Adjustment Criteria for Generalizing Experimental Findings

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Abstract

Generalizing causal effects from a controlled experiment to settings beyond the particular study population is arguably one of the central tasks found in empirical circles. While a proper design and careful execution of the experiment would support, under mild conditions, the validity of inferences about the population in which the experiment was conducted, two challenges make the extrapolation step to different populations somewhat involved, namely, transportability and sampling selection bias. The former is concerned with disparities in the distributions and causal mechanisms between the domain (i.e., settings, population, environment) where the experiment is conducted and where the inferences are intended; the latter with distortions in the sample's proportions due to preferential selection of units into the study. In this paper, we investigate the assumptions and machinery necessary for using *covariate adjustment* to correct for the biases generated by both of these problems, and generalize experimental data to infer causal effects in a new domain. We derive complete graphical conditions to determine if a set of covariates is admissible for adjustment in this new setting. Building on the graphical characterization, we develop an efficient algorithm that enumerates all possible admissible sets with poly-time delay guarantee; this can be useful for when some variables are preferred over the others due to different costs or amenability to measurement.

1. Introduction

Scientific inferences in data-driven disciplines entail some understanding of the laws of nature and a web of cause and effect relationships. For instance, policy-makers aiming to improve the economical condition of a certain population need to understand how a tax increase would affect consumers' behavior and, in turn, economic activity; or, health scientists trying to develop a new treatment for prostate cancer would have to understand how their new drug interacts with the body and affects the cancer's progression (Pearl, 2000; Spirtes et al., 2001; Bareinboim and Pearl, 2016).

Controlled experimentation is one of the most pervasive methods to probe for such effects, deemed the "gold standard" for scientific research in empirical circles. The main idea is to generate a controlled environment where the behavior of an outcome variable can be observed under two regimes: one where a certain condition (e.g., drug A) is present and another where it isn't (placebo), under the *ceteris paribus* condition. If all other factors are held constant, intuitively, any difference in the outcome can be attributed to the action, i.e., to a causal relationship between them. In the medical sciences, this appears under the rubric of *Randomized Controlled Trials* (RCTs). In fact, the Food and Drug Administration (FDA) spends billions of dollars every year to support systematic, controlled, and large-scale experimentation (National Academy of Medicine, 2010).

Science is largely about generalization. Most experimental findings are intended to be generalized to a broader, or even different, *target domain* (in other words, population, setting, environment). In medicine, for instance, some of the most important pharmaceutical discoveries were first developed and tested using rats as subjects, while the goal was to use the results to treat humans. In psychology, college students are usually the subject of experimentation, so as to answer questions about human cognition, which, broadly speaking, include subjects with and without exposure to higher education. In many machine learning settings, agents are trained by performing actions in simulated environments, where the goal is to deploy these systems in other, maybe real, environment, which doesn't match the training ground. In all these settings, an extrapolation step from the causal distribution where the experiment was conducted to where the inference is intended is required. If the source distribution is such that its conclusions can be extrapolated to the target domain, the same is said to have *external validity*.

External validity has been considered one of the main re-

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search challenges by the current generation of data (empirical) scientists (Altman et al., 2001). In particular, we'll discuss two challenges that threaten external validity, namely, *transportability* and *sampling selection bias*.

Example 1. *Greenhouse et al., discussed the challenges of generalizability in the risk of suicidality among pediatric antidepressant users. On investigating the causal relationship between antidepressant use and the risk of suicide attempt, the FDA performed several RCTs, finding that youths receiving antidepressants (X) had approximately twice the amount of suicidal thoughts and behaviors (Y) compared to the control groups. These results led to a new policy and the issue of a strict warning in the drugs' label.*

Surprisingly, following the warning, reports suggested a decrease in the number of prescriptions and an increase in suicidal events in the corresponding age groups. Furthermore, several observational studies found a decrease in the risk of suicide in patients being treated with the same antidepressants, even after adjusting for access to mental health-care and other confounding factors. Some of the possible explanations for this discrepancy are:

- *Transportability: There is a mismatch between the study population and the general clinical population regarding ethnicity, race, and income (covariates named E).*
- *Sampling selection bias: FDA's studies sampled from a distinct population by excluding youths with elevated baseline risk for suicide (B) from their cohorts.*

The problem of extrapolating experimental findings across domains that differ both in their distributions and inherent causal characteristics (e.g., rats to humans) is usually called *transportability* (Bareinboim and Pearl, 2016). Special cases of transportability are found in the literature under different rubrics, including "lack of external validity" (Campbell and Stanley, 1963; Manski, 2007), "heterogeneity" (Höfler et al., 2010) and "meta-analysis" (Glass, 1976; Hedges and Olkin, 1985). Issues of transportability can be represented graphically in a causal diagram by adding a special variable in the form of a square, $\mathbf{T}$, which represents the unobserved disparity-generating factors. For instance, Fig. 1(a) represents the causal diagram of Example 1.

Sampling selection bias appears due to preferential exclusion of units from the sample. The data-gathering process will, therefore, reflect a distortion in the sample's proportions and, since the data is no longer a faithful representation of the underlying population, biased estimates will be produced regardless of the number of samples collected (even if the treatment is controlled). Different biases fall under the umbrella of sampling selection bias, including censoring, self-selection/volunteering and non-response (Hernán et al., 2004). Selection bias can be represented graphically through a special hollow node S, see Fig. 1(a). S can be seen as an indicator where $S{=}1$ if a unit is included in the sample, and $S{=}0$ otherwise (Bareinboim and Pearl, 2012).

Our goal here is to explicate the general principle that licenses extrapolation across settings when issues of transportability and selection bias are both present. We'll address this problem using the *covariate adjustment* technique
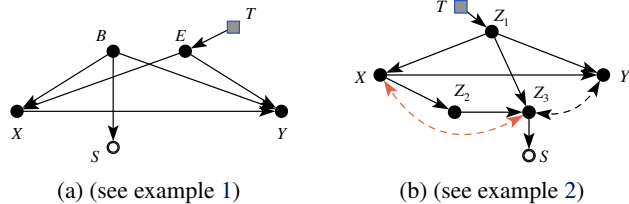

(a) (see example 1)   (b) (see example 2)

Figure 1. Selection diagrams with $\mathbf{T}$ and S nodes indicating differences between populations and the sampling selection mechanism.

(Pearl, 2000). Adjusting by a set of covariates is arguably the most widely used technique for causal effects estimation. Although usually used to control for confounding bias in observational data, it has recently been shown to be suitable to control for when selection bias is present as well (Correa and Bareinboim, 2017; Correa et al., 2018).

In this paper, we investigate the challenge of estimating causal effects when the input distribution is *experimental*, plagued with selection bias, and collected from a population that is structurally different than the one where the inferences are intended. We introduce a covariate adjustment formulation to overcome the challenges due to both transportability and selection bias. More specifically, our contributions are as follows:

1. **Generalization Adjustment Formula.** We introduce a covariate adjustment formulation that uses selection-biased experimental data from a source population and unbiased data from a target population, to produce an unbiased and valid estimand of a target causal effect.
2. **Graphical Characterization.** We prove a necessary and sufficient graphical condition for the admissibility of a set of covariates for this adjustment.
3. **Algorithmic Characterization.** We develop a complete algorithm that runs with polynomial delay and enumerates *all* sets suitable for adjustment according to the causal distribution and model, from which the researcher can pick with arbitrary criteria (e.g., low measurement cost, higher statistical precision).

2. Preliminaries and Related Work

Structural Causal Models. The systematic analysis of transportability and selection bias requires a formal language where the characterization of the underlying data-generating model can be encoded explicitly. We use the language of Structural Causal Models (SCMs) (Pearl, 2000). Formally, a SCM M is a 4-tuple $\langle \mathbf{U}, \mathbf{V}, F, P(\mathbf{u}) \rangle$, where $\mathbf{U}$ is a set of exogenous (latent) variables and $\mathbf{V}$ is a set of endogenous (measured) variables. F represents a collection of functions such that each variable $V_i \in \mathbf{V}$ is determined by $f_i \in F$, where f_i is a mapping from the respective domain of $U_i \cup Pa_i$ to V_i, $U_i \subseteq \mathbf{U}$, $Pa_i \subseteq \mathbf{V} \backslash \{V_i\}$, and the

entire set F forms a mapping from $\mathbf{U}$ to $\mathbf{V}$. Uncertainty is encoded through a probability distribution over the exogenous variables, $P(\mathbf{u})$. We will denote variables by capital letters, and their realized values by small letters. Sets of variables are denoted in bold.

Within the structural semantics, performing an action/intervention of setting $\mathbf{X}=\mathbf{x}$ is represented through the do-operator, $do(\mathbf{X}=\mathbf{x})$, which encodes the operation of replacing the original equation of $\mathbf{X}$ by the constant $\mathbf{x}$ inducing a submodel $M_{\mathbf{x}}$ and an experimental distribution $P_{\mathbf{x}}(\mathbf{v})$. An experiment can be thought of as physically replacing this equation by assigning a treatment, instead of letting it occur naturally. The causal effect of $\mathbf{X}$ on a set of variables $\mathbf{Y}$ is defined as $P_{\mathbf{x}}(\mathbf{y})$, that is, the distribution over $\mathbf{Y}$ in the intervened model $M_{\mathbf{x}}$. We will also use do-calculus to derive causal expressions from other causal quantities. For a detailed discussion of SCMs and do-calculus, we refer readers to (Pearl, 2000).

Every SCM M induces a causal diagram $\mathcal{G}$ represented as a directed acyclic graph where every variable $V_i \in \mathbf{V}$ is a vertex, and there exists a directed edge from every variable in Pa_i to V_i. Also, for every pair $V_i, V_j \in \mathbf{V}$ such that $U_i \cap U_j \neq \emptyset$, there exists a bidirected edge between V_i and V_j. A distribution is said to be *compatible* with $\mathcal{G}$ if it could be generated by an SCM that induces $\mathcal{G}$. We denote as $\mathcal{G}_{\overline{\mathbf{X}}\underline{\mathbf{Z}}}$ the graph resulting from removing all incoming edges to $\mathbf{X}$ and all outgoing edges from $\mathbf{Z}$ in $\mathcal{G}$. We use typical graph-theoretic terminology with the abbreviations $Pa(\mathbf{C}), De(\mathbf{C}), An(\mathbf{C})$, which stand for the union of $\mathbf{C}$ and its parents, descendants, and ancestors, respectively. The expression $(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})_{\mathcal{G}}$ denotes that $\mathbf{X}$ is independent of $\mathbf{Y}$ given $\mathbf{Z}$ in the graph $\mathcal{G}$ according to the d-separation criterion (Pearl, 2000) (subscript $\mathcal{G}$ may be omitted).

Transportability. Transportability theory is concerned with the conditions under which experimental data from one environment (π) can be used to establish a causal quantity in a different domain (π^*), while π and π^* are different but somewhat related domains, that is, assessing the causal effect of $\mathbf{X}$ on $\mathbf{Y}$ in the target domain (i.e., $P_{\mathbf{x}}^*(\mathbf{y})$) using measurements over a set of variables under experiments in a different environment (i.e., $P_{\mathbf{x}}(\mathbf{v})$). Different conditions were studied in the literature, for instance, in (Pearl and Bareinboim, 2011; Bareinboim et al., 2013; Bareinboim and Pearl, 2014). The first critical component of any transportability analysis is to formally express the assumptions about the differences between the domains of interest. In particular, the overlapping of two causal diagrams is used to express such difference, which is called *selection diagram*.

