Personalizing Path-Specific Effects

Abstract
Unlike classical causal inference, which often has an average causal effect of a treatment within a population as a target, in settings such as personalized medicine, the goal is to map a given unit’s characteristics to a treatment tailored to maximize the expected outcome for that unit. Obtaining high-quality mappings of this type is the goal of the dynamic regime literature (Chakraborty and Moodie 2013), with connections to reinforcement learning and experimental design. Aside from the average treatment effects, mechanisms behind causal relationships are also of interest. A well-studied approach to mechanism analysis is establishing average effects along with a particular set of causal pathways, in the simplest case the direct and indirect effects. Estimating such effects is the subject of the mediation analysis literature (Robins and Greenland 1992; Pearl 2001).

In this paper, we consider how unit characteristics may be used to tailor a treatment assignment strategy that maximizes a particular path-specific effect. In healthcare applications, finding such a policy is of interest if, for instance, we are interested in maximizing the chemical effect of a drug on an outcome (corresponding to the direct effect), while assuming drug adherence (corresponding to the indirect effect) is set to some reference level.

To solve our problem, we define counterfactuals associated with path-specific effects of a policy, give a general identification algorithm for these counterfactuals, give a proof of completeness, and show how classification algorithms in machine learning (Chen, Zeng, and Kosorok 2016) may be used to find a high-quality policy. We validate our approach via a simulation study.

Introduction
Establishing causal relationships between action and outcome is fundamental to rational decision-making. A gold standard for establishing causal relationships is the randomized controlled trial (RCT), which may be used to establish average causal effects within a population. Causal inference is a branch of statistics that seeks to predict effects of RCTs from observational data, where treatment assignment is not randomized. Such data is often gathered in observational studies, surveys given to patients during follow up, and in hospital electronic medical records.

While RCTs and causal inference methods that predict results of hypothetical RCTs establish whether a particular action is helpful on average, optimal decision making must tailor decisions to specific situations. In the context of causal inference this involves finding a map between characteristics of an experimental unit, such as baseline features, to an action that optimizes some outcome for that unit. Methods for finding such maps are studied in the dynamic treatment regime literature, and in off-policy reinforcement learning.

If an action is known to have a beneficial effect on some outcome, it is often desirable to understand the causal mechanism behind this effect. A popular type of mechanism analysis is mediation analysis, which seeks to decompose the average causal effects into direct and indirect components, or more generally into components associated with specific causal pathways. These components of the average causal effect are known as direct, indirect, and path-specific effects, and are also defined as a population average (Robins and Greenland 1992; Pearl 2001; Avin, Shpitser, and Pearl 2005). In this paper we introduce methods to personalize these types of effects, that is find mappings from unit characteristics to actions that maximize some path-specific effect.

Why Personalize Path-Specific Effects?
Just as it often makes sense to structure decision-making such that the overall effect of an action on the outcome is maximized for any specific unit, in some cases it is appropriate to choose an action such that only a part of the effect of an action on the outcome is maximized. Consider management of care for HIV patients. Since HIV is a chronic disease, care for HIV patients involves designing a long-term treatment plan to minimize chances of viral failure (an undesirable outcome). In designing such a plan, an important choice is initiation of primary therapy, and a switch to a second line therapy. Initiating or switching too early risks unneeded side effects and “wasting” treatment efficacy, while initiating or switching too late risks viral failure (Hernan et al. 2006).

However, in the context of HIV, treatment adherence is an important component of the overall effect of the drug on the outcome. Patients who do not take prescribed doses compromise the efficacy of the drug, and different drugs may have different levels of adherence. Thus, in HIV the overall effect of the drug can be viewed as a combination of the chemical
effect, and the adherence effect (Miles et al. 2017). Therefore, choosing an action that maximizes the overall effect of HIV treatment on viral failure entangles these two very different mechanisms. One approach to tailoring treatments to patients in a way that disentangles these mechanisms is to find a policy that optimizes a part of the effect, say the chemical (direct) effect of the drug, while hypothetically keeping the adherence levels to some reference level. Finding such a policy yields information on how best to assign drugs to maximize their chemical efficacy in settings where adherence levels can be controlled to a reference level – even if the only data available is one where patients have differential adherence.

Preliminaries

We will consider causal models represented by acyclic directed graphs (DAGs), and acyclic directed mixed graphs (ADMGs) representing classes of DAGs with hidden variables. A DAG is a graph with directed (→) edges with no directed cycles, an ADMG is a graph with directed (→) and bidirected (↔) edges with no directed cycles.

Graph Theory

We will define statistical and causal models as sets of distributions defined by restrictions associated with graphs. Thus we will use vertices and variables interchangeably – capital letters for a vertex or variable (V), bold capital letter for a set (V), small letters for values (v), and bold small letters for sets of values (v). For a set of values a of A, and a subset A† ⊆ A, we define aA† to be a restriction of a to elements in A†. We will assume graphs with a vertex set V. The state space of A will be denoted by xA, and the (Cartesian product) state space of A will be denoted by xA.

For a graph G, and any V ⊆ V, we will define the following genealogic sets: parents, children, ancestors, descendants, and siblings as: paG(V) = {W ∈ V | W → V}, chG(V) = {W ∈ V | V → W}, angG(V) = {W ∈ V | W → ... → V}, degG(V) = {W ∈ V | V → ... → W}, sibG(V) = {W ∈ V | V ↔ W}. By convention, angG(V) ∩ degG(V) ∩ sibG(V) = {V}. These sets generalize to V† ⊆ V disjunctively. For example, paG(V†) = U V∈V† paG(V).

For A ⊆ V, define paG(A) = paG(V) \ A.

We define the set ndG(V) = V \ degG(V). The district of V is defined as disG(V) = {W ∈ V | W ↔ ... ↔ V}. The set of districts will be denoted by D(G), and it always forms a partition of vertices in G. Given a graph G and A ⊆ V, denote by GA the subgraph of G containing only vertices in A and edges between these vertices.

Statistical And Causal Models Of A DAG

A statistical model of a DAG or a Bayesian network, associated with a DAG G, is the set of distributions p(V) such that p(V) = \prod_{V \in G} p(V | paG(V)). Such a p(V) is said to be Markov relative to G.

