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Simpson's Paradox and Related Phenomena

MYRA L. SAMUELS*

Simpson's paradox is viewed as one of a natural and coherent collection of *association reversal* phenomena that are of fundamental importance in statistical practice. Association reversal means that the direction of association between two variables X and Y is changed by collapsing (unconditioning) over a covariate Z ; an example is Simpson's paradox for contingency tables. This article gives necessary and sufficient conditions for Simpson's paradox and for more general forms of association reversal. Close connections are noted with amalgamation paradoxes, defined as situations where an unconditional measure of association between X and Y lies outside the range of the conditional (on Z) measures. Emphasis throughout is on statistical interpretation and on commonalities and contrasts between the paradoxical phenomena in various settings.

KEY WORDS: Amalgamation; Association; Confounding; Contingency table.

1. INTRODUCTION

Although Simpson's paradox has been recognized for many decades, it still retains some of its mystery. The purposes of this article are (1) to give statistically interpretable necessary and sufficient conditions for Simpson's paradox and relate them to necessary conditions given by Mittal (1991) and Lindley and Novick (1981) and to amalgamation paradoxes as defined by Good and Mittal (1987), and (2) to place Simpson's paradox in a general setting of association reversal phenomena and to extend certain results to this general setting.

1.1 Notation and Terminology

Consider random variables (X, Y, Z) with joint distribution F , and suppose that relations \uparrow , \downarrow , and \perp of directional association between X and Y have been defined. For instance, to represent the $2 \times 2 \times k$ contingency table, let X and Y each take values 0 or 1, let Z take values $1, 2, \dots, k$, and define \uparrow , \downarrow , and \perp as follows:

$$X \uparrow Y: \Pr(X = 1, Y = 1) > \Pr(X = 1)\Pr(Y = 1),$$

$$X \downarrow Y: \Pr(X = 1, Y = 1) < \Pr(X = 1)\Pr(Y = 1),$$

and

$$X \perp Y: \Pr(X = 1, Y = 1) = \Pr(X = 1)\Pr(Y = 1). \quad (1)$$

(Equivalently, the relation $X \uparrow Y$ [resp. $X \downarrow Y, X \perp Y$] means that the diagonal entries of the 2×2 table relating X and Y are greater than [resp. less than, equal to] the values that would be implied by independence.) Analogous relations conditional on Z will be denoted by $X \uparrow Y|Z$, and so on. In the classical Simpson's paradox (see Good and Mittal 1987 for a history), one of the relations (1) holds conditionally on $Z = z$ for all z , but a different one holds unconditionally.

To place Simpson's paradox in a more general context, we introduce the term *association reversal* (AR), which we now define. Consider the following relations, each conditional on a particular value z of Z :

- (a) $X \perp Y|Z = z$
- (b) $X \downarrow Y|Z = z$
- (c) $X \uparrow Y|Z = z.$ (2)

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In many applications, investigators are particularly interested in the null hypothesis

$$H_0: X \perp Y|Z, \quad (3)$$

which asserts that (a) holds for all z . We will say that F is a candidate for positive AR if either (a) or (b) holds for all z . Similarly, we will say that F is a candidate for negative AR if either (a) or (c) holds for all z . Finally, we will say that F exhibits positive [negative] AR if F is a candidate for positive [negative] AR and if either (1) $X \uparrow Y[X \downarrow Y]$ or (2) $X \perp Y$ but H_0 is not true.

Mittal (1991) called AR when H_0 is true "Yule's association paradox." Our definition of AR otherwise is slightly different from Mittal's.

Following Dawid (1979), we will use the notation \perp to denote independence. (The relation \perp as defined in (1) is indeed independence, but we will later use \perp in a more general way and reserve \perp for independence.)

We will say that Z is not doubly linked to (X, Y) if at least one of the following four conditions holds:

- (a) $Z \perp\!\!\!\perp X$
- (b) $Z \perp\!\!\!\perp Y$
- (c) $Z \perp\!\!\!\perp Y|X$
- (d) $Z \perp\!\!\!\perp X|Y.$ (4)

Otherwise, we will say that Z is doubly linked to (X, Y) . Thus double linkage expresses the idea that Z is related to both X and Y .