Definition 1 (Selection Diagram (Bareinboim and Pearl, 2014)). *Let $\langle M, M^* \rangle$ be a pair of SCMs relative to domains $\langle \pi, \pi^* \rangle$, sharing a diagram $\mathcal{G}$. $\langle M, M^* \rangle$ induces a selection diagram $\mathcal{D}$ consisting of $\mathcal{G}$ plus extra variables T_i with edge*

$T_i \to V_i$ *whenever there might exist a discrepancy $f_i \neq f_i^*$ or $P(U_i) \neq P^*(U_i)$ between M and M^*.*

We employ special indicator variables $\mathbf{T}$, drawn as squares to represent differences between the source and target populations, pointing to the variables that are affected by unobserved factors (causal mechanism or distribution) that are distinct across settings (e.g., see Fig. 1). As for selection bias, we use an indicator variable S (drawn round with double border) that is pointed to by every variable that affects the process by which a unit is included in the data.

Covariate Adjustment. Adjusting by a set of covariates is arguably the most common technique used to identify causal effects from an observational distribution $P(\mathbf{v})$, namely:

Definition 2 (Adjustment (Pearl, 2000)). *Given a causal diagram $\mathcal{G}$ over variables $\mathbf{V}$ and sets $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathbf{V}$, the set $\mathbf{Z}$ is called covariate adjustment for estimating the causal effect of $\mathbf{X}$ on $\mathbf{Y}$ (or, usually, just adjustment), if for every distribution $P(\mathbf{v})$ compatible with $\mathcal{G}$, it holds that*

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}} P(\mathbf{y} \mid \mathbf{x}, \mathbf{z}) P(\mathbf{z}). \tag{1}$$

In other words, the distribution $P(\mathbf{z})$ is used to re-weight the $\mathbf{z}$-specific distributions $P(\mathbf{y} \mid \mathbf{x}, \mathbf{z})$; for sets $\mathbf{Z}$ satisfying certain conditions (e.g., that would account for confounding bias), this mapping corresponds to the causal effect $P_{\mathbf{x}}(\mathbf{y})$.

Several criteria have been developed to determine whether a set $\mathbf{Z}$ is admissible for adjustment (Shpitser et al., 2010; Perković et al., 2015; 2018), including the celebrated "Backdoor criterion" (Pearl, 1993; 2000; Pearl and Paz, 2013), namely:

Definition 3 (Backdoor Criterion). *A set of variables $\mathbf{Z}$ satisfies the Backdoor Criterion relative to a pair of variables $(\mathbf{X}, \mathbf{Y})$ in a causal diagram $\mathcal{G}$ if:*

- *(i) No node in $\mathbf{Z}$ is a descendant of $\mathbf{X}$, and*
- *(ii) $\mathbf{Z}$ blocks every path between $\mathbf{X}$ and $\mathbf{Y}$ that contains an arrow into $\mathbf{X}$.*

Intuitively, this criterion identifies the variables that when conditioned on, block the "back-door" paths in the graph (those with arrows coming into $\mathbf{X}$ that carry spurious correlation), while keeping the causal paths unperturbed.

Covariate adjustment has been commonly used to control for confounding bias, nevertheless, some recent work demonstrated the validity of this technique to control for both confounding and selection biases (Correa and Bareinboim, 2017; Correa et al., 2018). As mentioned before, in the setting of this paper, the goal is not to control for confounding bias (solved by randomization), but for selection bias and transportability.

3. Generalizing Experimental Findings through Adjustment

A properly carried-out experiment will effectively control for confounding bias, and the resulting effect of the treatment $\mathbf{X}$ on the outcome $\mathbf{Y}$ will be valid for *the population represented in the experiment*, i.e., domain π. In most cases, as discussed earlier, the goal is not to make statements only about the units involved in the experiment, but to generalize the findings to a (usually much) larger and possibly different population (domain π^*). Invalid conclusions about the target population will be reached if the generalization biases are left uncontrolled. In other words, $P_{\mathbf{x}}(\mathbf{y})$, obtained in π may differ significantly from $P_{\mathbf{x}}^*(\mathbf{y})$, the corresponding causal quantity for the target population π^*.

Recall that we consider two challenges related to the generalizability of experimental findings, *transportability* and *selection bias*. For instance, consider the selection diagram in Fig. 1(a) corresponding to the situation described in Example 1. Background factors (E) affect both the use of antidepressants (X) and the formation of suicidal thoughts and behaviors (Y). The transportability node T pointing to E encodes the assumption that there is a discrepancy in the distributions of background factors between the population from the study and the target group of youths. Baseline risk for suicide (B), which affects both X and Y, also affects the inclusion of subjects into the randomized trials. This selective sampling process is encoded in the graph through the edge from B to the selection indicator S.

The aim here is to obtain the effect $P_x^*(y)$ in domain π^* (general population) from the data $P_x(y, b, e|S=1)$ coming from the domain π (controlled groups). In practice, experimental data from the source domain may be insufficient to identify the target effect. Still, it's not uncommon that non-experimental, unbiased data may be available in the target population, at least over some subset of the variables, $\mathbf{W}$ (i.e., $P^*(\mathbf{w})$). In these situations, the covariate adjustment technique provides a natural way of combining data from the two domains. For the model in Fig. 1(a), if $P^*(b, e)$ is available in the target population, then the target effect $P_x^*(y)$ can be computed by combining $P_x(y, b, e|S=1)$ with $P^*(b, e)$ in an adjustment expression, namely,

$$P_x^*(y) = \sum_{b,e} P_x(y \mid b, e, S = 1)P^*(b, e), \quad (2)$$

which will be proved later on in this section (Thm. 1).

A summary of this setting is provided in Fig. 2. In words, our task is: *Given qualitative causal assumptions in the form of a selection diagram $\mathcal{D}$, and given data $P_{\mathbf{x}}(\mathbf{v}|S = 1)$ in domain π and $P^*(\mathbf{w})$ in domain π^*, determine if $Q = P_{\mathbf{x}}^*(\mathbf{y})$ is estimable by adjustment on a set $\mathbf{Z} \subseteq \mathbf{W} \subset \mathbf{V}$. Specifically, we are looking for sufficient and necessary*
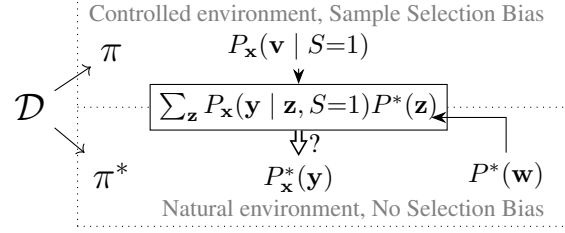

Figure 2. Summary of the task (see text for description).

conditions to determine if it holds that

$$P_{\mathbf{x}}^*(\mathbf{y}) = \sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}, S = 1)P^*(\mathbf{z}), \quad (3)$$

based on the assumptions encoded in a selection diagram $\mathcal{D}$. The right hand side of Eq. (3) contains two terms corresponding to different distributions – the first is the experimental one from the source (π) that may be affected by selection bias; the second is the distribution over a set of covariates measured in the target domain (π^*).

One may surmise that it's possible to get away by adjusting only for pre-treatment covariates, as customary in backdoor problems. However, adjusting for descendants of the treatment may be required to account for selection bias. To witness, consider the following scenario.

Example 2. *A randomized clinical trial is performed to measure the effect of a gene therapy (X) on a certain type of leukemia (Y). The selection diagram in Fig. 1(b) represents the corresponding causal model. One common side effect of X is the decrease in blood cells (Z_2), which in turn can affect the development of symptoms such as anemia and serious infections (Z_3). These symptoms are also caused by other background factors such as genetics, age, and family history (say Z_1). Outside the study, these factors affect the propensity of individuals choosing the treatment, and the outcome. There are also unmeasured factors affecting people using the treatment and developing the symptoms ($X \leftarrow\!-\!-\!-\!\rightarrow Z_3$) as well as latent variables that affect the symptoms and the outcome ($Z_3 \leftarrow\!-\!-\!-\!\rightarrow Y$).*

Due to the development of severe symptoms, subjects may drop from the study or be unable to attend the follow up consultations, resulting in their data being dropped from the study ($S = 0$). Considering only data from cases that did not drop out may lead to selection bias. Similarly, depending on the conditions of the study, the target population may differ in background factors compared to the units in the experiment. The possibility of such differences is accounted for by the transportability node T pointing to Z_1.

If one adjusts only for the set $\mathbf{Z} = \{Z_1\}$ to control for the transportability issue, there is still selection bias due to an active (open) path $S \leftarrow Z_3 \leftarrow\!-\!-\!-\!\rightarrow Y$.

It seems Z_3 is needed if selection bias is to be controlled as well. However, adjusting for some descendant of $\mathbf{X}$ may induce spurious correlation between $\mathbf{X}$ and $\mathbf{Y}$. In this case, conditioning on Z_3 induces a non-causal correlation between $\mathbf{X}$ and $\mathbf{Y}$, through, e.g., $X \leftarrow\!\dashrightarrow Z_3 \leftarrow\!\dashrightarrow Y$.

For convenience, when considering a set $\mathbf{Z}$ and treatment $\mathbf{X}$, let $\mathbf{Z_{nd}} = \mathbf{Z} \setminus De(\mathbf{X})$ denote the non-descendants of $\mathbf{X}$ in $\mathbf{Z}$, and $\mathbf{Z_d} = \mathbf{Z} \cap De(\mathbf{X})$ denote the descendants of $\mathbf{X}$. It turns out that conditioning on variables from $\mathbf{Z_d}$ that are independent of the outcome $\mathbf{Y}$ given $\mathbf{Z_{nd}}$ in the experimental distribution does not introduce spurious correlation into the adjustment. On the other hand, we need to pay special attention to those variables in $\mathbf{Z_d}$ d-connected with $\mathbf{Y}$ in the interventional graph $\mathcal{G}_{\overline{\mathbf{X}}}$ (given $\mathbf{X}$), that we will denote as

$$\mathbf{Z_p} = \left\{ Z \in \mathbf{Z_d} \mid (Z \not\perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z_{nd}}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}} \right\}. \quad (4)$$

We now introduce a graphical condition to characterize the sets $\mathbf{Z}$ that yield valid adjustments for $Q = P_x^*(\mathbf{y})$, i.e.:

Definition 4 (Generalization Adjustment (st-adjustment) Criterion (singleton treatment)). *Given a selection diagram $\mathcal{D}$ with transportability and selection bias variables, respectively, $\mathbf{T}$ and S, relative to domains π and π^*, a treatment X, and disjoint sets $\mathbf{Y}, \mathbf{Z} \subset \mathbf{V}$, the set $\mathbf{Z}$ is said to satisfy the st-adjustment criterion relative to $(X, \mathbf{Y})$ in $\mathcal{D}$ if*

(i) *The variables in $\mathbf{Z_p}$ are independent of the treatment given all other covariates, i.e., $(\mathbf{Z_p} \perp\!\!\!\perp X \mid \mathbf{Z} \setminus \mathbf{Z_p})$.*
(ii) *The outcome is independent of the transportability nodes and the selection bias mechanism given the covariates and X, i.e., $(\mathbf{Y} \perp\!\!\!\perp \mathbf{T}, S \mid \mathbf{Z}, X)_{\mathcal{D}_{\overline{X}}}$.*