Causal models of a DAG are also sets of distributions, but on counterfactual random variables. Given Y ∈ V and A ⊆ V \ {Y}, a counterfactual variable, also known as a potential outcome, and written as Y(a) represents variation in Y in a hypothetical situation where A were set to values a by an intervention operation (Pearl 2009). Given a set Y, define Y(a) = \{Y | a \in A\}. Given a DAG G, the joint distribution of the counterfactual variables p(V(a) | V ∈ V \ A) is identified, via the edge g-formula, which is the following generalization of (4):

\[ p(V(a) | V ∈ V \setminus A) = \prod_{V \in V \setminus A} p(V | paG(V) \setminus A, paG(V)). \] (4)

For example, in Fig 1 (a), p(Y((a1Y) → (a2'M) →) = \sum_{W,M} p(Y | a, M, W)p(M | a', W)p(W). This is sometimes known as the mediation formula (Pearl 2011).
Counterfactual responses to edge interventions represent effects of treatments A along some but not all causal pathways. In simplest cases, these responses can be used, often on the mean difference scale, to define direct and indirect effects (Robins and Greenland 1992; Pearl 2001). For example, in the model given by the DAG in Fig (a), the direct effect of A on Y is defined as $E[Y((aY)_{\perp\!\perp},(aM)_{\perp\!\perp})] - E[Y((aY)_{\perp\!\perp},(M)_{\perp\!\perp})]$ which is equal to $E[Y(a)] - E[Y(a', M(a))]$. The indirect effect may be defined similarly as $E[Y((aY)_{\perp\!\perp},(aM)_{\perp\!\perp})] - E[Y((aY)_{\perp\!\perp},(aM)_{\perp\!\perp})]$, which is equal to $E[Y(a', M(a))] - E[Y(a')]$. The direct and indirect effects defined in this way add up to the ACE.

Edge interventions represent a special case of a more general notion of a path-specific effect (Pearl 2001) which, unlike path-specific effects, happens to always be identified under an NPSEM-IE of a DAG, via (1). Path-specific effects may not be identified even in a DAG model, due to the presence of a recanting witness (Avin, Shpitser, and Pearl 2005).

Responses To Treatment Policies
In settings such as personalized medicine, counterfactual responses to conditional interventions that set treatment values in response to other variables via a known function are of frequent interest. Given a DAG $G$, a topological ordering $\prec$, and a set $A \subseteq V$, for each $A \in A$, define $W_A$ to be some subset of predecessors of $A$ according to $\prec$. Then, given a set of functions $f_A$ of the form $f_A : X_{W_A} \to X_A$, we define $Y(f_A)$, the counterfactual response $Y \in V$ to A being intervened on according to $f_A \equiv \{f_a | A \in A\}$, as

$$Y((f_A(W_Af_A)|A \in pa_G(Y) \cap A), \{pa_G(Y) \setminus A\}(f_A)),$$

As an example, in the graph in Fig. (b), if we are interested in evaluating the efficacy of a policy set $\{f_{A_1} : X_{W_0} \to X_{A_1}, f_{A_2} : X_{W_0,W_1} \to X_{A_2}\}$ as far as their effect on the outcome $W_2$, we could evaluate it via the random variable $Y(f_{A_1}, f_{A_2})$ defined as $W_5(f_{A_2}(W_1(f_{A_1}(W_0)), W_0), W_0).$ The efficacy of a particular set of policies may be evaluated on the mean scale as $E[Y(f_{A_1}, f_{A_2})]$. In a causal model of a DAG, given any policy set, the effect of $f_A$ on $V \setminus A$, represented by the distribution $p(V(f_A) | V \subseteq V \setminus A))$, is identified by the following modification of (2):

$$\prod_{V \subseteq V \setminus A} p(V(f_A(W_Af_A)|A \in A \cap pa_G(V)), \{pa_G(V) \setminus A\}(f_A)).$$

For example, $p(Y(f_{A_1}, f_{A_2}))$ is identified as

$$\sum_{W_0,W_1} p(W_2|W_0,f_{A_1}(W_0), W_1,f_{A_2}(W_0,W_1)) \times p(W_1|W_0,f_{A_1}(W_0)) p(W_0).$$

Identification In Hidden Variable DAGs
In a causal model of a DAG where some variables are unobserved, not every causal parameter is identifiable, that is not every parameter is a function of the observed data distribution. Given a DAG $G$ with a vertex set $V \cup H$, where $V$ are observed, and H hidden, define a latent projection $G(V)$ to be an ADMG with observed variables $V$ with an edge $(AB)_{\to}$ if there exists a directed path from $A$ to $B$ in $G$ with all intermediate vertices in H, and an edge $(AB)_{\to}$ if there exists a path without consecutive edges $\to o \leftarrow$ from $A$ to $B$ with the first edge on the path of the form $A \leftarrow$ and the last edge on the path of the form $B$. A variable pair in $G(V)$ may be connected by both a directed and a bidirected edge. It is known that all hidden variable DAGs which share latent projections share identification theory. Thus, we will describe identification results on latent projection ADMGs directly. General algorithms for identification of interventional distributions were given in (Tian and Pearl 2002), for responses to edge interventions in (Shpitser 2006), and for policies in (Tian 2008). Here we reformulate these results via simple one line formulas using conditional ADMGs and a fixing operator.

Conditional ADMGs, Kernels, And Fixing
A conditional ADMG (CADMG) $G(V,W)$ is an ADMG where $W$ are fixed vertices with the additional property that for all $W \in W$, $sg(W) \cap pa_G(W) = \emptyset$. A kernel $q(V|W)$ is a mapping from $X_W$ to normalized densities over $V$. A conditional distribution is one type of kernel, but others are possible. Conditioning and marginalization are defined in kernels in the usual way. For $A \subseteq V$,

$$q(V\setminus A|W) \equiv \sum_{V\setminus A} q(V|W); q(V \setminus A \cup W) \equiv \frac{q(V \setminus A|W)}{q(V|W)}.$$ For a $A \subseteq V$, a fixing operator $\phi_A(G(V,W))$ produces a new CADMG $G(V \setminus A, W \cup \{A\})$, where all edges into A are removed. For a CADMG $G(V,W)$ and kernel $q(V|W)$, and $A \subseteq V$, a fixing operator $\phi_A(q(V,G))$ produces a new kernel $q(V \setminus A|W \cup \{A\}) \equiv q(V|W) / q(V|A \cup \{A\}$.