1.2 Overview

Section 2 deals with the $2 \times 2 \times k$ contingency table. Sections 2.1 and 2.2 give necessary and sufficient conditions for F to exhibit AR if F is a candidate for AR. In particular, F cannot exhibit AR unless Z is doubly linked to (X, Y) . Section 2.3 discusses applications to sampling designs and interpretation of data. Finally, Section 2.4 gives sufficient conditions for preventing various amalgamation paradoxes and mentions an important case where avoiding AR can tend to produce an amalgamation paradox.

Section 3 investigates AR and amalgamation paradoxes in a more general setting. Sections 3.1 and 3.2 give definitions

and general results, and Section 3.3 gives stronger results for the case of dichotomous X . Sections 3.4 and 3.5 discuss the special cases of linear regression and logistic regression. The Appendixes present proofs and counterexamples.

It is assumed throughout that all conditional distributions discussed are well defined and that the conditional distributions of X given $Z = z$ and of Y given $Z = z$ are nondegenerate for all z .

2. ASSOCIATION REVERSAL IN THE $2 \times 2 \times k$ CONTINGENCY TABLE

Throughout Section 2 it is assumed that X and Y take values 0 and 1 and that Z takes values $1, \dots, k$. For $i = 1, \dots, k$, let

$$\begin{aligned} r_i &= \Pr(Z = i) \\ q_i &= \Pr(X = 1 | Z = i) \\ p_i &= \Pr(Y = 1 | X = 0, Z = i) \\ p'_i &= \Pr(Y = 1 | X = 1, Z = i) \\ \delta_i &= p'_i - p_i. \end{aligned} \quad (5)$$

The sequential conditioning in (5) is natural if X is an “explanatory” variable and Y is a “response” variable. As an illustration, visualize a population of individuals, some of whom receive a “treatment” ($X = 1$) and some of whom do not ($X = 0$); moreover, some individuals respond with “success” ($Y = 1$) and some do not ($Y = 0$); think of Z as determining strata in the population. Then q_i is the probability that an individual in stratum i receives the treatment, and p'_i and p_i are the success rates among treated and untreated individuals in stratum i . The hypothesis H_0 of Equation (3) asserts that $p'_i = p_i$; that is, $\delta_i = 0$.

Also, let

$$\begin{aligned} p &= \sum p_i r_i \\ p' &= \sum p'_i r_i \\ q &= \sum q_i r_i = \Pr(X = 1). \end{aligned} \quad (6)$$

2.1 Necessary and Sufficient Conditions for AR

The following theorem gives necessary and sufficient conditions for a candidate F actually to exhibit AR. (The theorem is a special case of Theorem 3.5, which is proved in Appendix A.)

Theorem 2.1. Suppose that F is a candidate for positive [negative] AR. Then F exhibits positive [negative] AR if and only if $\phi > 0$ [$\phi < 0$] and

$$|\phi| \geq |\delta| q(1 - q), \quad (7)$$

where

$$\begin{aligned} \phi &= \sum [p_i - p][q_i - q]r_i \\ \delta &= q^{-1} \sum \delta_i q_i r_i. \end{aligned} \quad (8)$$

Corollary 2.1. If H_0 is true, then F exhibits positive [negative] AR if and only if $\phi > 0$ [$\phi < 0$].

Theorem 2.1 has a natural statistical interpretation. The

parameter ϕ is simply the covariance between p_Z and q_Z . Thus, for example, the condition $\phi > 0$ says that strata where the treatment is more common also tend to be those with relatively high success rates even among untreated individuals; it is intuitively reasonable that this state of affairs would spuriously favor the treatment and, therefore, tend to produce positive AR. Similar remarks apply to $\phi < 0$. The parameter q is the fraction of individuals treated, and δ is an average of the δ_i with respect to the probability distribution $\{q^{-1}q_i r_i\}$. Theorem 2.1 anatomizes AR in a straightforward way; it shows clearly the competition between the parameter ϕ pulling toward AR and the parameter δ pulling away from it, with the factor $q(1 - q)$ setting the scale of the competition.

Although the phenomenon of AR can be discussed quite separately from causality, the preceding interpretation of Theorem 2.1 is even more vivid if expressed in causal language. Note that the covariance ϕ is calculated not with respect to the distribution of Z among individuals who actually have $X = 0$, but rather with respect to the distribution $\{r_i\}$ of Z in the entire population. This dovetails nicely with the causal model (see, for instance, Holland 1986; Rosenbaum and Rubin 1983), in which each individual in the population has two potential responses, one with treatment and one without treatment. If treatment assignment is Z -adjustable (Rosenbaum 1987), then p_i can be interpreted as the probability that a randomly chosen individual in stratum i would respond successfully even without treatment, and δ_i can be interpreted as the increment in success probability due to treatment. With this interpretation, the condition $\phi > 0$ says that individuals who are more likely to receive the treatment tend to be those who would more likely respond positively even in the absence of treatment; positive AR occurs if this tendency outweighs the treatment effect δ .