Since the variables in $\mathbf{Z_p}$ are correlated with the outcome (by definition), the first condition requires them to be independent of the treatment X, given the other covariates, so as to prevent spurious correlation or the disturbance of causal paths when employing such variables. The second condition accounts for the generalizability issues – it requires the outcome to be independent of the transportability (T) and selection bias nodes (S) in the effect specific to the levels of the set $\mathbf{Z}$; the criterion owes its name, st-adjustment, to this condition. In contrast to similar criteria, no condition is required for controlling confounding due to the experimental nature of the data. To build intuition on reading the conditions, consider the following examples:

Example 3. *Recall the selection diagram in Fig. 1(a) and consider the set $\mathbf{Z} = \{B, E\}$. It turns out that $\mathbf{Z_p} = \emptyset$ since neither B nor E are descendants of X, so the first condition is satisfied. For the second, one can immediately verify that $(Y \perp\!\!\!\perp T, S \mid B, E, X)_{\mathcal{D}_{\overline{X}}}$ holds.*

Example 4. *Consider the diagram in Fig. 1(b). For the set $\mathbf{Z} = \{Z_1\}$, condition (i) is trivially satisfied because $\mathbf{Z_p} = \emptyset$. However, there is an active path $S \leftarrow Z_3 \leftarrow\!\dashrightarrow Y$ that violates (ii). In fact, Z_3 needs to be included in $\mathbf{Z}$, but then*

$(Z_3 \not\perp\!\!\!\perp X \mid Z_1)$ *because of the directed path $X \to Z_2 \to Z_3$. We have to include Z_2 in $\mathbf{Z}$ to block this path, which leads to the same $\mathbf{Z_p}$, but now there is still a path $X \leftarrow\!\dashrightarrow Z_3$ that violates the first condition. It turns out, there is no set $\mathbf{Z}$ satisfying the criterion for this case. If the bidirected edge between X and Z_3 (shown in red color) was not present, $(Z_3 \perp\!\!\!\perp X \mid Z_1, Z_2)$ would hold and (as we will show next)*

$$P_x^*(y) = \sum_{z_1, z_2, z_3} P_x(y \mid z_1, z_2, z_3, S{=}1) P^*(z_1, z_2, z_3). \quad (5)$$

We show next that the st-adjustment criterion licenses, and it's also necessary for, the extrapolation of causal findings from a source to a target domain through covariate adjustment on a set $\mathbf{Z}$ in the context of singleton treatments.

Theorem 1 (st-adjustment (singleton treatment)). *Given a selection diagram $\mathcal{D}$, a singleton X, and disjoint sets $\mathbf{Y}$ and $\mathbf{Z}$, the causal effect $P_x^*(\mathbf{y})$ is given by*

$$P_x^*(\mathbf{y}) = \sum_{\mathbf{z}} P_x(\mathbf{y} \mid \mathbf{z}, S{=}1) P^*(\mathbf{z}) \quad (6)$$

if and only if $\mathbf{Z}$ satisfies the st-adjustment criterion relative to $(X, \mathbf{Y})$.

The proof for Thm. 1 will be given as a lemma (Lemma. 1) after stating a more general st-adjustment theorem (Thm. 3) in the next section. All proofs are provided in the appendix.

Example 5. *As discussed in Example 3, the set $\{B, E\}$ satisfies the st-adjustment criterion relative to (X, Y) in the diagram Fig. 1(a), which implies that $P_x^*(y)$ is given by Eq. (2), following Thm. 1. In words, the assumptions encoded in $\mathcal{D}$ license the extrapolation of the causal distribution – experiments on the effect of antidepressants on suicide risk carried out in RCTs (source) to a target population consisting of the general clinical population of youths with depression – combining the conditional effect segregated by each stratum of B, E (baseline risk for suicide and background factors), re-weighted by the probability of each level of those variables as observed in the target domain.*

Example 6. *For a case such as Fig. 1(b), where no set $\mathbf{Z}$ satisfies the criterion, Thm. 1 states that for any model consistent with the assumptions in $\mathcal{D}$, no adjustment in the form of Eq. (6) gives a correct estimation of the target effect.*

4. Adjusting for Multiple Treatments

Even though controlling for one treatment variable at a time may be sufficient in some applications, in practice, there are settings where multiple factors need to be tested concurrently. In this section, we address more challenging settings involving causal effects of multiple treatment variables. For example, in online marketing, experiments are used to test the effectiveness of a combination of variables

such as content position, media, and audience, on user interaction, clicks, or conversion. Due to cost and number of user participation required to carry out these experiments, it is desirable to be able to generalize them to alternative audiences and correct for sampling issues.

To handle multiple treatments, adjusting for the descendants of $\mathbf{X}$ may again induce spurious correlation between $\mathbf{X}$ and $\mathbf{Y}$. More attention is needed to the variables in $\mathbf{Z_p}$ (defined in Eq. (4)) and how they are related to the multiple treatments $\mathbf{X}$. Consider the two models in Fig. 3 and set $\mathbf{Z} = \{Z_1, Z_2, Z_3, Z_4\}$[1] leading to $\mathbf{Z_p} = \{Z_2, Z_4\}$. Note that $\mathbf{Z_p}$ is not independent of $\mathbf{X} = \{X_1, X_2\}$ given $\mathbf{Z} \backslash \mathbf{Z_p} = \{Z_1, Z_3\}$ in either one of the diagrams, hence condition (i) of Def. 4 fails in both cases. Even so, there is a subtle difference between the two models: while adjusting for $\mathbf{Z}$ is not valid in Fig. 3(a), it is guaranteed to yield $P_{\mathbf{x}}^*(y)$ in Fig. 3(b). To witness, note that $P_{\mathbf{x}}^*(y)$ can be derived as

$$P_{\mathbf{x}}^*(y)$$

$$= P_{\mathbf{x}}^*(y) \sum_{z_1} P^*(z_1) \tag{7}$$

$$= \sum_{z_1} P_{\mathbf{x}}^*(y|z_1) P^*(z_1) \tag{8}$$

$$= \sum_{z_1, z_2} P_{\mathbf{x}}^*(y|z_1, z_2) P_{\mathbf{x}}^*(z_2|z_1) P^*(z_1) \tag{9}$$

$$= \sum_{z_1, z_2} P_{\mathbf{x}}^*(y|z_1, z_2) P^*(z_1, z_2) \tag{10}$$

$$= \sum_{z_1, z_2, z_3} P_{\mathbf{x}}^*(y|z_1, z_2, z_3) P^*(z_1, z_2, z_3) \tag{11}$$

$$= \sum_{\mathbf{z}} P_{\mathbf{x}}^*(y|\mathbf{z}) P_{\mathbf{x}}^*(z_4|z_1, z_2, z_3) P^*(z_1, z_2, z_3) \tag{12}$$

$$= \sum_{\mathbf{z}} P_{\mathbf{x}}^*(y|\mathbf{z}) P^*(\mathbf{z}) \tag{13}$$

$$= \sum_{\mathbf{z}} P_{\mathbf{x}}(y|\mathbf{z}, S=1) P^*(\mathbf{z}) \tag{14}$$

In the derivation above, we first introduced Z_1 into the adjustment (Eq.(7)) using the fact that it was independent of Y given $\mathbf{X}$ in $\mathcal{D}_{\overline{\mathbf{X}}}$, hence it does not introduce any spurious correlation (8). Next, we added Z_2 by conditioning (9), and since X_2 has no effect on $\{Z_1, Z_2\}$, $P_{\mathbf{x}}(z_2 \mid z_1) = P_{x_1}(z_2 \mid z_1)$. Also, given Z_1, Z_2 is independent of X_1, so no spurious correlation is added (10). Similarly, Z_1, Z_3 is independent of Y given the already introduced $\{Z_1, Z_2\}$ (11). Finally, Z_4 is independent of $\{X_1, X_2\}$ given $\{Z_1, Z_2, Z_3\}$ (13). After both Z_2 and Z_4 have been adjusted for, the outcome is independent of the selection mechanism S, and the causal effect can be expressed in the form of the st-adjustment (14).

Remarkably, no other set $\mathbf{Z}$ is valid for adjustment in this model, and the steps described can only be performed in the given order. As a matter of fact, the reason why $\mathbf{Z}$ will not work for Fig. 3(a) is that in the last step, we have a distribution $P_{\mathbf{x}}(Z_4|Z_1, Z_2, Z_3)$ and since X_1 has a causal effect

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[1]The two selection diagrams do not have $\mathbf{T}$ nodes, meaning the populations are the same in source and target domains with only selection bias issue occurring.
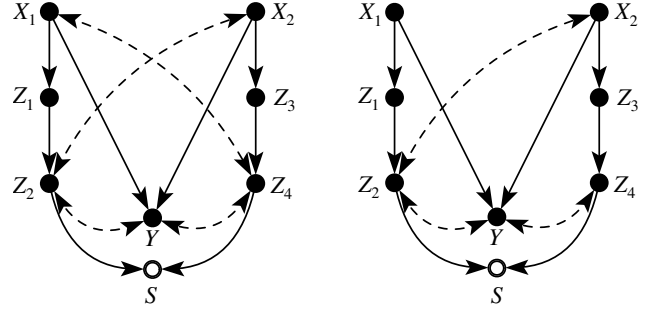
(a) No order over Z_1, Z_2, Z_3, Z_4 is suitable for adjustment.

(b) Order $Z_1 < Z_2 < Z_3 < Z_4$ is suitable for adjustment.

Figure 3. Models with multiple treatment variables $\mathbf{X} = \{X_1, X_2\}$.

over $\{Z_1, Z_2\}$, this conditional probability is not guaranteed to be equal to $P_{x_2}(Z_4|Z_1, Z_2, Z_3)$, if it was, we could employ $(Z_4 \perp\!\!\!\perp X_2 \mid Z_1, Z_2, Z_3)$ to finish the derivation. A symmetric problem with Z_2 arises If we change the order so that Z_4 is added before $\{Z_1, Z_2\}$.

To solve the generalization of experimental findings across domains, it turns out to be helpful to first deal with the generalization in the same domain. That is, what are the conditions for the causal effect $P_{\mathbf{x}}^*(\mathbf{y})$ to be computable in the form of Eq. (13). In practical applications, this may be an interesting question by itself. For example, consider settings where covariate-specific causal effects are measured, such as experiments where the units are separated in groups according to a combination of variables and studied independently. We could use adjustment in Eq. (13) to compute an average causal effect combining such experimental results. The following definition characterizes the adjustment sets that allow this extrapolation to take place.

Definition 5 (Experimental Adjustment (e-adjustment) Criterion). *Given a causal diagram $\mathcal{G}$ and disjoint $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subset \mathbf{V}$, $\mathbf{Z}$ is said to satisfy the e-adjustment criterion relative to $(\mathbf{X}, \mathbf{Y})$ in $\mathcal{G}$ if there exists an order over $\mathbf{Z}$: $Z_1 < Z_2 < \cdots$, such that $\mathbf{Z_{nd}} < \mathbf{Z_d}$, and for each $Z_i \in \mathbf{Z_d}$ we have*

$$\left(Z_i \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}^{\leq i-1}, \mathbf{X}\right)_{\mathcal{G}_{\overline{\mathbf{X}}}}, \text{ or} \tag{15}$$

$$\left(Z_i \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}^{\leq i-1}\right)_{\mathcal{G}_{\overline{\mathbf{x}\left(\mathbf{z}^{\leq i-1}\right)}}}, \tag{16}$$

where $\mathbf{Z}^{\leq i}$ denotes the set $\{Z_1, \ldots, Z_i\}$.

