat{\psi}_1^{\text{eff}}(a, l) \hat{P}(A = 1 - a \mid L = l) - \hat{\psi}_1(a, l) \frac{I[L = l]}{\hat{P}(L = l)} (I[A = 1 - a] - \hat{P}(1 - a \mid L = l)) \right) \hat{P}(A = a \mid L = l)$$

$$+ \hat{\mathbb{E}}[Y \mid A = a, L = l] \hat{P}(A = a \mid L = l) \frac{I[L = l]}{\hat{P}(L = l)} (I[A = 1 - a] - \hat{P}(1 - a \mid L = l)) \right) \hat{P}(A = a \mid L = l)$$

$$+ \hat{\mathbb{E}}[Y \mid A = a, L = l] \hat{P}(A = a \mid L = l) \frac{I[L = l]}{\hat{P}(L = l)} (I[A = 1 - a] - \hat{P}(1 - a \mid L = l)) \right) \hat{P}(A = a \mid L = l)$$

This estimator requires the following models to be correctly specified:

- the model for $\psi_1(a, l)$,
- the model for $P(A = a^\dagger \mid L = l)$, and
- the model for $\mathbb{E}[Y \mid A = a, L = l]$.

Semi-parametric multiple robust estimators for expressions similar to $\psi_1(a, l)$ have been suggested, see e.g. Cui (2021), which can be used to estimate $\Psi(a, l)$. In Appendix C.1 we also give the efficient influence function for identification of the $L$-superoptimal regime without necessarily identifying the value function.

Furthermore, the results in this section motivate a (new) simple semi-parametric estimator, which can be used to estimate value functions under both $L$-optimal and $L$-superoptimal regimes with standard regression models when $\Psi(a, l)$ identifies $\mathbb{E}(Y^a \mid A = 1 - a, L)$, as stated in Appendix D.

**B.1. Influence function of the marginal value function.** Let $g(a, l)$ be a known regime which is a function of $a$ and $l$. Now we derive the influence function of the marginal value function $\mathbb{E}[Y^{g(A, L)}]$. 
First,

$$
\mathbb{E}[Y^{g(a,L)}] = \sum_{a,l} \mathbb{E}[Y^{g(a,l)} | A = a, L = l] P(A = a, L = l).
$$

Because \(g(a,l)\) is a constant given \(a\) and \(l\), we can use differentiation rules for influence functions,

$$
\mathbb{IF} (\mathbb{E}[Y^{g(a,l)}]) = \sum_{a,l} I[g(a,l) = a] \frac{I[A = a, L = l]}{P(A = a, L = l)} (Y - \mathbb{E}[Y | A = a, L = l]) P(A = a, L = l)
$$

$$
\quad + I[g(a,l) = 1 - a] \Psi^{\text{eff}}(1 - a, l) P(A = a, L = l)
$$

$$
\quad + \mathbb{E}[Y^{g(a,l)} | A = a, L = l](I[A = a, L = l] - P(A = a, L = l)),
$$

assuming \(L\) is discrete. The argument extends to continuous (real-valued) \(L\) by replacing sums with integrals.

**Appendix C. One-step estimator**

C.1. **Identification and estimation of the sign of the superoptimal regime.** Estimating the \(L\)-superoptimal regime \(g_{\text{super}}\) often requires fewer model assumptions than estimating the value function \(\mathbb{E}[Y^{g_{\text{super}}}]\). Indeed, it follows from Corollary 5 that we only need to identify and estimate the difference \(\mathbb{E}(Y | L = l) - \psi_1\), which has the non-parametric influence function stated in the following corollary:

**Corollary 5.** The efficient influence function of \(\mathbb{E}(Y | L = l) - \psi_1\) in \(\mathcal{M}_{np}\) is given by

$$
\frac{1(L = l)}{P(L = l)} (Y - \mathbb{E}(Y | L = l)) - \psi_1^{\text{eff}}.
$$
Proof. Corollary [3] follows immediately from Proposition [3]. The influence of \( \mathbb{E}(Y \mid L = l) \) is

\[
\frac{1(L = l)}{P(L = l)} (Y - \mathbb{E}(Y \mid L = l)).
\]