A sequence $(A_1, A_2, \ldots, A_k)$ of vertices in $V$ is said to be fixable if $A_1$ is fixable in $G$, $A_2$ is fixable in $\phi_{A_1}(G)$, and so on, with $A_k$ being fixable in $\phi_{A_{k-1}}(\ldots \phi_{A_2}(\phi_{A_1}(G)) \ldots)$. A consequence of a theorem in (Richardson et al. 2017) states that if $p(H \cup V)$ is Markov relative to $G(H \cup V)$, for any two sequences $\langle A_1, \ldots, A_k \rangle$, $\langle A_1, \ldots, A_k \rangle$ fixable in $G(V)$, graphs and kernels obtained

![Figure 1: (a) A simple causal DAG, with a single treatment A, a single outcome Y, a vector W of baseline variables, and a single mediator M. (b) A more complex causal DAG with two treatments $A_1$, $A_2$, an intermediate outcome $W_1$, and the final outcome $W_2$. (c) A graph where $p(Y(A, M(a')))$ is identified, but $p(Y(f_A(W), M(a)))$ is not.](image-url)
from applying these sequences to \( G(V) \) and \( p(V) \) are the same. For this reason, we will consider fixable sets. A set is fixable in \( G \) if it is possible to arrange its elements into a fixable sequence. All sequences are fixable in a DAG. For a fixable in \( G \), we will define \( \phi_A(.) \), applied to either graphs or kernels, to be a composition of \( \phi \) applied in order to some fixable sequence of elements in \( A \). If \( A \subseteq V \) is fixable in \( G \), then the set \( V \setminus A \) is reached a called a reachable set.

Given a kernel \( q_V(V \setminus W) \equiv q_W(p(V \cup W); G(V \cup W)) \), and given \( a \in X_A \), for \( A \subseteq W \), define \( \phi_Aa \) \((p(V \cup W); G(V \cup W)) \) to be a kernel \( q_V(V \setminus W \setminus A) \) such that for any \( w \in X_W^A \), \( q_V(V \setminus w) = q_V(V \setminus w, a) \).

**Identification Algorithms Via The Fixing Operator**

A complete algorithm for identifying interventional distributions of the form \( p(Y(a)) \) for \( Y \subseteq V \setminus A \) was given in ([Tian and Pearl 2007]). This algorithm can be rephrased using the fixing operator as follows. Let \( Y^* \equiv \alpha \cap G^V \setminus A \). Then if for every \( D \in D(G_Y^* \setminus A) \), \( D \) is reachable in \( G \), then for \( Y \subseteq V \setminus A \),

\[
p(Y(a)) = \sum_{Y \setminus Y^*} \prod_{D \in D(G_Y^* \setminus A)} \phi^*_V(D) (p(V); G). \tag{8}
\]

If some \( D \in D(G_Y^* \setminus A) \) is not reachable in \( G \), \( p(Y(a)) \) is not identifiable. See theorem 60 in ([Richardson et al. 2017]).

Identification of path-specific effects where each path is associated with one of two possible value sets \( a, a' \) was given a general characterization in ([Shpitser 2013]) via the recanting district criterion. Here, we reformulate this result in terms of the fixifying operator in a way that generalizes \( \beta \), and applies to the response of any edge intervention, including those that set edges to multiple values rather than two. This result can also be viewed as a generalization of node consistency of edge interventions in DAG models, found in ([Shpitser and Tchetgen Tchetgen 2016]).

Given \( A_\alpha \equiv \{ A \mid (AB) \in \alpha \} \), and an edge intervention given by the mapping \( \alpha \), define \( Y^* \equiv \alpha \cap G^V \setminus A_\alpha \). The joint distribution of the counterfactual response \( p(V \setminus A_\alpha) \{\alpha\} \) is identified, under the NPSEM-IE, if and only if \( p(V \setminus A_\alpha) \{\alpha\} \) is identified via \( \beta \), and for every \( D \in D(G_Y^* \setminus A) \), for every \( A \subseteq A_\alpha \), either every directed edge out of \( A \) into \( D \) is in \( \alpha \) and \( \alpha \) agrees on values assignments to those edges, or every directed edge out of \( A \) into \( D \) is not in \( \alpha \).

**Theorem 1** Under above assumptions, \( p(V \setminus A_\alpha) \{\alpha\} \) is

\[
\sum_{Y \setminus Y^*} \prod_{D \in D(G_Y^* \setminus A)} \phi^*_V(D) (p(V); G). \tag{9}
\]

A general algorithm for identification of responses to a set of policies \( f_A \) is given in ([Tian 2008]). We again reformulate this algorithm in terms of the fixing operator. Define a graph \( G_{f_A} \) to be a graph obtained from \( G \) by removing all edges into \( A \), and adding for any \( A \subseteq A \), directed edges from \( W_A \) to \( A \). Define \( Y^* \equiv \alpha \cap G^V \setminus A_\alpha \). Then \( Y^* \{f_A(a)\} \) is identified in \( G \) if \( p(Y^* \{a\}) \) is identified. Moreover, the identification formula is

\[
\sum_{Y^* \cup A \subseteq V} \prod_{D \in D(G_Y^* \setminus A)} \phi^*_V(D) (p(V); G). \tag{10}
\]

where \( \bar{a} \equiv \{ A \mid f_A(W_A) \mid A \in \alpha \} \) if \( \alpha \cap \emptyset \) is not empty, and is defined to be the empty set otherwise. The sum over \( A \) is vacuous if \( f_A \) is a set of deterministic policies.