Note that although it may seem computationally expensive to determine the existence of an order over $\mathbf{Z}$ satisfying e-adjustment, we will show in Section 4.1 that this can in fact be verified efficiently. Also, if $\mathbf{Z_p}$ is empty, Def. 5 is trivially satisfied. The following theorem ties the definition of e-adjustment with the adjustment expression.

Theorem 2. *Given a causal diagram $\mathcal{G}$ and disjoint sets of variables $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subset \mathbf{V}$, the distribution $P_{\mathbf{x}}(\mathbf{y})$ is given by*

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}) P(\mathbf{z}) \qquad (17)$$

if and only if $\mathbf{Z}$ *satisfies the e-adjustment criterion relative to* $(\mathbf{X}, \mathbf{Y})$.

Leveraging e-adjustment, the definition below will characterize the adjustment sets that will allow generalizing experiments across domains with multiple treatments.

Definition 6 (st-adjustment criterion (multiple treatments)). *Given a selection diagram* $\mathcal{D}$ *with transportability and selection bias variables, respectively,* $\mathbf{T}$ *and* S, *relative to domains* π *and* π^*, *and disjoint sets* $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subset \mathbf{V}$, *the set* $\mathbf{Z}$ *is said to satisfy the st-adjustment criterion relative to* $(\mathbf{X}, \mathbf{Y})$ *in* $\mathcal{D}$ *if*

(i) $\mathbf{Z}$ *satisfies the e-adjustment criterion (Def. 5), and*
(ii) $(\mathbf{Y} \perp\!\!\!\perp \mathbf{T}, S \mid \mathbf{Z}, \mathbf{X})_{\mathcal{D}_{\overline{\mathbf{X}}}}$.

Theorem 3. *Given a selection diagram* $\mathcal{D}$ *and disjoint sets of variables* $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$, *the causal effect* $P_{\mathbf{x}}^*(\mathbf{y})$ *is given by*

$$P_{\mathbf{x}}^*(\mathbf{y}) = \sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}, S{=}1) P^*(\mathbf{z}) \qquad (18)$$

if and only if $\mathbf{Z}$ *satisfies the st-adjustment criterion relative to* $(\mathbf{X}, \mathbf{Y})$.

Example 7. *In Fig. 3(b), the set* $\mathbf{Z} = \{Z_1, Z_2, Z_3, Z_4\}$ *satisfies the st-adjustment criterion with order* $Z_1 < Z_2 < Z_3 < Z_4$. *Therefore* $P_{x_1,x_2}^*(y)$ *can be computed by Eq. (18) as explicitly derived in Eqs. (7)-(14).*

From Thm. 3, the st-adjustment criterion provides a complete characterization of valid adjustment sets. Next we discuss some special situations that may be of practical interests. First given Thm. 3, the following lemma provides a proof for the single treatment case in Thm. 1.

Lemma 1. *When* $\mathbf{X}$ *is a singleton, Definition. 6 is equivalent to Definition. 4.*

Consider adjusting for only pre-treatment variables, which is often what many practitioners are looking for due to the wide use of the Backdoor Criterion. In fact, if $\mathbf{Z}$ contains no descendants of $\mathbf{X}$ then it trivially satisfies the e-adjustment criterion. The result below immediately follows.

Proposition 1. *If* $\mathbf{Z} \cap De(\mathbf{X}){=}\emptyset$, *and* $(\mathbf{Y} \perp\!\!\!\perp \mathbf{T}, S | \mathbf{Z}, \mathbf{X})_{\mathcal{D}_{\overline{\mathbf{X}}}}$, *then* $\mathbf{Z}$ *satisfies the st-adjustment criterion w.r.t.* $(\mathbf{X}, \mathbf{Y})$.

Finally in situations where there is no selection bias problem (only transportability issues), we can safely restrict our attention to covariates that are non-descendants of the treatment $\mathbf{X}$, as shown in the following statement.

Theorem 4. *In the absence of selection bias (i.e.,* S *node disconnected from any other variable), if a set* $\mathbf{Z}$ *satisfies st-adjustment and* $\mathbf{Z} \cap De(\mathbf{X}) \neq \emptyset$, *then there exists* $\mathbf{Z}' \subseteq \mathbf{Z}$ *such that* $\mathbf{Z}' \cap De(\mathbf{X}) = \emptyset$ *and* $\mathbf{Z}'$ *satisfies st-adjustment.*
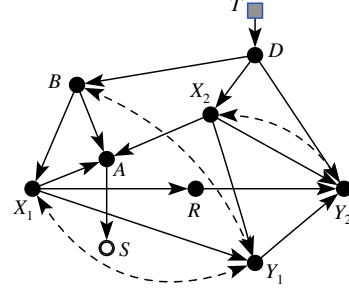

Figure 4. Example where the target effect is $P_{x_1,x_2}(y_1, y_2)$.

Algorithm 1 IsEAdmissible$(\mathcal{G}, \mathbf{X}, \mathbf{Y}, \mathbf{Z})$

Input: causal diagram $\mathcal{G}$, disjoint subsets $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathbf{V}$.
Output: **true** if $\mathbf{Z}$ satisfies e-adjustment, **false** otherwise.
1: **if** $\mathbf{Z} \cap De(\mathbf{X}) = \emptyset$ **then**
2:     **return true**
3: **end if**
4: **for each** $Z \in \mathbf{Z} \cap De(\mathbf{X})$ **do**
5:     **if** $(Z \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z} \setminus \{Z\}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$ **or**
      $(Z \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z} \setminus \{Z\})_{\mathcal{G}_{\overline{\mathbf{X}(\mathbf{Z} \setminus \{Z\})}}}$ **then**
6:       **return** *IsEAdmissible*$(\mathcal{G}, \mathbf{X}, \mathbf{Y}, \mathbf{Z} \setminus \{Z\})$
7:     **end if**
8: **end for**
9: **return false**

Example 8. *Consider the model in Fig. 4 where the target query is* $Q{=}P_{x_1,x_2}(y_1, y_2)$. *Thm. 3 licenses adjustment for the set* $\{D, B, A\}$. *We have that* D, B *are non-descendants of* $\mathbf{X}$, *an order* $D < B < A$ *such that* A *satisfies* $(A \perp\!\!\!\perp Y_1, Y_2 \mid D, B, X_1, X_2)_{\mathcal{D}_{\overline{X_1, X_2}}}$, *and* $(Y_1, Y_2 \perp\!\!\!\perp \mathbf{T}, S \mid D, B, A, X_1, X_2)_{\mathcal{D}_{\overline{X_1, X_2}}}$.

Another valid set is $\{B, D\}$, *which satisfies Proposition 1 since we have* $(Y_1, Y_2 \perp\!\!\!\perp \mathbf{T}, S \mid B, D, X_1, X_2)_{\mathcal{D}_{\overline{X_1, X_2}}}$.

4.1. Verifying e-adjustment Efficiently

Evaluating condition (i) of the st-adjustment (Def. 6), that is, the existence of an order over $\mathbf{Z}$ satisfying e-adjustment (Def. 5), may seem computationally hard. However, we will show in this section that in fact it can be verified efficiently, by establishing first some properties of e-adjustment.

Lemma 2. *A set* $\mathbf{Z}$ *satisfies e-adjustment if and only if there exists* $Z_i \in \mathbf{Z}$ *such that* Z_i *satisfies (15) or (16), and* $\mathbf{Z} \setminus \{Z_i\}$ *satisfies e-adjustment.*

Lemma 2 provides a recursive characterization of the order condition. Based on this result, we can verify the existence of an order by finding, at each step, any variable satisfying (15) or (16) in the set and removing it, as described next:

Lemma 3. *If* $\mathbf{Z}$ *satisfies e-adjustment, then for any* $Z_i \in \mathbf{Z}$ *satisfying (15) or (16), the set* $\mathbf{Z} \setminus \{Z_i\}$ *satisfies e-adjustment.*

Leveraging these results, we introduce an algorithm called *IsEAdmissible* (Alg. 1) that efficiently checks if **Z** satisfies the e-adjustment criterion.

Theorem 5. **Z** *satisfies e-adjustment (Def. 5) w.r.t.* (**X**,**Y**) *in* $\mathcal{G}$ *if and only if IsEAdmissible (Alg. 1) returns true.*

To illustrate how *IsEAdmissible* works, consider again the diagram in Fig. 3(b) with the set $\{Z_1, Z_2, Z_3, Z_4\}$. Line 5 will evaluate true only for Z_4, then the process reduces to verifying if $\{Z_1, Z_2, Z_3\}$ has an order. Next, the same condition will evaluate true for Z_3 reducing the problem to $\{Z_1, Z_2\}$. The process continues by removing Z_2 and after removing Z_1 the condition on line 1 is satisfied, so line 2 executes and returns true. In the case of Fig. 3(a) also with $\{Z_1, Z_2, Z_3, Z_4\}$, none of the variables in the set will satisfy the condition in line 5 and line 9 returns false.

Let n and m stand, respectively, for the number of variables and edges in the graph. Then *IsEAdmissible* performs at most $n^2 - n$ conditional independence tests. Constructing the graphs $\mathcal{G}_{\overline{\mathbf{X}}}$ and $\mathcal{G}_{\overline{\mathbf{X}(\mathbf{Z}\setminus\{Z\})}}$, as well as determining the descendants of **X** is achievable in $O(n + m)$ time. Testing an independence in the graph can be done in $O(n + m)$ (van der Zander et al., 2014). Therefore, the overall time complexity of *IsEAdmissible* is $O(n^2(n + m))$.

5. Enumerating Valid Sets for st-adjustment

Armed with a graphical condition to test if a set **Z** is valid for adjustment, the natural question is how to find sets satisfying the st-adjustment criterion systematically, as efficiently as possible. In practice, what variables are suitable for adjustment may be determined by factors such as feasibility, cost and effort required to measure such variables, as well as the quality and number of obtainable samples. In this paper, we assume data is available in the target domain over a set **W** of variables (see Fig. 2) and our task here is to list all sets $\mathbf{Z} \subseteq \mathbf{W}$ satisfying the st-adjustment.

The number of sets satisfying the st-adjustment is possibly exponential depending on the topology of the diagram and the target effect. In this sense, it is impossible to construct a procedure that runs in polynomial time since just outputting an exponential number of answers takes exponential time.

Under these conditions, the best guarantee we can provide is that the time to output the first valid set or indicate fail (if there is no satisfying set), and the time between consecutive outputs, is polynomial. Algorithms with this property are said to run with *polynomial delay* (Takata, 2010).