Using differentiation rules, we find that the influence function of \( \mathbb{E}(Y \mid L = l) - \mathbb{E}(Y^a \mid L = l) \) is

\[
\frac{1(L = l)}{P(L = l)} (Y - \mathbb{E}(Y \mid L = l)) - \psi_{\text{eff}}
\]

which is the formula given in the statement.

\[\square\]

Thus, a one-step estimator of \( \mathbb{E}(Y \mid L = l) - \mathbb{E}(Y^a \mid L = l) \) is

\[
\hat{\mathbb{E}}(Y \mid L = l) - \hat{\psi}_1 + \mathbb{P}_n \left( \frac{1(L = l)}{P(L = l)} (Y - \hat{\mathbb{E}}(Y \mid L = l)) - \hat{\psi}_{\text{eff}} \right).
\]

This estimator requires one of the six following combination of models to be correctly specified:

1. \( \mathcal{M}_1 \): models for \( f(Z \mid L) \) and \( \delta(L) \),
2. \( \mathcal{M}_2 \): models for \( f(Z \mid L) \) and \( \gamma(L) \) := \( \sum_z \{ z \mathbb{E}[A Y I\{A = a\} \mid Z = z, L = l]\}/\delta(L) \),
3. \( \mathcal{M}_3 \): models for \( \gamma(L) \), \( \gamma'(L) = \mathbb{E}[A Y I\{A = a\} \mid Z = 0, L] \) and \( \delta(L) \), \( \mathbb{E}[A \mid Z = 0, L] \),
4. \( \mathcal{M}_4 \): models for \( f(Z \mid L) \), \( \delta(L) \) and \( \mathbb{E}(Y \mid L = l) \),
5. \( \mathcal{M}_5 \): models for \( f(Z \mid L) \), \( \gamma(L) \) and \( \mathbb{E}(Y \mid L = l) \), or
6. \( \mathcal{M}_6 \): models for \( \gamma(L) \), \( \gamma'(L) \), \( \mathbb{E}[A \mid Z = z, L = l] \) and \( \mathbb{E}(Y \mid L = l) \).

Here, we have also assumed that \( \hat{P}(L = l) \) is estimated empirically, so it will not be misspecified.
Appendix D. Estimation algorithm of a simple semi-parametric estimator

Suppose that positivity, consistency and Assumptions 8-13 from Appendix A hold. Under these assumptions, the identification result in Proposition 4 is valid. A standard M-estimator argument implies that the following estimation algorithm, which was applied in Section 8, is consistent when the parametric regression models are correctly specified. We use greek letters to denote parameters indexing statistical models, and we use hats to denote estimates. As before, let $W(a) = \frac{(2Z-1)Y(2A-1)I(A=a)}{\delta(L)f(Z|L)}$, and $\psi_1(a,l) = \mathbb{E}(W(a) | L = l)$.

1. Using data from all individuals, compute an estimate of $\delta(L)$ by
   - first computing the MLE $\hat{\beta}_z$ for $z = 0, 1$ using the (parametric) models $P(A = 1 | Z = 1, L; \beta_1)$ and $P(A = 1 | Z = 0, L; \beta_0)$ of $P(A = 1 | Z = z, L)$, e.g. a logistic regression model with the dependent variable $A$ and the independent variable is a specified function of $Z$ and $L$.
   - Compute an estimate $\delta(L; \hat{\beta}_0, \hat{\beta}_1) = P(A = 1 | Z = 1, L; \hat{\beta}_1) - P(A = 1 | Z = 0, L; \hat{\beta}_0)$.

2. Using data from all individuals, compute an estimate $\hat{\mathbb{E}}[W(a) | L]$ of $\mathbb{E}(W(a) | L)$ as follows:
   - For each $a \in \{0, 1\}$, compute the MLE $\hat{\theta}_{az}$ of $\theta_{az}$ for $a, z \in \{0, 1\}$ for the model $\mathbb{E}[Y(2A - 1)I(A = a) | L = l, Z = z; \theta_{az}]$ of $\mathbb{E}[Y(2A - 1)I(A = a) | L = l, Z = z]$ with independent variables $l$; that is, fit models
     