**Path-Specific Policies**

Fix a set of directed edges \( \alpha \), and define \( A_\alpha \equiv \{ A \mid (AB) \in \alpha \} \) as before. Denote \( \bar{\alpha} \) to be the set of outgoing edges from elements in \( A_\alpha \) not in \( \alpha \). Consider a set \( \{ W_A \mid A \in A_\alpha \} \) defined as before with respect to a topological ordering \( \prec \). We are going to consider a simple version of path-specific policies where for variables in \( A \) we wish to intervene on, all outgoing edges for every \( A \subseteq A \) are either associated with a reference policy \( f_A^0 : X_{W_A} \mapsto X_A \) (for edges not in \( \alpha \), or a policy of interest \( f_A : X_{W_A} \mapsto X_A \) (for edges in \( \alpha \)). Our results generalize to more complex types of path-specific policies, but we do not pursue this here in the interests of space. Generally, we will let \( f_A^0 \) be a simple policy that sets \( A \) to a reference value \( \alpha \), ignoring \( W_A \). Such reference policies are the most relevant in practice.

We now define counterfactual responses to these types of policies, which we denote by \( (f_A)^{0,\alpha} \equiv (f_A)^{0,\alpha}(f_A^{\alpha}, f_A^\alpha) \), where \( f_A \equiv \{ f_A \mid A \in A \} \), \( f_A^\alpha \equiv \{ f_A^\alpha \mid A \in A \} \), \( f_A^{0,\alpha} \equiv \{ f_A^{0,\alpha} \mid A \in A \} \), and the subscripts \( \alpha, \bar{\alpha} \) are meant to denote that these policies only apply for the purposes of those respective edge sets. Define \( Y((f_A)^{0,\alpha}) \) as

\[
Y(f_A^0(W_A((f_A^{0,\alpha}) \cap \{AY\}) \in \bar{\alpha}), \{ f_A(W_A((f_A^{0,\alpha}) \cap \{AY\}) \in \alpha \}, \{ W((f_A^{0,\alpha}) \cap \{WY\} \in \alpha \}) \}
\]

This definition generalizes both \( \beta \) and \( \gamma \) in an appropriate way. As an example, in Fig. 10 (a), a policy \( f_{12}^0(W) \) that sets \( A \) to a value only with respect to the edge \( \{AY\} \), and a reference value \( a \) that \( A \) assumes with respect to the edge \( \{AM\} \), results in the counterfactual \( Y(f_{12}^0(W), M(a,W), W) \). In the graph in Fig. 10 (b), the response of \( W_2 \) to \( A_1 \), \( A_2 \) being set according to

\[
W_2 = f_{12}(W_1(a_1, W_1, a_2, W_1, W_1(a_1, W_1)), f_{12}(W_1(a_1, W_1, a_2, W_1, W_1)), f_{12}(W_1, W_1), a_1, W_1, W_1).
\]

**Identification Of Path-Specific Policies**

Having condensed existing identification results on responses to policies \( f_A \) and responses to edge interventions arising in mediation analysis \( \beta \), we generalize these results to give an identification result for responses to path-specific policies, via the following theorem.

**Theorem 2** Define \( G_{f_A^{0,\alpha}} \) as \( G_{f_A} \) before, and let \( Y^* \equiv \alpha \cap G^V \setminus A_\alpha \). Then \( p(Y((f_A)^{0,\alpha})) \) is identified if \( p(Y^* \{a\}) \) is identified, and for every \( D \in D(G_Y^* \setminus A) \), for every \( A \subseteq A_\alpha \), either every directed edge out of \( A \) into \( D \) is in \( \alpha \), or every directed edge out of \( A \) into \( D \) is not in \( \alpha \). Moreover, the identifying formula is

\[
\sum_{Y^* \cup A \subseteq V} \prod_{D \in D(G_Y^* \setminus A)} \phi^*_V(D) (p(V); G). \tag{12}
\]
Figure 2: (a) A causal model where \( p(W_3; \{ f_{A_1}(W_0) \}_{A_1}, a_{(A_1,M_1)}) \) is identified. (b) The graph \( \mathcal{G}_Y \), where \( Y^* = \{ W_0, M_1, W_2 \} \) obtained from (a). (c) A causal model representing the chemical effect of HIV mediation, and adherence on viral failure.

where \( p_{a_0}(D) \cap A_\alpha \) is defined to be \( \{ A = f_A(W_A) \mid A \in p_{a_0}(D) \cap A_\alpha \} \cup \{ A = f_A(W_A) \mid A \in p_{a_0}(D) \cap A_{\bar{\alpha}} \} \), and \( p_{a_0}(D) \cap A_{\bar{\alpha}} \) is not empty, and is defined to be the empty set otherwise.

Responses to path-specific policies are identified in strictly fewer cases compared to responses to edge interventions. This is because \( Y^* \) is a larger set in the former case. As an example, consider the graph in Fig. 1 (c), where we are interested either in the counterfactual \( p(Y(a, M(a'))) \), used to define pure direct effects, and the counterfactual \( p(Y(f_A(W), M(a'))) \).

For the former, we have \( Y^* = \{ Y, M \} \), and \( p(Y(a, M(a'))) \) equal to

\[
\sum_{m} \left( \frac{p(Y, m | a, w)p(w)}{\sum_w p(m | a, w)p(w)} \right) \sum_w p(m | a', w)p(w)
\]

We omit the detailed derivation in the interests of space.

For the latter, however, \( Y^* = \{ Y, M, W \} \), and since \( \alpha = \{ \{ Y \} \} \) and \( \bar{\alpha} = \{ \{ AM \} \} \), Theorem 2 is insufficient to conclude identification. An example where identification is possible is shown in Fig. 1(b). Here, we are interested in optimizing the direct effect of \( A_1 \) and \( A_2 \) on \( W_2 \) via policies \( f_{A_1}(W_0) \) and \( f_{A_2}(W_1, W_0) \), while keeping the indirect effect of \( A_1 \) on \( W_2 \) through \( W_1 \) at a reference level \( W_1(a_1) \). This yields the counterfactual \( \mathbf{1} \), which is identified as

\[
\sum_p p(W_2 | f_{A_2}(W_1, W_0), W, f_{A_1}(W_0), a_{1a_1}, W_0)p(W_1(a_1), W_0)p(W_0).
\]

Generalizations of the example in Fig. 1(b) are the most relevant in practice, as their causal structure corresponds to longitudinal observational studies, of the kind considered in [Robins 1986], and many other papers. However, we illustrate complications that may arise in identifyability of responses to path-specific policies with the following, more complex, example in Fig. 2 (a). Here, the distribution \( p(W_2; \{ f_{A_1}(W_0) \}_{A_1}, a_{(A_1,M_1)}) \) is identified via:

\[
\sum_{W_0, A_1, M_1, W_1} \left[ \sum_{W_0, A_1} p(W_1 | M_1, f_{A_1}(W_0), W_0) [p(M_1 | a_1, W_0)p(W_0)] \right] \times
\]

with the detailed derivation given in the Appendix. In this example, the graph entails an identifying formula that does not resemble a factorization where a conditional distribution of the treatment \( A_1 \) is replaced by a policy \( f_{A_1} \), such as [7]. Instead, due to the presence of a bidirected arrow connecting \( A_1 \) and \( W_2 \), the identifying functional resembles the functional arising from the front-door criterion [Pearl 2009].