In a related article with a different emphasis from the present one, Zidek (1984) investigated the “Simpson disaggregation” of given probabilities $\Pr(X = 1 | X = 0)$ and $\Pr(Y = 1 | X = 1)$ into a $2 \times 2 \times 2$ table that exhibits AR. Zidek gave bounds on the magnitude of the AR that can occur if q_1 and q_2 are constrained to vary within fixed limits.

Theorem 2.1 assigns different roles to the values $X = 0$ and $X = 1$. Reversing the roles yields the following companion theorem.

Theorem 2.1'. Theorem 2.1 remains true if ϕ and δ are replaced by

$$\begin{aligned} \phi' &= \sum [p'_i - p'][q_i - q]r_i \\ \delta' &= (1 - q)^{-1} \sum \delta_i (1 - q_i) r_i. \end{aligned} \quad (9)$$

The parameters ϕ and ϕ' that appear in Theorems 2.1 and 2.1' are, of course, not the same. If $\delta_i = \delta$, then $\phi = \phi'$, and if F exhibits AR, then ϕ and ϕ' must have the same sign. Otherwise, however, ϕ and ϕ' can have different signs.

In applications it is helpful to have conceptually simple conditions that are sufficient to prevent AR. The following corollary gives two such conditions.

Corollary 2.2. F cannot exhibit AR if either of the following holds:

$$(a) \quad \phi = 0 \quad (10)$$

or

$$(b) \quad p_i = p \quad \text{or} \quad q_i = q. \quad (11)$$

If $k = 2$, then (10) \Leftrightarrow (11); thus we have the following additional corollary to Theorem 2.1.

Corollary 2.3. For the $2 \times 2 \times 2$ contingency table, suppose that H_0 is true. Then the condition (11) is both necessary and sufficient to prevent AR.

The phenomenon of AR is loosely related to the more subtle concept of confounding, whose precise definition is still debated (see, for example, Greenland, Holland, and Mantel 1989 and references therein). Many epidemiological textbooks give a verbal definition of confounding that is reminiscent of (11); for instance, Kelsey, Thompson, and Evans (1986, p. 12) defined a confounder of the relationship between disease occurrence (Y) and exposure (X) as “a variable that (a) is causally related to the disease . . . and (b) is associated with the exposure . . . but is not a consequence of this exposure.” More formally, Wickramaratne and Hollard (1987) gave sufficient conditions for “no confounding in the population,” which are essentially the requirement that (11) hold.

2.2 Conditions Symmetric in X and Y

The phenomenon of AR is symmetric in X and Y , but Theorems 2.1 and 2.1' are not. One might also consider the reverse parameterization given by \tilde{q}_i , \tilde{p}_i , \tilde{p}'_i , and $\tilde{\delta}_i$, defined as in (5) but with X and Y interchanged. Of course, Theorems 2.1 and 2.1' and their corollaries remain true if ϕ , δ , ϕ' , δ' , p , p' , and q are replaced by $\tilde{\phi}$, $\tilde{\delta}$, $\tilde{\phi}'$, $\tilde{\delta}'$, \tilde{p} , \tilde{p}' , and \tilde{q} , defined in analogy with (6), (8), and (9) but using the reverse parameterization.

The conditions (4) for absence of double linkage can be expressed in the present notation as

- (a) $Z \perp X: q_i = q$
- (b) $Z \perp Y: \tilde{q}_i = \tilde{q}$
- (c) $Z \perp Y|X: p_i = p \quad \text{and} \quad p'_i = p'$
- (d) $Z \perp X|Y: \tilde{p}_i = \tilde{p} \quad \text{and} \quad \tilde{p}'_i = \tilde{p}'$.

An additional corollary to Theorem 2.1 follows.

Corollary 2.4. F cannot exhibit AR if Z is not doubly linked to (X, Y) .

To state necessary and sufficient conditions for AR that are symmetric in X and Y , we let

$$\eta_i = \delta_i q_i (1 - q_i). \quad (12)$$

Good and Mittal (1987, p. 699) considered the measure η_i , attributing it to Yule. It is easy to show that $\delta_i q_i (1 - q_i) = \tilde{\delta}_i \tilde{q}_i (1 - \tilde{q}_i)$, so that η_i is symmetric in X and Y .