     $\mathbb{E}[-YI(A = 0) | L = l, Z = 0; \theta_{00}] = \mathbb{E}[Y(2A - 1)I(A = 0) | L = l, Z = 0; \theta_{00}],$
     $\mathbb{E}[-YI(A = 0) | L = l, Z = 1; \theta_{01}] = \mathbb{E}[Y(2A - 1)I(A = 0) | L = l, Z = 1; \theta_{01}],$
     $\mathbb{E}[YI(A = 1) | L = l, Z = 0; \theta_{10}] = \mathbb{E}[Y(2A - 1)I(A = 1) | L = l, Z = 0; \theta_{10}],$
     $\mathbb{E}[YI(A = 1) | L = l, Z = 1; \theta_{11}] = \mathbb{E}[Y(2A - 1)I(A = 1) | L = l, Z = 1; \theta_{11}].$
When $A$ and $Y$ are binary, then $\mathbb{E}[Y(2A-1)I(A = 0) \mid L = l, Z = z] + 1 \in \{0, 1\}$ and $\mathbb{E}[Y(2A-1)I(A = 1) \mid L = l, Z = z] \in \{0, 1\}$. We can thus fit regression models to estimate each of the four conditional expectations, and then we compute estimates $\hat{\psi}_1(a,l) := \hat{\mathbb{E}}[W(a) \mid L = l]$ of $\psi_1(a,l) := \mathbb{E}(W(a) \mid L = l)$ by

$$\hat{\psi}_1(a,l) = \hat{\mathbb{E}}[W(a) \mid L = l] = \sum_z \frac{(2z - 1)}{\delta(l)} \mathbb{E}[Y(2A-1)I(A = a) \mid L = l, Z = z; \hat{\theta}_{az}],$$

where $\hat{\theta}$ is the MLE.

(3) Using data from all individuals, compute the MLE $\hat{\gamma}$ of $\gamma$ for a model $\mathbb{E}(Y \mid L = l; \gamma)$ of $\mathbb{E}(Y \mid L = l)$. If $Y$ is binary, use e.g. a logistic regression with dependent variable $Y$ and independent variables a specified function of $L$.

(4) For all $a,l$, the estimated superoptimal regime $\hat{g}_{sup}(a,l)$ is

$$\hat{g}_{sup}(a,l) = \arg \max_{a^*} I[a^* = a] \mathbb{E}(Y \mid L = l; \hat{\gamma}) + I[a^* \neq a] \hat{b}(a^*, l),$$

where $\mathbb{E}(Y \mid L = l; \hat{\gamma})$ and $\hat{\psi}_1(a^*, l) = \hat{\mathbb{E}}[W(a^*) \mid L = l]$ are estimated expected conditional means from the models specified earlier.

- Similarly, if the interest is the regime $\hat{g}_{opt}(l)$,

$$\hat{g}_{opt}(a,l) = \hat{g}_{opt}(l) = \arg \max_{a^*} \hat{b}(a^*, l),$$

because $\hat{\psi}_1(a^*, l)$ can be interpreted as an estimator of $E(Y^a \mid L = l)$, as shown in Cui and Tchetgen Tchetgen (2021b).

(5) To find the value function, we first use that

$$\mathbb{E}(Y^{\hat{g}_{sup}} - Y) = \mathbb{E}\left\{ \mathbb{E}\left[I[\hat{g}_{sup}(A, L) \neq A] [\psi_1(\hat{g}_{sup}(A, L), L) - \mathbb{E}(Y \mid L)] \mid L, A \right] \right\},$$

When $Y$ is binary we know that, for each $a$, $0 \leq \mathbb{E}(W(a) \mid L) \leq 1$ w.p.1.
which can be estimated by

\[
\hat{E}(Y^{\hat{g}_{sup}} - Y) = \\
\frac{1}{n} \sum_i \left\{ I[A_i = 0, \hat{g}_{sup}(0, L_i) \neq 0] \{ \hat{E}(W(\hat{g}_{sup}(0, L_i)) | L_i) - E(Y | L_i; \hat{\gamma}) \} \\
+ I[A_i = 1, \hat{g}_{sup}(1, L_i) \neq 1] \{ \hat{E}(W(\hat{g}_{sup}(1, L_i)) | L_i) - E(Y | L_i; \hat{\gamma}) \} \right\},
\]

and

\[
\hat{E}(Y^{\hat{g}_{sup}}) = \hat{E}(Y^{\hat{g}_{sup}} - Y) + \hat{E}(Y),
\]

where \( \hat{E}(Y) = n^{-1} \sum_i E(Y | L_i; \hat{\gamma}) \).