We have developed the algorithm *ListGAdjSets* (Alg. 2) which systematically lists valid adjustment sets, using the recursive subroutine *ListGAdjIR*. *ListGAdjIR* outputs all sets $\mathbf{Z}, \mathbf{I} \subseteq \mathbf{Z} \subseteq \mathbf{R}$, that satisfy the st-adjustment. At each step, it chooses a variable A and splits the problem

---

Algorithm 2 ListGAdjSets$(\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{W})$

Input: selection diagram $\mathcal{D}$ over variables **V** and indicators **T**, S; disjoint subsets of $\mathbf{X}, \mathbf{Y}, \mathbf{W} \subseteq \mathbf{V}$.
Output: list of subsets $\mathbf{Z}_1, \mathbf{Z}_2, \ldots, \mathbf{Z}_k \subseteq \mathbf{W}$ satisfying def. 6
1: $\mathbf{F} \leftarrow De\big((De(\mathbf{X})_{\mathcal{D}_{\overline{\mathbf{X}}}} \setminus \mathbf{X}) \cap An(\mathbf{Y})_{\mathcal{D}_{\overline{\mathbf{X}}}}\big)$
2: $\mathbf{R} \leftarrow \mathbf{W} \setminus (\mathbf{X} \cup \mathbf{Y} \cup \mathbf{F})$
3: *ListGAdjIR*$(\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{T}, S, \emptyset, \mathbf{R})$
function ListGAdjIR$(\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{I}, \mathbf{R})$
4: **if** *ExistsSep*$(\mathcal{D}_{\overline{\mathbf{X}}}, \mathbf{T} \cup \{S\}, \mathbf{Y}, \mathbf{I}, \mathbf{R})$ **then**
5:    **if** $\mathbf{I} = \mathbf{R}$ **then**
6:       **output** **I**
7:    **else**
8:       $A \leftarrow$ variable from $(\mathbf{R} \setminus \mathbf{I})$ such that
           $A \notin De(\mathbf{X})$, else
           $(A \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{I}, \mathbf{X})_{\mathcal{D}_{\overline{\mathbf{X}}}}$, else
           IsEAdmissible$(\mathcal{D}, \overline{\mathbf{X}}, \mathbf{Y}, \mathbf{I} \cup \{A\})$
9:       **if** A exists **then**
10:          *ListGAdjIR*$(\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{I} \cup \{A\}, \mathbf{R})$
11:          *ListGAdjIR*$(\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{I}, \mathbf{R} \setminus \{A\})$
12:       **else**
13:          *ListGAdjIR*$(\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{I}, \mathbf{I})$
14:       **end if**
15:    **end if**
16: **end if**

---

into two: listing sets containing A (line 10) and those with no A (line 11), while pruning branches yielding no valid sets (lines 4,13). This strategy is similar to those used in (Takata, 2010), (van der Zander et al., 2014), and (Correa et al., 2018) for listing separating sets in a graph. Here, it has been augmented to recognize the conditions in Def. 6 (See appendix. B for details).

Theorem 6. *ListGAdjSets on input* $\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{W}$, *lists all sets* $\mathbf{Z} \subseteq \mathbf{W}$ *satisfying st-adjustment relative to* $\mathbf{X}, \mathbf{Y}$ *in* $\mathcal{D}$, *with* $O(n^4(n + m))$ *delay.*

6. Conclusions

We study in this paper the problem of generalizing experimental findings across heterogeneous populations using the language of causal models. We introduced necessary and sufficient graphical conditions (Defs. 4,6) to decide whether biased experimental distributions can be used to infer a causal effect in a different population by adjusting for a set of covariates measured in that target population (Thms. 1,3). We further developed efficient algorithms to test whether a set of covariates is admissible for adjustment (Alg. 1) and to list all admissible sets, subject to the available measurements (Alg. 2). Experiments are, almost invariably, performed with the intent of being used outside the "laboratory" setting (i.e., the source population), so we hope that this work can be helpful for data scientists to understand, model, and solve the challenging issues of generalizability of experimental findings across disparate settings.

Acknowledgements

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A. Appendix: Proofs in Section 4

A.1. Proof for Theorem 2

Theorem 2. *Given a causal diagram $\mathcal{G}$ and disjoint sets of variables $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subset \mathbf{V}$, the distribution $P_{\mathbf{x}}(\mathbf{y})$ is given by*

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}) P(\mathbf{z}) \qquad (17)$$

if and only if $\mathbf{Z}$ satisfies the e-adjustment criterion relative to $(\mathbf{X}, \mathbf{Y})$.

Proof. (if) Let $Z_1 < \cdots < Z_m$ be such order, then we have:

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}^{\leq j}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq j}\right) P_{\mathbf{x}}\left(\mathbf{z}^{\leq j}\right) \qquad (19)$$

$$= \sum_{\mathbf{z}^{\leq j}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq j}\right) P\left(\mathbf{z}^{\leq j}\right), \qquad (20)$$

where eq. (19) follows from summing over the set $\mathbf{Z}^{\leq j}$, and eq. (20) from using rule 3 of do-calculus licensed by the fact that no element in $\mathbf{Z}^{\leq j}$ is a descendant of $\mathbf{X}$, hence the intervention on $\mathbf{X}$ can be removed from the second term.

Let $i \geq j$, we will show by induction on i that

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}^{\leq i}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i}\right) P\left(\mathbf{z}^{\leq i}\right). \qquad (21)$$

The base case, $i = j$, is given by eq. (20). Now suppose this is true for $i-1$, we will demonstrate it holds for i.

By inductive hypothesis:

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}^{\leq i-1}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i-1}\right) P\left(\mathbf{z}^{\leq i-1}\right) \qquad (22)$$

If (15) holds for Z_i:

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}^{\leq i-1}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i-1}\right) \sum_{z_i} P\left(\mathbf{z}^{\leq i}\right) \qquad (23)$$

$$= \sum_{\mathbf{z}^{\leq i-1}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i}\right) \sum_{z_i} P^*\left(\mathbf{z}^{\leq i}\right) \qquad (24)$$

$$= \sum_{\mathbf{z}^{\leq i}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i}\right) P\left(\mathbf{z}^{\leq i}\right) \qquad (25)$$

If (16) is the independence that holds:

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}^{\leq i-1}} \sum_{z_i} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i}\right) P_{\mathbf{x}}\left(z_i \mid \mathbf{z}^{\leq i}\right) P\left(\mathbf{z}^{\leq i-1}\right) \qquad (26)$$

$$= \sum_{\mathbf{z}^{\leq i}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i}\right) P\left(z_i \mid \mathbf{z}^{\leq i}\right) P\left(\mathbf{z}^{\leq i-1}\right) \qquad (27)$$

$$= \sum_{\mathbf{z}^{\leq i}} P_{\mathbf{x}}\left(\mathbf{y} \mid \mathbf{z}^{\leq i}\right) P\left(\mathbf{z}^{\leq i}\right) \qquad (28)$$

Whatever the case, eq. (21) is proven correct. For $i = m$ (all variables in $\mathbf{Z}$), the effect is equal to the expression given by e-adjustment.

(only if) To show the necessity of the criterion we will prove that whenever its conditions fail, we can find a model inducing $\mathcal{G}$ where the causal distribution $P_{\mathbf{x}}(\mathbf{y})$ is different than $\sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}) P(\mathbf{z})$.

Consider the right hand side of (17) the first factor in the sum is equal to

$$P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}) = \frac{P_{\mathbf{x}}(\mathbf{y}, \mathbf{z})}{P_{\mathbf{x}}(\mathbf{z})} \qquad (29)$$

$$= \frac{P_{\mathbf{x}}(\mathbf{y}, \mathbf{z_{nd}}) P_{\mathbf{x}}(\mathbf{z_0}|\mathbf{y}, \mathbf{z_{nd}}) P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0})}{P_{\mathbf{x}}(\mathbf{z_{nd}}) P_{\mathbf{x}}(\mathbf{z_0}|\mathbf{z_{nd}}) P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0})} \qquad (30)$$

Since $\mathbf{Z_0}$ is not in $\mathbf{Z_p}$, it must be the case that $(\mathbf{Z_0} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z_{nd}}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$, hence $P_{\mathbf{x}}(\mathbf{z_0}|\mathbf{y}, \mathbf{z_{nd}}) = P_{\mathbf{x}}(\mathbf{z_0}|\mathbf{z_{nd}})$ and that term can be simplied because it also appears in the denominator, leading to

$$= \frac{P_{\mathbf{x}}(\mathbf{y}, \mathbf{z_{nd}}) P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0})}{P_{\mathbf{x}}(\mathbf{z_{nd}}) P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0})}, \qquad (31)$$

and the second factor

$$P(\mathbf{z}) = P(\mathbf{z_{nd}}) P(\mathbf{z_0}|\mathbf{z_{nd}}) P(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0}). \qquad (32)$$

When replacing (31) and (32) in the right hand side of (17), the term $P(\mathbf{z_{nd}})$ in both expressions cancels out. Rearranging some factors yields:

$$\sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y}, \mathbf{z_{nd}}) P(\mathbf{z_0}|\mathbf{z_{nd}}) \frac{P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0})}{P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0})} P(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0}). \qquad (33)$$

Moving inwards the sums over $\mathbf{Z_p}$ and $\mathbf{Z_0}$, and letting

$$h(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0}) = \sum_{\mathbf{z_p}} \frac{P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0})}{P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0})} P(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0}), \qquad (34)$$

we have:

$$\sum_{\mathbf{z_{nd}}} P_{\mathbf{x}}(\mathbf{y}, \mathbf{z_{nd}}) \sum_{\mathbf{z_0}} P(\mathbf{z_0}|\mathbf{z_{nd}}) h(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0}). \qquad (35)$$

Now, let

$$g(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}) = \sum_{\mathbf{z_0}} P(\mathbf{z_0}|\mathbf{z_{nd}})h(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0}), \quad (36)$$

then the adjustment functional can be written as

$$\sum_{\mathbf{z_{nd}}} P_{\mathbf{x}}(\mathbf{y}, \mathbf{z_{nd}})g(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}). \quad (37)$$

The three terms in $h(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0})$:

$$P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0}), \quad (38)$$
$$P_{\mathbf{x}}(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0}), \text{ and} \quad (39)$$
$$P(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0}).; \quad (40)$$

are very similar and, by definition, we have that $(\mathbf{Z_p} \not\perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z_{nd}}, \mathbf{Z_0}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$ and we can find a model such that (38) is not equal to (39) for at least one $\mathbf{z_p}$. Not satisfying this condition also implies that (39) is not equal to (40), to prove this, suppose this is not the case, then: there exists an order over $\mathbf{Z_p}$, such that:

$$P(\mathbf{z_p}|\mathbf{z_{nd}}, \mathbf{z_0}) = \prod_{\{i|Z_i \in \mathbf{Z_p}\}} P\left(z_i|\mathbf{z_{nd}}, \mathbf{z_0}, \mathbf{z_{\bar{p}}^{\leq i-1}}\right) \quad (41)$$

$$= \prod_{\{i|Z_i \in \mathbf{Z_p}\}} P_{\mathbf{x}}\left(z_i|\mathbf{z_{nd}}, \mathbf{z_0}, \mathbf{z_{\bar{p}}^{\leq i-1}}\right) \quad (42)$$

$$= P_{\mathbf{x}}(\mathbf{z_p} \mid \mathbf{z_{nd}}, \mathbf{z_0}). \quad (43)$$

For each factor in (41) to be equal to each factor in (42) the independence $(Z_i \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z_{nd}}, \mathbf{Z_0}, \mathbf{Z_{\bar{p}}^{\leq i-1}})_{\mathcal{G}_{\overline{\mathbf{x}\left(\mathbf{z_{nd}}, \mathbf{z_0}, \mathbf{z_{\bar{p}}^{\leq i-1}}\right)}}}$ must hold. In this case we can construct an order over $\mathbf{Z}$ that satisfies the condition in the theorem by appending $\mathbf{Z_{nd}} < \mathbf{Z_0} < \mathbf{Z_p}$.

Accordingly, we can construct a model such that the terms (38), (39) and (40) are all distinct for at least one configuration $\mathbf{z_p}$. Hence, a model such that $h(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}, \mathbf{z_0}) \neq 1$ for each possible assignment $\mathbf{z_0}, \mathbf{z_{nd}}$. Then, the term $g(\mathbf{x}, \mathbf{y}, \mathbf{z_{nd}}) \neq 1$ for each assignment $\mathbf{z_{nd}}$, then the sum in equation (37) is different to $P_{\mathbf{x}}(\mathbf{y})$.