On Completeness

The ID algorithm phrased in terms of \( \mathbf{8} \) via the fixing operator is known to be complete for non-parametric identification [Huang and Valtorta 2006; Shpitser and Pearl 2006]. Completeness here means that failure of identification means no other method is able to yield identification under the same model. A similar result does not, to the authors’ knowledge, exist for the identification algorithm for responses to policies in [Tian 2008], and rephrased as \( \mathbf{10} \).

Here we give an argument for completeness of algorithms corresponding to \( \mathbf{10} \), and \( \mathbf{13} \) under the assumption that not only is the causal model non-parametric, but the set of policies \( f_{A} \) consists of arbitrary functions. In other words, to show non-identifyability it will suffice to exhibit two unrestricted elements in the causal model, and any set of functions \( f_{A} \) such that the two elements agree on \( p(V) \) but disagree on \( p(Y(f_{A})) \). If the set of policies of interest \( f_{A} \) is restricted, or alternatively if the causal model has parametric restrictions, completeness may no longer hold. To see this, consider Fig. 3 (c) where we pick functions \( f_{A}(W) \) that sets \( A \) to \( a \) for the purposes of \( (AY)_{\alpha} \), and \( f_{A}(W) \) that sets \( A \) to \( a' \) for the purposes of \( (AM)_{\bar{\alpha}} \). In other words, both functions ignore \( W \). In this restricted class, \( p(Y((f_{A}(AY)_{\alpha}), (f_{A}(AM)_{\bar{\alpha}})) \) is in fact identifiable, since this distribution is equal to \( p(Y(a, M(a'))) \), which was shown to be identifiable in the previous section. We defer all proofs to the Appendix.

**Lemma 1** Assume \( p_1(Y(a) | W) \neq p_2(Y(a) | W) \), and a fixed \( p_1(W), p_2(W) \) (either equal or not). Then there exists \( \hat{p}(A | W) \) such that \( \sum_{w} p_1(A | W)p(a | W)p(w) \neq \sum_{w} p_2(A | W)p(a | W)p(w) \).

**Theorem 3** Assume \( p(Y(a) | Y \in Y^*) \) is not identifiable, where \( Y^* = a_{\alpha_{\bar{\alpha}}} \). Then \( p(Y(f_{A}) | Y \in Y) \) is not identifiable.

**Lemma 2** Assume a fixed \( p_1(W), p_2(W) \) (equal or not), and \( p_1(Y_1(a_1, a_2), Y_2(a_1, a_2)) \neq p_2(Y_1(a_1, a_2), Y_2(a_1, a_2)) \). Then there exists \( \hat{p}(A_1 | W), \hat{p}(A_2 | W) \) such that

\[
\sum_{w, a_1, a_2} p_1(Y_1(a_1, a_2), Y_2(a_1, a_2) | w) \hat{p}(a_1 | w) \hat{p}(a_2 | w)p(w) \neq \sum_{w, a_1, a_2} p_2(Y_1(a_1, a_2), Y_2(a_1, a_2) | w) \hat{p}(a_1 | w) \hat{p}(a_2 | w)p(w).
\]

**Theorem 4** Let \( Y^* = a_{\alpha_{\bar{\alpha}}} \). Then if \( p(Y^*(a_\alpha)) \) is not identifiable, \( p(Y((f_{A}), \alpha_{\bar{\alpha}})) \) is not identifiable.

Finding Optimal Total Effect Policies

Generally, having defined counterfactual responses to policies, the goal is to find an optimal policy. Optimality may
be quantified in a number of ways, but a common approach is maximizing expected counterfactual outcome under a policy, that is finding \( \arg \max_{\pi} \mathbb{E}[Y(f_{\pi}(W))] \).

Consider a simple example in Fig. 1(a), where we wish to learn the optimal policy \( f_A(W) \), by which we mean a policy that maximizes \( \mathbb{E}[Y(f_{\pi}(W))] \). Assume we happen to know the correct parametric specification for \( Q(A, W; \gamma) = \mathbb{E}[Y(A) \mid W; \gamma] = \mathbb{E}[Y[A, W; \gamma]] \) (this type of specification is sometimes known as a Q-function in the reinforcement learning literature). Then for a binary treatment \( A \) (with values 0, 1), it is fairly easy to show that for any given \( w \in \mathcal{X}_W \), the optimal policy has the form \( I(Q(1, w; \gamma) > Q(0, w; \gamma)) \), where \( I(.) \) is the indicator function.

Consider a general version of Fig. 1(b), with a vector of baseline factors \( W_0 \), a set of treatments \( A_t \), and outcomes \( W_i \) for \( i = 1, \ldots, k \), and a temporal order on variables \( W_0, A_1, W_1, \ldots, A_k, W_k \), where all variables earlier in the order are assumed to causally influence variables later in the order, and an unobserved common parent \( U \) of \( W_0, \ldots, W_k \). Given \( A_t \), denote \( \mathcal{A}_t \) to be all variables earlier in the ordering than \( A_t \), similarly for \( W_i \) and \( \mathcal{W}_i \). Finally, denote by \( \mathcal{A}_t^{<} \) to be all variables earlier in the ordering than \( A_t \) except \( A_j \), similarly for \( \mathcal{W}_i^{<} \). Assume we are interested in choosing a set of policies \( f_A = \{ f_A(\mathcal{A}_i) \mid i = 1, \ldots, k \} \) which maximize \( \mathbb{E}[W_k(f_A)] \).