(6) To obtain confidence intervals for the value function,

(a) estimate \( \hat{g}_{sup}(a, l) \) from the entire data, and

(b) for each bootstrap sample \( b \), estimate \( \hat{E}_b(Y^{\hat{g}_{sup}}) \) as in step 5, where subscript \( b \) indicates the bootstrap sample.

In our data example in Section 8 of the main text we performed the algorithm on sample split data; that is, we estimated the optimal regime in 60% of the data, and subsequently estimated the value function with confidence intervals in the remaining 40% of the data. We parameterized the following terms with logistic regression models:

- \( P(A = 1 | Z = 1, L) \),
- \( P(A = 1 | Z = 0, L) \),
- \( E[-Y I[A = 0] | L = l, Z = 0] \),
- \( E[-Y I[A = 0] | L = l, Z = 1] \),
- \( E[Y I[A = 1] | L = l, Z = 0] \),
- \( E[Y I[A = 1] | L = l, Z = 1] \), and
- \( E[Y | L = l] \).
Appendix E. Leveraging Identification with Instrumental Variables

Consider the following regimes, which are functions of baseline covariates \( L \) and the instrument \( Z \).

**Definition 4** \((L,Z)\)-optimal regimes. The \((L,Z)\)-optimal regime, \( g_{\text{opt}} \), assigns treatment \( A^{g_{\text{opt}}} = a \) given a vector \( L = l \) and instrument \( Z = z \) by

\[
g_{\text{opt}}(l, z) \equiv \arg \max_{a \in \{0,1\}} \mathbb{E}(Y^a | L = l, Z = z).
\]

Because \( Z \perp Y^a | L \) under the classical IV assumptions 8-11, see Appendix A, the \((L,Z)\)-optimal is equal to the \(L\)-optimal regime; that is,

\[
\mathbb{E}(Y^a | L = l, Z = z) = \mathbb{E}(Y^a | L = l) \quad \text{for all } a, l, z.
\]

Consider now the \((L,Z)\)-Superoptimal regimes.

**Definition 5** \((L,Z)\)-Superoptimal regimes. The \((L,Z)\)-superoptimal regime, \( g_{\text{sup}} \) assigns treatment \( A^{g_{\text{sup}}} = a \) given \( A = a'\), \( L = l \) and \( Z = z \) by

\[
g_{\text{sup}}(a', l, z) \equiv \arg \max_{a \in \{0,1\}} \mathbb{E}(Y^a | A = a', L = l, Z = z).
\]

Interestingly,

\[
Z \not\perp Y^a | L, A,
\]

which e.g. can be read off of the SWIG in Figure 1. Indeed, there could exist \( a, a', z \) and \( l \) such that

\[
\mathbb{E}(Y^a | A = a', L = l, Z = z) \neq \mathbb{E}(Y^a | A = a, L = l).
\]

Thus, using the instrument as input to the decision function could further improve expected outcomes under the regime. This result is not only of theoretical interest, because under positivity, consistency and identification assumptions 8-13 we can identify these regimes without additional assumptions, as confirmed by the following proposition.
Proposition 6. Under consistency and positivity, $E(Y^a | A = a', L = l, Z = z)$ can be expressed as

$$E(Y^a | A = a', L = l, Z = z) = \begin{cases} 
E(Y | A = a', L = l, Z = z), & \text{if } a = a', \\
\frac{E(Y^a | L = l, Z = z) - E(Y | A = a, L = l, Z = z)P(A = a' | L = l, Z = z)}{P(A = a' | L = l, Z = z)}, & \text{if } a \neq a'.
\end{cases}$$

Furthermore, under Assumptions 8-(13), we have that $E(Y^a | L = l, Z = z) = E(Y^a | L = l) = \psi_1(a, l)$, and thus $E(Y | A = a', L = l, Z = z)$ is identified.