□

A.2. Proof for Theorem 3

To prove this theorem we will use the following definitions and results:

Definition 7 (Generalized Adjustment Criterion (Correa and Bareinboim, 2017; Correa et al., 2018)). *Given a causal diagram $\mathcal{G}$ augmented with selection bias variable S and disjoint sets of variables $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathbf{V}$; $\mathbf{Z}$ satisfies the criterion relative to $\mathbf{X}, \mathbf{Y}$ in $\mathcal{G}$ if:*

(i) $\mathbf{Z} \cap Dpcp(\mathbf{X}, \mathbf{Y}) = \emptyset$,

(ii) $(\mathbf{Y} \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}, S)_{\mathcal{G}_{\mathbf{XY}}^{pbd}}$, and
(iii) $(\mathbf{Y} \perp\!\!\!\perp S \mid \mathbf{X}, \mathbf{Z})$.

Lemma 4 (Selection Bias Adjustment Criterion (Correa and Bareinboim, 2017; Correa et al., 2018)). *Given $\mathcal{G}$ a causal diagram augmented with a variable S, $\mathbf{Z}$ and a pair of disjoint sets of variables $\mathbf{X}, \mathbf{Y} \subseteq \mathbf{V}$,*

$$P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}} P(\mathbf{y} \mid \mathbf{x}, \mathbf{z}, S{=}1)P(\mathbf{z}), \quad (44)$$

holds in every model inducing $\mathcal{G}$ if and only if $\mathbf{Z}$ satisfy definition 7 relative to $\mathbf{X}, \mathbf{Y}$.

Definition 8 (Adjustment Criterion (Shpitser et al., 2010)). *Let $\mathcal{G}$ be a DAG over $\mathbf{V}$, and $\mathbf{X}, \mathbf{Y}, \mathbf{Z} \subseteq \mathbf{V}$ be pairwise disjoint subsets of variables. The set $\mathbf{Z}$ satisfies the adjustment criterion relative to $(\mathbf{X}, \mathbf{Y})$ in $\mathcal{G}$ if:*

(i) No element in $\mathbf{Z}$ is a descendant in $\mathcal{G}$ of any $W \in \mathbf{V}\backslash\mathbf{X}$ lying on a proper causal path from $\mathbf{X}$ to $\mathbf{Y}$ and
(ii) All proper non-causal paths in $\mathcal{G}$ from $\mathbf{X}$ to $\mathbf{Y}$ are blocked by $\mathbf{Z}$.

Lemma 5 (Adjustment (Shpitser et al., 2010)). *The set of variables $\mathbf{Z}$ and $\mathbf{X}, \mathbf{Y}$ in a causal diagram $\mathcal{G}$ satisfy the adjustment criterion if and only if for every model inducing $\mathcal{G}$, we have $P_{\mathbf{x}}(\mathbf{y}) = \sum_{\mathbf{z}} P(\mathbf{y} \mid \mathbf{x}, \mathbf{z})P(\mathbf{z})$.*

Now we are ready to prove the following

Theorem 3. *Given a selection diagram $\mathcal{D}$ and disjoint sets of variables $\mathbf{X}$, $\mathbf{Y}$, $\mathbf{Z}$, the causal effect $P_{\mathbf{x}}^*(\mathbf{y})$ is given by*

$$P_{\mathbf{x}}^*(\mathbf{y}) = \sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}, S{=}1)P^*(\mathbf{z}) \quad (18)$$

if and only if $\mathbf{Z}$ satisfies the st-adjustment criterion relative to $(\mathbf{X}, \mathbf{Y})$.

Proof. (if) Since $\mathbf{Z}$ satisfies condition (i), by Thm. 2 we have,

$$P_{\mathbf{x}}^*(\mathbf{y}) = \sum_{\mathbf{z}} P_{\mathbf{x}}^* (\mathbf{y} \mid \mathbf{z}) P^* (\mathbf{z}), \quad (45)$$

and by condition (ii) we have that $P_{\mathbf{x}}^* (\mathbf{y} \mid \mathbf{z}) = P_{\mathbf{x}} (\mathbf{y} \mid \mathbf{z}, S{=}1)$ therefore:

$$P_{\mathbf{x}}^*(\mathbf{y}) = \sum_{\mathbf{z}} P_{\mathbf{x}} (\mathbf{y} \mid \mathbf{z}, S{=}1) P^* (\mathbf{z}). \quad (46)$$

(only if) To show the necessity of the criterion we will prove that whenever its conditions fail, there exists two models inducing $\mathcal{D}$ (i.e., $\langle M, M^* \rangle$) that generate distributions distributions $P_{\mathbf{x}}(\mathbf{y}, \mathbf{z} \mid S{=}1)$ and $P^*(\mathbf{z})$ where $P_{\mathbf{x}}^*(\mathbf{y}) \neq \sum_{\mathbf{z}} P_{\mathbf{x}} (\mathbf{y} \mid \mathbf{z}) P^* (\mathbf{z})$.

If condition (i) is not satisfied, consider any two models M, M' for which $P_{\mathbf{x}}^* (\mathbf{y} \mid \mathbf{z}) = P_{\mathbf{x}} (\mathbf{y} \mid \mathbf{z}, S{=}1)$, then by

the e-adjustment criterion we have that the causal distribution is different that the g-adjustment.

Now, suppose condition (i) holds while condition (ii) does not. This is the case when there exists a path $\bar{p}$ from some T-node or S-node to $Y' \in \mathbf{Y}$ that is active given $\mathbf{Z}$ in $\mathcal{D}_{\overline{\mathbf{X}}}$.

First assume it is a T-node. Then, we will show that there exists a pair of models compatible with $\mathcal{D}'$, a graph where all edges but those in $\bar{p}$ have been removed, that is also compatible with $\mathcal{D}$.

Note that $\bar{p}$ does not contain any variable in $\mathbf{X}$ otherwise it would be blocked in $\mathcal{D}_{\overline{\mathbf{X}}}$ given $\mathbf{X}$. Without loss of generality assume that Y' is the only element in $\mathbf{Y}$ also in $\bar{p}$, else select the other element in $\mathbf{Y}$ closer to T as Y'. Consequently, we have that

$$P_{\mathbf{x}}^*(\mathbf{y}) = P^*(\mathbf{y}) = P^*(\mathbf{y} \setminus \{y'\})P^*(y') \qquad (47)$$

Consider the possible structures of $\bar{p}$:

(a) Suppose that the path between T and Y' is directed: Assume that S is pointing to a node W at the beginning of the path (if T points directly to Y' we can use the same argument and sum-out W from the obtained distributions while substituting W with f_W in the equations). From eq. (47) we can sum over W and obtain

$$P_{\mathbf{x}}^*(\mathbf{y}) = P^*(\mathbf{y} \setminus \{y'\}) \sum_w P^*(y' \mid w)P^*(w) \quad (48)$$

$$= P(\mathbf{y} \setminus \{y'\}) \sum_w P(y' \mid w)P^*(w), \quad (49)$$

while the adjustment functional is equal to

$$\sum_{\mathbf{z}} P(\mathbf{y} \mid \mathbf{z})P^*(\mathbf{z}) \qquad (50)$$

$$= \sum_{\mathbf{z}} P(\mathbf{y})P^*(\mathbf{z}) \qquad (51)$$

$$= P(\mathbf{y}) \qquad (52)$$

$$= P^*(\mathbf{y} \setminus \{y'\})P^*(y') \qquad (53)$$

$$= P^*(\mathbf{y} \setminus \{y'\}) \sum_w P(y' \mid w)P(w). \qquad (54)$$

We can parametrize two models with all variables binary, such that W is not independent of Y, and all conditional distributions are the same except for $P^*(w) \neq P(w)$. In this case the mapping between W and Y is one-to-one, hence the adjustment is different to the causal effect of interest.

(b) If the path $\bar{p}$ is not directed, suppose, as before, that T points to a variable W, which also has a parent R with binary domain, and let M^* be a model such that

$$P_{R=1}^*(y') \neq \sum_{\mathbf{z}} P^*(y' \mid \mathbf{z}, R=1)P^*(\mathbf{z}), \quad (55)$$

which must exists by the completeness of the adjustment criterion (lemma 5) since $\mathbf{Z}$ does not satisfy it relative to (R, Y'). Now let M be a model such that $f_W(u_w) = f_W^*(u_w, R = 1)$. It is easy to see that $P_{R=1}^*(y') = P^*(y') = P^*(y' \mid \mathbf{x})$ and that $P^*(y' \mid \mathbf{z}, R = 1) = P(y' \mid \mathbf{z}) = P(y' \mid \mathbf{z}, \mathbf{x})$, hence equation (55) becomes

$$P_{\mathbf{x}}^*(y') \neq \sum_{\mathbf{z}} P(y' \mid \mathbf{z}, \mathbf{x})P^*(\mathbf{z}), \qquad (56)$$

implying that M^*, M serve as counterexamples for this case.

Second, if the condition is violated because of an S-node, consider two identical submodels compatible compatible with $\mathcal{D}'$, a diagram where all edges but those witnessing the violation to the condition have been disconnected. Note that in $\mathcal{D}'$ no edges incoming to $\mathbf{X}$ remain and the transportability nodes are disconnected, therefore we have

$$P_{\mathbf{x}}(\mathbf{y} \mid \mathbf{z}, S{=}1) = P^*(\mathbf{y} \mid \mathbf{x}, \mathbf{z}, S{=}1), \qquad (57)$$

because $(\mathbf{Y} \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}, S{=}1)_{\mathcal{D}'_{\underline{\mathbf{x}}}}$. Then, the adjustment functional becomes

$$\sum_{\mathbf{z}} P_{\mathbf{x}}(\mathbf{y}|\mathbf{z}, S{=}1)P^*(\mathbf{z}) = \sum_{\mathbf{z}} P^*(\mathbf{y}|\mathbf{x}, \mathbf{z}, S{=}1)P^*(\mathbf{z}).$$

$$(58)$$

Since $(\mathbf{Y} \not\perp\!\!\!\perp S \mid \mathbf{X}, \mathbf{Z})_{\mathcal{D}'}$, Lemma 4 implies that (58) is not equal to $P_{\mathbf{x}}^*(\mathbf{y})$ for some model compatible with $\mathcal{D}'$, which serves as a counter example to our case. $\qquad \square$

A.3. Proof for Lemma 1

First we state the following lemma:

Lemma 6. *Let $\mathbf{Z}$ satisfy e-adjustment. Then, for any order satisfying the condition, no element in $\mathbf{Z_p}$ satisfies independence* (15) *in that order.*

Proof. By definition $(\mathbf{Z_p} \not\perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z_{nd}}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$, so any element $Z' \in \mathbf{Z_p}$ does not satisfy (15) unless there exists some $W \in \mathbf{Z_d} \setminus \mathbf{Z_p}$ for every path from Z' to $\mathbf{Y}$ that was active given $\mathbf{Z_{nd}}$. But, any such W is also not independent of $\mathbf{Y}$ given $\mathbf{Z_{nd}}$ (to be able to block a path to $\mathbf{Y}$) so it must be in $\mathbf{Z_p}$, a contradiction. The conclusion follows. $\qquad \square$

Lemma 1. *When $\mathbf{X}$ is a singleton, Definition. 6 is equivalent to Definition. 4.*

Proof. The second condition in each criterion is the same, hence we need to show that the first condition in one is equivalent to the other when $|\mathbf{X}| = 1$.