Theorem 2.2. Suppose that F is a candidate for positive [negative] AR. Then F exhibits positive [negative] AR if and only if $\psi > 0$ [$\psi < 0$] and $|\psi| \geq |\eta|$, where $\psi = \sum [\eta_i - q_i][\tilde{q}_i - \tilde{q}] r_i$ and $\eta = \sum \eta_i r_i$.

Corollary 2.5. F cannot exhibit AR if $\psi = 0$.

Corollary 2.6. Suppose that $k = 2$ and F exhibits positive AR. Then either (a) $X \uparrow Z$ and $Y \uparrow Z$ or (b) $X \downarrow Z$ and $Y \downarrow Z$.

Theorem 2.2 is a special case of Theorem 3.2, which is proved in Appendix A. Corollary 2.6 was proposed by Lindley and Novick (1981), and a full proof was given by Mittal (1991).

The parameter ψ bears some resemblance to the covariance parameters ϕ and $\tilde{\phi}$; namely, ψ is the covariance between q_Z and \tilde{q}_Z . Thus, for instance, if $\psi > 0$, then those individuals who have a higher probability that $X = 1$ also tend to have a higher probability that $Y = 1$. In many applications this symmetric image involving unconditional probabilities may be less intuitive than the asymmetric image in which one of the probabilities is conditional. For instance, if one thinks of X as an “explanatory” variable and of Y as a “response” variable, then the interpretation in terms of ϕ , as illustrated in Section 2.1, is more natural.

Theorems 2.1 and 2.2 imply that ϕ , $\tilde{\phi}$, and ψ must have the same sign if F exhibits AR. Moreover, if H_0 is true, then $\tilde{p}_i = q_i$ and $\tilde{q}_i = p_i$, so that $\phi = \tilde{\phi} = \psi$. In general, however, the three parameters need not agree in sign, even if F is a candidate for AR (see Appendix B for counterexamples).

Mittal (1991) defined *homogeneous* strata by the requirement that any of the following four inequalities hold:

$$\max_i p_i \leq \min_i p'_i, \quad (13a)$$

$$\max_i p'_i \leq \min_i p_i, \quad (13b)$$

$$\max_i \tilde{p}_i \leq \min_i \tilde{p}'_i, \quad (13c)$$

and

$$\max_i \tilde{p}'_i \leq \min_i \tilde{p}_i. \quad (13d)$$

Mittal showed that homogeneity is sufficient to prevent AR. If H_0 is false, then homogeneity neither implies nor is implied by any of the conditions for preventing AR given in Corollaries 2.2, 2.4, and 2.5. If H_0 is true, then homogeneity is equivalent to (11) and to the absence of double linkage, and homogeneity implies that $\phi = \tilde{\phi} = \psi = 0$.

Mittal called the strata *row homogeneous* if (13a) or (13b) holds and *column homogeneous* if (13c) or (13d) holds. (This correspondence between Mittal’s terminology and our notation assumes that X represents the rows and Y represents the columns of the 2×2 table.) If H_0 is true, then (11) says that the strata are either row *or* column homogeneous. Mittal claims (Lemma 3.2) that if H_0 is true and $k = 2$, then AR occurs unless the strata are both row *and* column homogeneous. This claim contradicts our Corollary 2.3. But the claim is incorrect; Mittal’s proof of row [column] homogeneity assumes implicitly that column [row] homogeneity is absent.

2.3 Applications to Study Design

In the preceding sections the distribution F was taken to represent a population; with this interpretation, the entries in the $2 \times 2 \times k$ contingency table represent population probabilities. Alternatively, one could multiply all the entries by a number N without changing any of the relationships in

the table and take N to be the total number of observations in a data set. The values in the table could then be interpreted as (a) expected cell frequencies under some specified sampling scheme or (b) observed cell frequencies for a particular set of data. With this new interpretation the entire preceding discussion carries over unchanged.

The following corollary links the population results to simple sampling designs.

Corollary 2.7. If a contingency table is generated by either (a) simple random sampling from the population, (b) product binomial sampling with fixed marginal totals for X , or (c) product binomial sampling with fixed marginal totals for Y , then the table of expected cell frequencies cannot exhibit AR unless the population does.