It’s well-known that this counterfactual mean is identified, under the model we specified, via a version of the e-computation algorithm (Robins 1986), a special case of (10):

\[
\sum_{k=1}^{\infty} \mathbb{E}[W_k \mid W_0, \ldots, W_{k-1}, f_{A_1}(W_0), \ldots, f_{A_k}(\mathcal{A}_k)] \times \prod_{i=1}^{k} p(W_i \mid W_0, \ldots, W_{i-1}, f_{A_1}(W_0), \ldots, f_{A_i}(\mathcal{A}_i)). \tag{13}
\]

If we knew the correct specification of all these models, we could obtain the optimal \( f_{A_k} \) as \( \mathbb{I}[\mathbb{E}[W_k \mid A_k = 1, \mathcal{A}_k] > \mathbb{E}[W_k \mid A_k = 0, \mathcal{A}_k]] \), and the optimal \( f_{A_t}^{*} \) as

\[
\mathbb{I}[\mathbb{E}[W_k(f_{A_1}^{*}, \ldots, f_{A_{t-1}}^{*}, A_t = 1) \mid \mathcal{A}_t] > \mathbb{E}[W_k(f_{A_1}^{*}, \ldots, f_{A_{t-1}}^{*}, A_t = 0) \mid \mathcal{A}_t]] \tag{14}
\]

by an appropriate modification of (13). This approach is known as dynamic programming or backwards induction.

**Outcome Weighted Learning**

If models in (13) are not known precisely, but their parametric form is known, they may be estimated from data via usual maximum likelihood methods, and resulting estimates used to find the optimal policy given data. If we are uncertain whether these models are correctly specified, we are naturally no longer guaranteed to learn optimal policies directly in this way. In addition even under a correctly specified model, evaluating (13) may be computationally demanding, as it involves integrating over \( W_1, \ldots, W_{k-1} \).

A number of alternative strategies for finding policies where the optimal policy is not easily available in closed form have been considered in the literature, including grid search, and value search within a restricted class of policies. In this paper, we consider outcome weighted learning (Chen, Zeng, and Kosorok 2016), which translates the problem of picking optimal policies into a weighted classification problem in machine learning.

The key idea is if we had any method for learning \( \mathbb{E}[W_k(f_{A_1}, \ldots, f_{A_{t-1}}, A_t) \mid \mathcal{A}_t] \) for any \( A_t \), the task for finding \( f_{A_t}^{*} \), assuming \( f_{A_1}^{*}, \ldots, f_{A_{t-1}}^{*} \) were already found recursively, reduces to training a classifier mapping features \( \mathcal{A}_t \) to a class label \( A_t^{*} \) (either 0 or 1). In typical binary classification problems, training a classifier entails minimizing the 0-1 loss, where a correct classification is not penalized, while an incorrect classification is penalized by 1. In our case, we solve a sequence of recursive classification problems with a weighted 0-1 loss. In the base case, choosing \( A_t^{*} \) correctly yields no penalty, while choosing \( A_t^{*} \) incorrectly yields the penalty

\[
\mathbb{E}[W_k(1 - A_t^{*}) \mid \mathcal{A}_t].
\]

A number of approaches have been developing for minimizing these types of non-convex losses. While any choice that specifies some inductive bias may imply the true optimal policy is no longer within the considered class, a flexible classification strategy minimizes this risk in practice. In our simulations, we used support vector machines (SVMs) (Cortes and Vapnik 1995), because of their flexibility and relative simplicity. Note that the choice of classifier implicitly defines the restricted set of policies where we seek to find the optimum. In the case of SVMs, this choice is all policies defined by a hyperplane through a high dimensional space defined by a kernel function. We now consider how outcome weighted learning and dynamic programming translate to optimizing path-specific policies.

**Finding Optimal Path-Specific Effect Policies**

Consider the generalization of Fig. 1(b) to the longitudinal setting with mediators, shown (for two time points) in Fig. 2(c). This causal model corresponds to the setting described in detail in (Miles et al. 2017), representing an observational longitudinal study of HIV patients. Here, \( W_0 \) represents the baseline variables of a patient, \( A_1, A_2 \) represent treatment assignments, which were chosen based on observed treatment history according to physician’s best judgement, \( W_1, W_2 \) are intermediate and final outcomes (such as CD4 count or viral failure), and \( M_1, M_2 \) are measures of patient adherence to their treatment regimen. We are interested in finding policies \( f_{A_1}(W_0), f_{A_2}(W_0, W_1, A_1, M_1) \) that optimize the effect of \( A_1, A_2 \) on \( W_2 \) that is either direct or via intermediate outcomes, but not via adherence, and where adherence is kept to that of a reference treatment \( a_1, a_2 \). Specifically, we are interesting in choosing \( f_{A_1}, f_{A_2} \) to optimize the following counterfactual expectation:

\[
\mathbb{E} \left[ W_2 \left( W_0, f_{A_1}(W_0), M_1(a_1), W_1(f_{A_1}(W_0), M_1(a_1)), M_2(a_1, a_2), W_3(f_{A_1}(W_0), M_1(a_1)), M_2(a_1) \right) \right].
\]
which is identified as
\[
\sum_{W_2} E[W_2|W_0, W_1, M_1, M_2, f_{A_1}(W_0), f_{A_2}(W_0, f_{A_1}(W_0)), M_1, W_1] \times p(W_0)p(M_1|a_1, W_0)p(W_1|W_0, f_{A_1}(W_0), M_1)p(M_2|W_2, W_1, a_2)
\]  
(15)

More generally for \(k\) time points, we wish to learn policies \(f_{A_1}, \ldots, f_{A_k}\) that optimize
\[
E[W_k\left(\left\{f_{A_1}(A_1, W_1), \ldots, f_{A_k}(A_k, W_k)\right\}\right)],
\]
which is identified by the appropriate generalization of (15):
\[
\sum_{W_k} E[W_k|W_0, \ldots, W_{k-1}, M_1, \ldots, M_k, f_{A_1}(W_0), \ldots, f_{A_k}(\mathcal{A}_k)] \times
\left(\prod_{i=1}^{k-1} p(W_i|W_0, \ldots, W_{i-1}, f_{A_1}(W_0), \ldots, f_{A_i}(\mathcal{A}_i))\right) \times
\left(\prod_{i=1}^{k} p(M_i|W_0, \ldots, W_{i-1}, a_1, \ldots, a_i)\right)
\]  
(16)