Appendix F. Examples

Example 3. [Qiu et al. (2021)] developed theory for identification and estimation of $L$-optimal regimes in settings with unmeasured confounding, given that a valid binary instrument is available for a binary treatment. Whereas [Qiu et al. (2021)] gave identification results for regimes that are $L$-optimal with respect to pretreatment covariates $L$, they emphasized that these $L$-optimal regimes can be worse than the regime that was implemented in the observed data (Qiu et al., 2021, Remark 1), which also was illustrated by an explicit example (Qiu et al., 2021, Remark 5). Specifically:

1. Draw $W, U, Z \sim \text{Bernoulli}[p = 0.5]$ (mutually independent draws).
2. Draw $A^{z=0} \sim \text{Bernoulli}[p = 0.3U + 0.4]$.
3. Draw $A^{z=1} \sim \text{Bernoulli}[p = 0.3U + 0.6]$.
4. Draw $Y^{a=0} \sim \mathcal{N}[1 - 2U, 1]$.
5. Draw $Y^{a=1} \sim \mathcal{N}[2U - 1, 1]$.

Qiu et al. (2021) showed that $E(Y) = 0.3$ but $E(Y^{g_{opt}}) = 0$. However, a simple computation shows that $E(Y^{g_{sup}}) = 0.3$. Thus, the superoptimal regime is strictly better than the $L$-optimal regime.

Example 4. We also consider a modified version of Example 3, where only $P(A^z = a | L, U, Z)$ is changed, that is,
(1) Draw $W, U, Z \sim \text{Bernoulli}[p = 0.5]$ (mutually independent draws).

(2) Draw $A^{a=0} \sim 1 - \text{Bernoulli}[p = 0.3U + 0.4]$.

(3) Draw $A^{a=1} \sim 1 - \text{Bernoulli}[p = 0.3U + 0.6]$.

(4) Draw $Y^{a=0} \sim N[1 - 2U, 1]$.

(5) Draw $Y^{a=1} \sim N[2U - 1, 1]$.

Because everything except $P(A^{a} = a \mid W, U, Z)$ is identical to Example 3, the $L$-optimal regime in this example is equal to the $L$-optimal regime in Example 3; that is, $E(Y^{g_{\text{opt}}}) = 0$. A simple calculation shows that $E(Y) = -0.3$, and, thus, the observed regime is inferior to the $L$-optimal regime. Another simple calculation shows that $E(Y^{g_{\text{sup}}}) = 0.3$, which implies that the $L$-superoptimal is strictly better than the observed regime and the $L$-optimal regime. Thus, this example illustrates that the $L$-superoptimal regimes can be (strictly) better than regimes derived from approaches that could leverage the implicit regime (Kallus and Zhou, 2021; Cui and Tchetgen Tchetgen, 2021b; Qiu et al., 2021).

**Example 5.** IV assumptions 8-11 used to identify $L$-superoptimal regimes do impose restrictions on the counterfactual outcome distributions. However, in the following simple example, we nevertheless illustrate that these restrictions do not preclude the $L$-superoptimal regime from being better than the $L$-optimal regime.

Suppose IV assumptions 8-11 hold. Let $L = \emptyset$, and consider $U, Z, A, Y \in \{0, 1\}$ such that

- $P(U = 1) = (Z = 1) = 0.5$
- $P(A = 1 \mid Z = z, U = u) = 0.5c + cz + cu$, where $0 < c < 0.4$
- $E(Y^{a=1}) = 0.5$, $E(Y^{a=1} \mid U = 1) = 0.1$, $E(Y^{a=1} \mid U = 0) = 0.9$
- $E(Y^{a=0}) = 0.4$, $E(Y^{a=0} \mid U = 1) = 0.7$, $E(Y^{a=0} \mid U = 0) = 0.1$

This example is consistent with the SWIG in Figure 1 if we had removed $L$ from the graph.