Suppose (i) holds in def.4. Then, an order with $\mathbf{Z_{nd}} < \mathbf{Z_d} \setminus \mathbf{Z_p} < \mathbf{Z_p}$ satisfies e-adjustment (by definition of $\mathbf{Z_d}$

and $(\mathbf{Z_p} \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z} \setminus \mathbf{Z_p})$). Accordingly, condition (i) in def.6 is satisfied too.

For the other direction, suppose (i) in def. 6 is satisfied, hence there exists an order over $\mathbf{Z}$ that satisfies e-adjustment. The first element Z_1 in the order cannot be in $\mathbf{Z_p}$ because then has to satisfy $(Z_1 \perp\!\!\!\perp X)$, which is not possible since $Z_1 \in De(X)$. Also, for any $Z_i, i > 1$, the graph $\mathcal{D}_{\overline{\mathbf{X}(\mathbf{Z}^{\leq i-1})}} = \mathcal{D}$. Let Z_i and Z_{i+1} two contiguous variables in the order such that $i > 1$ and $Z_i \in \mathbf{Z_p}$ and $Z_{i+1} \notin \mathbf{Z_p}$. Then we have $(Z_i \perp\!\!\!\perp X \mid \mathbf{Z}^{\leq i-1})$ and $(Z_{i+1} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}^{\leq i})_{\mathcal{D}_{\overline{\mathbf{X}}}}$. We want to claim that

- $(Z_i \perp\!\!\!\perp X \mid \mathbf{Z}^{\leq i-1} \cup \{Z_{i+1}\})$ holds: If this is not the case Z_{i+1} has to be a descendant of a collider in a path from Z_i to X. However, by lemma 6, Z_i must be d-connected to $\mathbf{Y}$ given $\mathbf{Z}^{\leq i-1}$ in which case Z_{i+1} is also d-connected to $\mathbf{Y}$ and is in $\mathbf{Z_p}$ (a contradiction) unless Z_i is a collider in the this path between Z_{i+1} and $\mathbf{Y}$, but then Z_{i+1} is d-connected to $\mathbf{Y}$ given $\mathbf{Z}^{\leq i}$ in $\mathcal{D}_{\overline{\mathbf{X}}}$, contradicting our assumption.
- $(Z_{i+1} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}^{\leq i-1})_{\mathcal{D}_{\overline{\mathbf{X}}}}$ holds: Suppose this is not the case, then Z_{i+1} is not a descendant of a collider in a path from Z_{i+1} to $\mathbf{Y}$, in which case any node in the portion of the path from Z_i to Z_{i+1} (including the latter) are by definition in $\mathbf{Z_p}$, a contradiction.

From these new independences, we conclude that Z_i and Z_{i+1} can be swapped while maintaining the invariance of property of the order. Repeating this process yields an order where $\mathbf{Z_{nd}} < \mathbf{Z_d} \setminus \mathbf{Z_p} < \mathbf{Z_p}$ which implies that $(\mathbf{Z_p} \perp\!\!\!\perp X \mid \mathbf{Z} \setminus \mathbf{Z_p})$.

$\square$

A.4. Proof for Theorem 4

Theorem 4. *In the absence of selection bias (i.e., S node disconnected from any other variable), if a set $\mathbf{Z}$ satisfies st-adjustment and $\mathbf{Z} \cap De(\mathbf{X}) \neq \emptyset$, then there exists $\mathbf{Z}' \subseteq \mathbf{Z}$ such that $\mathbf{Z}' \cap De(\mathbf{X}) = \emptyset$ and $\mathbf{Z}'$ satisfies st-adjustment.*

Proof. (by contradiction) We will show that given $\mathbf{Z}$ if no $\mathbf{Z}' \subseteq \mathbf{Z} \setminus De(\mathbf{X})$ exists satisfying the conditions, then $\mathbf{Z}$ violates at least one of them. By proposition 1, any $\mathbf{Z}'$ always satisfies condition (i). It must be the case, that $\mathbf{Z}'$ could only be violating condition (ii). Accordingly, there exists a path $\overline{p}$ between some $S \in \mathbf{S}$ to $Y \in \mathbf{Y}$ that is blocked given $\mathbf{Z}$ but active given $\mathbf{Z}'$ in $\mathcal{D}_{\overline{\mathbf{X}}}$ which implies there exists $Z \in \mathbf{Z} \setminus \mathbf{Z}'$ that blocks $\overline{p}$, and that $\overline{p}$ does not intersect $\mathbf{X}$. If $Z \notin De(\mathbf{X})$ we could just add Z to $\mathbf{Z}'$ and restart the argument from there, so we will further assume that $Z \in De(\mathbf{X})$. S has only outgoing edges, so $\overline{p}$ is either directed or contains one or more colliders. In the former case, Z has to be an ancestor of Y to be able to block $\overline{p}$. In the latter, Z has to be an ancestor of a collider or of Y, but if

it is the ancestor of a collider, that collider is also in $De(\mathbf{X})$, hence not in $\mathbf{Z}'$ contradicting the assumption that $\overline{p}$ is active given $\mathbf{Z}'$. In consequence, Z is an ancestor of Y. Under this assumptions, and by lemma 7, $\mathbf{Z}$ may not contain any such Z else it does not satisfy e-adjustment and we have a contradiction. $\square$

A.5. Proof for Lemma 2

Lemma 2. *A set $\mathbf{Z}$ satisfies e-adjustment if and only if there exists $Z_i \in \mathbf{Z}$ such that Z_i satisfies (15) or (16), and $\mathbf{Z} \setminus \{Z_i\}$ satisfies e-adjustment.*

Proof. (if) Suppose $\mathbf{Z}$ satisfies e-adjustment, then there exists an order such that each element satisfies (15) or (16). Let Z_i be the last element in that order and notice that $\mathbf{Z} \setminus \{Z_1\}$ is also E-Admissible by the same order minus Z_i.

(only if) If $\mathbf{Z}$ satisfies e-adjustment and some Z_i satisfies (15) or (16) with $\mathbf{Z}^{\leq i-1} = \mathbf{Z}$, then the order over $\mathbf{Z}$ with Z_i appended at the end witnesses that $\mathbf{Z} \cup \{Z_i\}$ satisfies e-adjustment. $\square$

A.6. Proof for Lemma 3

Lemma 3. *If $\mathbf{Z}$ satisfies e-adjustment, then for any $Z_i \in \mathbf{Z}$ satisfying (15) or (16), the set $\mathbf{Z} \setminus \{Z_i\}$ satisfies e-adjustment.*

Proof. Define the predicates:

$\mathcal{E}(\mathbf{Z})$: $\mathbf{Z}$ satisfies e-adjustment,
$\mathbf{A}(Z_i, \mathbf{Z})$: Z_i satisfies (15) with $\mathbf{Z}^{\leq i-1} = \mathbf{Z} \setminus \{Z_1\}$, and
$\mathbf{B}(Z_i, \mathbf{Z})$: Z_i satisfies (16) with $\mathbf{Z}^{\leq i-1} = \mathbf{Z} \setminus \{Z_1\}$.

Then from lemma 2 we have that

$$\mathcal{E}(\mathbf{Z}) \implies \tag{59}$$
$$\exists_{Z_i \in \mathbf{Z}} \left(\mathbf{A}(Z_i, \mathbf{Z}) \text{ or } \mathbf{B}(Z_i, \mathbf{Z}) \right) \text{ and } \mathcal{E}(\mathbf{Z}). \tag{60}$$

Equivalently,

$$\neg(\forall_{Z_i \in \mathbf{Z}} \left(\neg\mathbf{A}(Z_i, \mathbf{Z}) \text{ and } \neg\mathbf{B}(Z_i, \mathbf{Z}) \right) \text{ or } \neg\mathcal{E}(\mathbf{Z} \setminus \{Z_i\})). \tag{61}$$

In particular, for any Z_i satisfying (15) or (16) this is implies

$$\mathcal{E}(\mathbf{Z}) \implies \neg(\textit{false} \text{ and } \neg\mathcal{E}(\mathbf{Z} \setminus \{Z_i\})) \tag{62}$$
$$\mathcal{E}(\mathbf{Z}) \implies \mathcal{E}(\mathbf{Z} \setminus \{Z_i\}) \tag{63}$$

$\square$

A.7. Proof for Theorem 5

Theorem 5. *$\mathbf{Z}$ satisfies e-adjustment (Def. 5) w.r.t. $(\mathbf{X}, \mathbf{Y})$ in $\mathcal{G}$ if and only if IsEAdmissible (Alg. 1) returns true.*

Proof. (if) the procedure will return true only if it was able to remove all elements $\mathbf{Z} \cap De(\mathbf{X})$ one by one while they satisfied either independence (15) or (16), witnessing that there exists an order satisfying the condition.

(only if) Suppose for the sake of contradiction that the algorithm returned false but $\mathbf{Z}$ satisfies e-adjustment. The procedure returns false when there is $\mathbf{Z}' \subseteq \mathbf{Z}$ such that no element in $\mathbf{Z}'$ satisfies (15) or (16) and all elements in $\mathbf{Z} \setminus \mathbf{Z}'$ removed in some order $Z'_\ell < \ldots < Z'_1$ did (Z_ℓ was the last removed before obtaining $\mathbf{Z}'$). By Lemma. 3 we have that $\mathbf{Z}' \cup \{Z_\ell\}$ does not satisfy the criteria, and by repeatedly applying the same theorem we conclude that $\mathbf{Z}$ is not admissible, a contradiction.

$\square$

B. Appendix: Proofs in Section 5

B.1. Proof for Lemma 10

First, we will need some results.

Lemma 7. *If $\mathbf{Z}$ includes some $W \notin \mathbf{X}$, that is a descendant of $\mathbf{X}$ and also an ancestor of $\mathbf{Y}$ in $\mathcal{G}_{\overline{\mathbf{X}}}$, or a descendant of such W in $\mathcal{G}$, then $\mathbf{Z}$ does not satisfy g-adjustment.*

Proof. Let W be a variables as described in the statement. This variables does not satisfy (15) because of the directed path $\overline{p}$ from some $X' \in \mathbf{X}$ to W. It also does not satisfy (16) due to the directed path $\overline{q}$ from W to some $Y' \in \mathbf{Y}$. Therefore, a viable set $\mathbf{Z}$ including W must also include at least another variable W' that goes before W in the order and blocks $\overline{p}$ or $\overline{q}$. However, W' has the same characteristics as W and requires some W'' to be also in the order. Following this argument, we must reach a W that is directly connected to X' or Y' and conclude that the order required by def. 5 cannot not exists. $\square$

Lemma 8. *Let $\mathbf{Z}$ be such that $\mathbf{Z_p} = \emptyset$. Then, $\mathbf{Z}$ satisfies e-adjustment criterion.*

Proof. Since $\mathbf{Z_d} = \mathbf{Z} \cap De(\mathbf{X})$ contains no element from $\mathbf{Z_p}$, it follows $(\mathbf{Z_d} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z} \setminus \mathbf{Z_d}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$ which implies (by decomposition graphoid) that for any order over $\mathbf{Z_d}$ we have $(Z_i \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z^i}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$. We conclude that an order where $\mathbf{Z_{nd}} < \mathbf{Z_d}$ satisfies def. 5. $\square$