The dynamic programming approach to learning optimal policies within a restricted class given by our chosen classification method proceeds as follows. We solve a sequence of recursive classification problems with a weighted 0-1 loss. In the base case, choosing \(A_2^*\) correctly yields no penalty, while choosing \(A_2^*\) incorrectly yields the penalty
\[
\sum_{M_2} \{E[W_k|A_2^*, \mathcal{A}_k] - E[W_k|1 - A_2^*, \mathcal{A}_k]\} p(M_2|a_2, \mathcal{A}_k).
\]

Assuming \(f_{A_1}^*, \ldots, f_{A_{k-1}}^*\) were already selected via classifiers minimizing appropriate loss, choosing \(A_2^*\) correctly yields no penalty, while choosing \(A_2^*\) incorrectly yields a penalty \(E[\mathcal{R}(A_2^*) - \mathcal{R}(1 - A_2^*) | \mathcal{A}_2]\), where \(\mathcal{R}(A_2)\) is
\[
W_k\left[\left\{f_{A_{k-1}}^*\right\}(A_{k-1}, W_{k-1}, \ldots, (A_{k-1} + W_{k-1})) \cdots \left\{f_{A_k}^*\right\}(A_k, W_k)\right],
\]
and identified by the appropriate modification of (16). In the subsequent section, we report the results of a simulation study illustrating this dynamic programming approach with an SVM classifier, for the two time point case \((k = 2)\).

### A Simulation Study

We demonstrated our method via a simulation study for the model given in Fig. 2(c). We used a 5-variate normal for \(W_0\), logistic regression models for binary \(A_1, M_1, A_2, M_2\), and linear regressions for continuous-valued \(W_2\) and \(W_1\) (the latter was a 6-variable vector). We will make our simulation code available upon request. We used softmargin SVMs which allowed row weights, as implemented in the libsvm library, to optimize the weighted 0-1 loss, as defined in the previous section, using an appropriate hinge loss convex surrogate.

Table 1 summarizes the performance of the SVM classifiers in Stage 2 and Stage 1, respectively. We report the accuracy of the classifiers trained using both linear and polynomial (poly) kernels of various degrees \(d\). Table 2 summarizes the average weighted 0-1 loss incurred during policy evaluation in both stages. As expected, it is straightforward to optimize the second stage policy, since significant information is available at that point via the vector \(\mathcal{A}_2\). At stage 1, only \(W_0\) is available, which complicates deriving an optimal decision surface. In addition, while flexible decision surfaces are helpful at the second stage, they appear to be counterproductive for the first stage. We leave a detailed investigation of weighted classification algorithms for this problem to future work.

| Stage 2 | Stage 1 training accuracy (%) |
|---------|-------------------------------|
| Linear | Poly (d=3) | Poly (d=5) | Poly (d=7) |
| Linear | 78.69 | 83.47 | 75.56 | 67.08 | 67.67 |
| Poly (d=3) | 93.53 | 82.21 | 74.15 | 64.61 | 65.11 |
| Poly (d=5) | 99.18 | 82.10 | 73.75 | 64.76 | 64.87 |
| Poly (d=7) | 99.30 | 82.59 | 74.48 | 65.15 | 66.19 |

| Stage 2 average weighted 0-1 loss | Stage 1 average weighted 0-1 loss (3 sig.figures) |
|-----------------------------------|-----------------------------------------------|
| Linear | Poly (d=3) | Poly (d=5) | Poly (d=7) |
| Linear | 3.762 | 145 | 252 | 508 | 491 |
| Poly (d=3) | 0.302 | 148 | 257 | 520 | 508 |
| Poly (d=5) | 0.007 | 152 | 261 | 532 | 513 |
| Poly (d=7) | 0.022 | 143 | 248 | 532 | 498 |

### Conclusion

In this paper, we defined counterfactual responses to policies that set treatment value in such a way that they affect outcomes with respect to certain causal pathways only. Such counterfactuals arise when we wish to personalize only some portion of the causal effect of the treatment, while keeping other portions to some reference values. An example might be optimizing the chemical effect of a drug, while keeping drug adherence to a reference value.

We gave a general algorithm for identifying these responses from data, which generalizes similar algorithms due to Tian (2008) and Shpitser (2013) for dynamic treatment regimes, and path-specific effects, respectively, shown that given an unrestricted class of policies the algorithm is, in some sense, complete, and demonstrated how path-specific policies may be optimized using outcome weighted learning (Chen, Zeng, and Kosorok 2016).
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Appendix

Example Derivation For An Identifiable Path-Specific Policy

We seek to identify the distribution \( p(W_2 | (f_{A_1}(W_0))_{A_1=1}^{M_1=1} g_{A_1(M_1)}) \) in Fig. 2 (b). Thus, we have three terms, a term \( \phi(W_1, A_1, M_1, W_2) (p; G) \) for \( W_2 \), a term \( \phi(W_0, A_1, M_1, W_2) (p; G) \) for \( W_1 \), and a term \( \phi(A_1, W_1, W_2) (p; G) \) for \( \{W_0, M_1\} \).

We have

\[
\sum_{W_0, A_1, M_1, W_2} p(W_2 | W_1, A_1, M_1, W_0) p(A_1) = p(W_0 | (f_{A_1}(W_0))_{A_1=1}^{M_1=1} g_{A_1(M_1)})
\]

where \( G^{(a)}, G^{(b)}, G^{(c)} \) are CADMGs in Figs. 3 (a), (b), and (c), respectively. Similarly, \( \phi(W_0, A_1, M_1, W_2) (p; G) \) is equal to

\[
\sum_{W_0, A_1, M_1, W_2} p(W_2 | W_1, A_1, M_1, W_0) p(A_1) = p(W_0 | (f_{A_1}(W_0))_{A_1=1}^{M_1=1} g_{A_1(M_1)})
\]

Finally,

\[
\sum_{W_0, A_1, M_1, W_2} p(W_2 | W_1, A_1, M_1, W_0) p(A_1) = p(W_0 | (f_{A_1}(W_0))_{A_1=1}^{M_1=1} g_{A_1(M_1)})
\]

where \( G^{(a)}, G^{(b)}, G^{(c)} \) are CADMGs in Figs. 3 (a), (b), and (c), respectively.