Trivially, $g_{\text{opt}} = 1$. To calculate $g_{\text{sup}}$, we use law of total probability to find the values of $P(U = u \mid Z = z, A = a)$ for all $u, z$ and $a$, and then compute $E(Y^{a'} \mid A = a, Z = z)$.
from
\[ E(Y^{a'} \mid A = a, Z = z) = \sum_u E(Y^{a'} \mid U = u) P(U = u \mid A = a, Z = z). \]

In particular, for \( c = \frac{4}{5} \) we find that

- \( E(Y^{a=1} \mid A = 1, Z = 1) = 4/10 < E(Y^{a=0} \mid A = 1, Z = 1) = 19/40, \)
- \( E(Y^{a=1} \mid A = 0, Z = 0) = 11/20 > E(Y^{a=0} \mid A = 0, Z = 0) = 17/80. \)

Thus, \( g_{\text{sup}}(a = 1, z = 1) = 0 \neq g_{\text{sup}}(a = 0, z = 0) = 1, \) which is sufficient to illustrate that the superoptimal regime is better than the optimal regime.

APPENDIX G. A STRATEGY FOR TESTING THE PRESENCE OF UNMEASURED CONFounding

The following proposition follows by the same logic of Corollary 3 in the main text, and states constraints on counterfactual parameters that motivate a test for unmeasured confounding.

**Proposition 7.** Let \( \Pi \equiv \{ g : L \rightarrow \{0, 1\} \} \) be the class of regimes \( g \) that depend only on \( L \), and let \( \Pi^* \) be the analogous class of regimes \( g^* \) that may depend additionally on \( A \). Then consider \( B \) and \( C \) to be coarsenings of \( A \) of \( L \), respectively. Define the interval \( I^g_c \) constructed from the following upper and lower bounds:

\[ \max_{g \in \Pi} E[Y^g \mid C = c] \quad \text{and} \quad \min_{g \in \Pi} E[Y^g \mid C = c]. \]

Likewise define the interval \( I_{b,c}^{g^*} \) to be the analogous interval constructed by minimizing and maximizing over \( g^* \in \Pi^* \), and additionally conditioning on \( B = b \).

Suppose \( Y^a \perp \perp A \mid L \) for \( a \in \{0, 1\} \). Then, for each \( c \),

\[ I_{b,c}^{g^*} \equiv I_c^g \text{ for all } b. \]
Proof. If $Y^a \indep A \mid L$, then for any $g^* \in \Pi^*$, $E[Y^{g^*} \mid B = b, C = c]$ is equal to $E[Y^{g_{\text{rand}}} \mid B = b, C = c]$ where $g_{\text{rand}}$ is some regime that is maximally dependent on $L$ and an exogenous randomizer term $\delta$. Robins (1986) showed that $E[Y^{g_{\text{rand}}} \mid C = c]$ is equal to some convex combination of the values in the set $\{E[Y^g \mid C = c] : g \in \Pi\}$. The result then follows immediately.

Corollary 6. If $Y^a \indep A \mid L$ then $E[Y \mid B = b, C = c]$ and $E[Y^{g_{\text{sup}}} \mid B = b, C = c]$ are contained in the interval $I^a_{bc}$ for all $b, c$.

Proof. Corollary 6 follows immediately because $Y^{g_{\text{sup}}}$ is obviously an element in $\Pi^*$ and also because $Y = Y^{g^*}$ with probability 1 for the special regime in $\Pi^*$ that assigns $A^{g^*} = A$.

Remark 8. When the conditions of Proposition 2 hold, then $I^a_{bc}$ is identified, as are the conditional average outcomes under the superoptimal regime $g_{\text{sup}}$. This would allow us to re-express Proposition 7 in terms of constraints on the law of the observed data. Consideration of the contrapositive of this re-expressed Proposition 7 then ostensibly motivates a simple test for unmeasured confounding. If any of the constraints are violated, then $Y^a \not\indep A \mid L$ for some $a \in \{0, 1\}$. The practical utility of this test, however, is questionable, because it will have low (or zero) power in many settings. In particular, common identification strategies, such as those based on the g-formula (Robins, 1986), would rely on no unmeasured confounding assumptions for identification, e.g. $Y^a \indep A \mid L$, $a \in \{0, 1\}$. Whenever such conditions are (possibly erroneously) assumed, the test has zero power. In IV settings, however, the test could reject the null hypothesis of no unmeasured confounding. We illustrate one such setting in Example 3. Thus, this simple test adds to the small number of existing tests for unmeasured confounding, which, to our knowledge, critically rely on instrumental variables (Guo et al., 2014; de Luna and Johansson, 2014).