Lemma 9. *Let $\mathbf{I}$ and $\mathbf{Z}$ be two set satisfying e-adjustment relative to $\mathbf{X}, \mathbf{Y}$ such that $\mathbf{I} \subset \mathbf{Z}$. Then, there exists $Z_i \in \mathbf{Z} \setminus \mathbf{I}$ such that $\mathbf{I} \cup \{Z_i\}$ satisfies e-adjustment.*

Proof. Assume for the sake of contradiction that for every $Z_i \in \mathbf{Z} \setminus \mathbf{I}, \mathbf{I} \cup \{Z_i\}$ has no valid order. Then, for every Z_i there exists $Z_j \in (\mathbf{Z} \setminus \mathbf{I}) \setminus \{Z_i\}$ that comes after Z_i in the order, and $Z_k \in \mathbf{I}$ that satisfied the conditions in the order

over $\mathbf{I}$, failed when Z_i is added and satisfy it again when Z_j is also added. That is $(Z_k \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}^{<\mathbf{k}}, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$, $(Z_k \not\perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}^{<\mathbf{k}}, Z_i, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$ and $(Z_k \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}^{<\mathbf{k}}, Z_i, Z_k, \mathbf{X})_{\mathcal{G}_{\overline{\mathbf{X}}}}$. Or $(Z_k \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}^{<\mathbf{k}})_{\mathcal{G}_{\overline{\mathbf{X}(\mathbf{Z}^{<\mathbf{k}})}}}$, $(Z_k \not\perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}^{<\mathbf{k}}, Z_i)_{\mathcal{G}_{\overline{\mathbf{X}(\mathbf{Z}^{<\mathbf{k}}, Z_i)}}}$ and $(Z_k \perp\!\!\!\perp \mathbf{X} \mid \mathbf{Z}^{<\mathbf{k}}, Z_i)_{\mathcal{G}_{\overline{\mathbf{X}(\mathbf{Z}^{<\mathbf{k}}, Z_i, Z_k)}}}$. These constraints cannot be satisfied for every Z_i simultaneously. $\square$

Lemma 10. *ListGAdjIR outputs all sets $\mathbf{Z}$, $\mathbf{I} \subseteq \mathbf{Z} \subseteq \mathbf{R}$, that satisfy g-adjustment, with $O(n(n+m))$ delay. , $\mathbf{I} = \emptyset$ and $\mathbf{R} = \mathbf{W} \setminus De\big((De(\mathbf{X})_{\mathcal{D}_{\overline{\mathbf{X}}}} \setminus \mathbf{X}) \cap An(\mathbf{Y})_{\mathcal{D}_{\overline{\mathbf{X}}}}\big)$*

Proof. (Correctness) The algorithm outputs $\mathbf{I}$ (line 6), if $\mathbf{I}$ d-separates $\mathbf{T}, S$ and $\mathbf{Y}$ in $\mathcal{D}_{\overline{\mathbf{X}}}$ (condition in line 4); hence $\mathbf{I}$ satisfies condition (ii) in def. 6. Because of the order in which variables for A are picked, variables in $\mathbf{Z_p}$ are added last to $\mathbf{I}$. While $\mathbf{I} \cap \mathbf{Z_p} = \emptyset$, proposition 1 and lemma 8 guarantee that $\mathbf{I}$ satisfies e-adjustment. If $\mathbf{I}$ contains an element in $\mathbf{Z_p}$ it must have been picked at line 8 and *IsEAdmissible* returned true for $\mathbf{I}$; hence $\mathbf{I}$ always satisfies condition (i). We conclude that every time the algorithm outputs a set, it satisfies g-adjustment criterion.

(Completeness) Note that at each recursion the search branches into to disjoint families of sets. Those sets that contain A (line 10) and those that do not (line 11).

Consider any set $\mathbf{Z}$ satisfying definition 6, there should a branch in this recursion such that $\mathbf{Z} = \mathbf{I} = \mathbf{R}$ (when $\mathbf{Z}$ is outputted), unless (1) the condition in line 4 failed while $\mathbf{I} \subseteq \mathbf{Z} \subseteq \mathbf{R}$ or (2) line 13) was executed while $\mathbf{I} \subseteq \mathbf{Z} \subseteq \mathbf{R}$ and A was empty.

In case (1), failing the condition implies (by lemma 11) that there exists no set $\mathbf{Z}$ such that $\mathbf{I} \subseteq \mathbf{Z} \subseteq \mathbf{R}$ that d-separates $\mathbf{T}, S$ from $\mathbf{Y}$ in $\mathcal{D}_{\overline{\mathbf{X}}}$, which contradicts the assumption that $\mathbf{Z}$ satisfies the conditions (in particular condition (ii).

In case (2), since A was empty, it means that $\mathbf{R} \setminus \mathbf{I}$ only contains variables in $\mathbf{Z_d}$ such that $(\mathbf{R} \setminus \mathbf{I} \not\perp\!\!\!\perp \mathbf{Y} \mid \mathbf{I})_{\mathcal{D}_{\overline{\mathbf{X}}}}$, (that is variables in $\mathbf{Z_p}$) and there is no $A \in \mathbf{R} \setminus \mathbf{I}$ such that $\mathbf{I} \cup \{A\}$ satisfies e-adjustment criterion. By lemma 9 no such $\mathbf{Z}, \mathbf{I} \subset \mathbf{Z} \subseteq \mathbf{R}$ may exists, hence the only possibility left to explore is for $\mathbf{I}$ itself to be a valid set which is verified by the recursive call in line 13.

(Complexity) The recursion induced by the algorithm can be seen as a tree where each leaf produces an output. This is due to the fact that every time there is no valid set restricted to $\mathbf{I}$ and $\mathbf{R}$, the algorithm aborts that branch at line 4 if it is due to condition (i), and at line 13 if due to condition (ii). In the first case, it takes $O(n+m)$ time to perform this test.

In the second case, A has to be empty, meaning that no variable in $\mathbf{R} \setminus \mathbf{I}$ satisfied any of the conditions in line 8. From those, the first and second one can be tested in $O(n+m)$ time, while the third (that uses *IsEAdmissible*) may take

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Algorithm 3 ExistsSep($\mathcal{G}, \mathbf{X}, \mathbf{Y}, \mathbf{I}, \mathbf{R}$)

Input: causal diagram $\mathcal{G}$, disjoint subsets $\mathbf{X}, \mathbf{Y}, \mathbf{R} \subseteq \mathbf{V}$ and set $\mathbf{I} \subset \mathbf{R}$.
Output: true if there exists $\mathbf{Z}$ such that $\mathbf{I} \subseteq \mathbf{Z} \subseteq \mathbf{R}$ and $(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z})$ in $\mathcal{G}$.
  1: let $\mathbf{Z}' = An(\mathbf{X} \cup \mathbf{Y} \cup \mathbf{I}) \cap \mathbf{R}$
  2: **return** $(\mathbf{X} \perp\!\!\!\perp \mathbf{Y} \mid \mathbf{Z}')_{\mathcal{G}}$

$O(n^2(n+m))$. In the worst case each element in $\mathbf{R} \setminus \mathbf{I}$ has to be tested leading to time $O(n^3(n+m))$ for any particular call in the recursion.

The length of any branch (from the start to reaching a leaf) is at most n, because at every level $\mathbf{R} \setminus \mathbf{I}$ reduces in one variable and the process end when the difference is 0. It follows that the time spent on each output is $O(n^4(n+m))$. $\qquad\square$

B.2. Proof for Theorem 6

Theorem 6. *ListGAdjSets on input $\mathcal{D}, \mathbf{X}, \mathbf{Y}, \mathbf{W}$, lists all sets $\mathbf{Z} \subseteq \mathbf{W}$ satisfying st-adjustment relative to $\mathbf{X}, \mathbf{Y}$ in $\mathcal{D}$, with $O(n^4(n+m))$ delay.*

Proof. First, the algorithm identifies the set $\mathbf{F}$ that by lemma 7 can be discarded. Then, restrict the search to subsets of $\mathbf{R}$ which is equal to the available set $\mathbf{W}$ minus $\mathbf{X}, \mathbf{Y}$ and $\mathbf{F}$. Then, by calling *ListGAdjIR*, it lists all sets $\mathbf{Z}$ satisfying g-adjustment such that $\mathbf{Z} \subseteq \mathbf{R}$.

The complexity here is given by *ListGAdjIR*. $\qquad\square$

The algorithm *ExistsSep* used in *ListGAdjIR* is shown in algorithm 3 and it is correct due to the following

Lemma 11 ((van der Zander et al., 2014)). *Let $\mathbf{X}, \mathbf{Y}, \mathbf{I}, \mathbf{R}$ be sets of nodes with $\mathbf{I} \subseteq \mathbf{R}$, $\mathbf{R} \cap (\mathbf{X} \cup \mathbf{Y}) = \emptyset$. If there exists an separator $\mathbf{Z_0}$ for $\mathbf{X}, \mathbf{Y}$, with $\mathbf{I} \subseteq \mathbf{Z_0} \subseteq \mathbf{R}$ then $\mathbf{Z} = An(\mathbf{X} \cup \mathbf{Y} \cup \mathbf{I}) \cap \mathbf{R}$ is a separator for $\mathbf{X}, \mathbf{Y}$.*

C. Appendix: Other Results Used

We use the following rules to reason about causal distributions throughout the paper:

Theorem 7 (Do-Calculus (Pearl, 1995)). *Let $\mathcal{G}$ be a causal diagram compatible with a structural causal model M, and let $P(\mathbf{v})$ be a probability distribution induced by M over the endogenous variables $\mathbf{V}$. For any disjoint subsets of endogenous variables $\mathbf{X}, \mathbf{Y}, \mathbf{Z}$, and $\mathbf{W}$, the following rules are valid for every interventional distribution compatible with $\mathcal{G}$.*

Rule 1 *(Insertion/Deletion of observations):*

$$P(\mathbf{y} \mid do(\mathbf{x}), \mathbf{z}, \mathbf{w}) = P(\mathbf{y} \mid do(\mathbf{x}), \mathbf{w}) \qquad (64)$$
$$if\ (\mathbf{Y} \perp\!\!\!\perp \mathbf{Z} \mid \mathbf{X}, \mathbf{W})_{\mathcal{G}_{\overline{\mathbf{X}}}}. \qquad (65)$$

Rule 2 *(Action/Observation exchange):*

$$P(\mathbf{y} \mid do(\mathbf{x}), do(\mathbf{z}), \mathbf{w}) = P(\mathbf{y} \mid do(\mathbf{x}), \mathbf{z}, \mathbf{w}) \qquad (66)$$
$$if\ (\mathbf{Y} \perp\!\!\!\perp \mathbf{Z} \mid \mathbf{X}, \mathbf{W})_{\mathcal{G}_{\overline{\mathbf{X}}\underline{\mathbf{Z}}}}. \qquad (67)$$

Rule 3 *(Insertion/Deletion of actions):*

$$P(\mathbf{y} \mid do(\mathbf{x}), do(\mathbf{z}), \mathbf{w}) = P(\mathbf{y} \mid do(\mathbf{x}), \mathbf{w}) \qquad (68)$$
$$if\ (\mathbf{Y} \perp\!\!\!\perp \mathbf{Z} \mid \mathbf{X}, \mathbf{W})_{\mathcal{G}_{\overline{\mathbf{X}\mathbf{Z}(\mathbf{W})}}}, \qquad (69)$$

where $\mathbf{Z}(\mathbf{W})$ is the set of $\mathbf{Z}$-nodes that are not ancestors of any $\mathbf{W}$-node in $\mathcal{G}_{\overline{\mathbf{X}}}$.