Note that whenever the fixing operation for a kernel \( q_{V}(V | W) \) that fixes \( V \in \mathcal{V} \) is such that \( \mathcal{V} \neq \mathcal{V} \), the resulting kernel can be viewed as \( q_{V}(V | \mathcal{V}) \mathcal{V} \cup \mathcal{V} \) for \( \sum_{V} q_{V}(V | W) \). We now combine these terms, evaluating \( \phi(A_1, W_1, W_2) (p; G) \), as appropriate, yielding the following expression for \( p(W_2 | (f_{A_1}(W_0))_{A_1=1}^{M_1=1}, W_0) \):

\[
\sum_{W_0, A_1, M_1, W_2} p(W_1 | M_1, f_{A_1}(W_0), W_0) p(M_1 | A_1, W_0) p(A_1) p(W_0) = p(W_2 | (f_{A_1}(W_0))_{A_1=1}^{M_1=1}, W_0) \times \sum_{W_0, A_1, M_1, W_2} p(W_2 | W_1, M_1, A_1, W_0) p(A_1, W_0) \]
Lemma 1 Assume $p_1(Y(a) \mid w) \neq p_2(Y(a) \mid w)$, and a fixed $p_1(W), p_2(W)$ (either equal or not). Then there exists $\tilde{p}(A \mid W)$ such that $
abla_{w,a} p_1(Y(a) \mid w)\tilde{p}(a \mid w)p_1(w) \neq \nabla_{w,a} p_2(Y(a) \mid w)\tilde{p}(a \mid w)p_2(w)$.

Proof: Since $\tilde{p}_1(Y)$ and $\tilde{p}_2(Y)$ are weighted averages, to assure their inequality it suffices to pick $\tilde{p}(A \mid W)$ in such a way that $\tilde{p}(a \mid w)p_1(w)$ and $\tilde{p}(a \mid w)p_2(w)$ are both sufficiently close to 1.

Theorem 3 Assume $p\{\{Y(a) \mid Y \in Y^*\} \mid a \in A_0\}$ is not identifiable, where $Y^* = \text{an}_{\tilde{g}_A}(Y) \setminus A$. Then $p\{\{Y(f_A) \mid Y \in Y^*\} \mid A \in A_0\}$ is not identifiable.

Proof: Order variables in $Y^*$ topologically as $Y_1, \ldots, Y_k$ with $Y_j$ being the set of variables in $Y^*$ earlier in the ordering than $Y_j$. Pick the earlier $Y_j$ in the ordering such that $p(Y_j(a) \mid Y_j(a))$ is not identified. Such a variable is guaranteed to exist, since $p(Y(a) \mid Y \in Y^*))$ is not identifiable. If $Y_j = \emptyset$, our conclusion is trivial since $p(Y_j(a)) = p(Y(f_A))$ is not identifiable. Otherwise, by a simple extension of Lemma 2, $p\{\{Y(f_A) \mid Y \in Y^*\} \mid A \in A_0\}$ is not identified, and thus, neither is $p\{\{Y(f_A) \mid Y \in Y^*\} \mid A \in A_0\}$.

Lemma 2 Assume a fixed $p_1(W), p_2(W)$ (equal or not), and $p_1(Y_1(a_1, a_2), Y_2(a_1, a_2) \mid w) \neq p_2(Y_1(a_1, a_2), Y_2(a_1, a_2) \mid w)$. Then there exists $\tilde{p}_1(A_1 \mid W), \tilde{p}_2(A_2 \mid W)$ such that

$$\nabla_{w,a_1, a_2} \sum_{p_1(Y_1(a_1, a_2), Y_2(a_1, a_2) \mid w)\tilde{p}(a_1|w)p(a_2|w)p(w) \neq \nabla_{w,a_1, a_2} \sum_{p_2(Y_1(a_1, a_2), Y_2(a_1, a_2) \mid w)\tilde{p}(a_1|w)p(a_2|w)p(w).$$

Proof: Since $\tilde{p}_1(Y_1, Y_2)$ and $\tilde{p}_2(Y_1, Y_2)$ are weighted averages, to assure their inequality it suffices to pick $\tilde{p}(A_1 \mid W), \tilde{p}(A_2 \mid W)$ such that $\tilde{p}(a_1 \mid w)p(a_2 \mid w)\tilde{p}(w) \neq \tilde{p}(a_1 \mid w)p(a_2 \mid w)\tilde{p}(w)$ and $\tilde{p}(a_1 \mid w)p(a_2 \mid w)\tilde{p}(w)$ are both sufficiently close to 1.

Theorem 4 Assume $p\{Y^*(a_0) \mid a_0 \in A_0\}$ is not identifiable, and let $Y^* = \text{an}_{\tilde{g}_A}(Y) \setminus A_0$. Then $p\{Y^*(f_A) \mid A \in A_0\}$ is not identifiable.

Proof: Order variables in $Y^*$ topologically as $Y_1, \ldots, Y_k$ with $Y_j$ being the set of variables in $Y^*$ earlier in the ordering than $Y_j$. Pick the earlier $Y_j$ in the ordering such that $p(Y_j(a) \mid Y_j(a)) = p(Y_j(f_A))$ is not identifiable. Such a variable is guaranteed to exist, since $p\{Y^*(a_0) \mid A \in A_0\}$ is not identifiable. If $Y_j = \emptyset$, our conclusion is trivial since $p(Y_j(a_0)) = p(Y_j(f_A))$ is not identifiable. Otherwise, by a simple extension of Lemma 2, $p\{Y^*(f_A) \mid A \in A_0\}$ is not identified, and thus, neither is $p\{Y^*(f_A) \mid A \in A_0\}$.