We now ask how a sampling design can remedy an AR that may exist in the population. In particular, consider *stratum-matched sampling*; that is, any sampling scheme that uses random sampling within the cells but for which the observed distributions of Z for $X = 0$ and $X = 1$ (or, similarly, for $Y = 0$ and $Y = 1$) are forced to agree. Examples are matched cohort studies and matched case-control studies in epidemiology.

Corollary 2.8. If a contingency table is generated by stratum-matched sampling, then AR cannot occur either in the data or in the table of expected cell frequencies.

Corollary 2.8 says that matching prevents AR, so that a summary statistic calculated for the collapsed 2×2 table cannot misrepresent the direction of association in the separate tables. This does not mean, however, that matching is always a good thing nor that the resulting data should be analyzed using only the collapsed table (see, for example, Samuels 1981).

In designing a study, investigators often need to consider whether AR is a potential problem. A practical guideline is the concept of double linkage. In some cases an investigator can reason a priori that double linkage is absent. The paradigm case is a randomized experiment. If individuals are randomly allocated to levels of X , then X is automatically rendered independent of all covariates Z . This means that randomization prevents AR with respect to any conceivable Z which may affect Y . In a nonrandomized study the investigator might know a priori that $Z \perp\!\!\!\perp X$ or that $Z \perp\!\!\!\perp Y | X$. As an example of the former (due to Miettinen and Cook 1981), let Y = presence or absence of coronary heart disease, X = blood group (Type O or non-O) and Z = gender; it is known that $Z \perp\!\!\!\perp X$. As an example of the latter (taken from Anderson et al. 1980, p. 14), let Y = presence or absence of thromboembolism in women, X = use of oral contraceptives, and Z = religion; one can plausibly argue (although some might reasonably disagree) that $Z \perp\!\!\!\perp Y | X$, at least approximately.

2.4 Amalgamation Paradoxes and AR

Let α be a measure of association between X and Y and let α_i and α_C denote the values of α for $Z = i$ and for the collapsed 2×2 table. Good and Mittal (1987) defined an *amalgamation paradox* (AMP) as a situation where $\alpha_C < \min_i \alpha_i$ or $\alpha_C > \max_i \alpha_i$. Clearly, AR implies AMP. The

following theorem gives, for four measures α , sufficient conditions for avoiding AMP.

Theorem 2.3.

- (a) If $\phi = 0$, then F cannot exhibit AMP with respect to the measures $\alpha_i^{(1)} = \delta_i = p'_i - p_i$, $\alpha_i^{(2)} = p'_i/p_i$, or $\alpha_i^{(3)} = (1 - p'_i)/(1 - p_i)$.
- (b) If $\psi = 0$, then F cannot exhibit AMP with respect to $\alpha_i^{(4)} = \eta_i$ defined in (12).

Good and Mittal (1987, thms. 4.1 and 4.2) showed that the condition $q_i = q$ is sufficient to prevent AMP with respect to $\alpha^{(j)}$, $j = 1, 2, 3, 4$; Theorem 2.3 strengthens Good and Mittal's results. (Theorem 2.3(b) and 2.3(a) for $\alpha^{(1)}$ are special cases of Theorems 3.3 and 3.6, which are proved in Appendix A; Theorem 2.3(a) for $\alpha^{(2)}$ and $\alpha^{(3)}$ also is proved in Appendix A.)

Taken together, Theorems 2.1, 2.2, and 2.3 give an impression of harmony between the twin goals of avoiding AR and avoiding AMP. But the relationship is more dissonant for the most commonly used association measure, the odds ratio (say θ), defined for $Z = i$ by

$$\theta_i = \{p'_i(1 - p_i)\} / \{p_i(1 - p'_i)\}. \quad (14)$$

Let θ_C denote the odds ratio for the collapsed 2×2 table. The following theorem collects known results concerning AMP for the odds ratio.

Theorem 2.4.

- (a) If $Z \perp\!\!\!\perp X | Y$ or $Z \perp\!\!\!\perp Y | X$, then the odds ratio is both constant and collapsible; that is,

$$\theta_i = \theta_C. \quad (15)$$

In particular, F cannot exhibit AMP with respect to θ (Bishop, Fienberg, and Holland 1975).

- (b) If $Z \perp\!\!\!\perp X$ and $Z \perp\!\!\!\perp Y$, then F cannot exhibit AMP with respect to θ (Good and Mittal 1987).
- (c) If $Z \perp\!\!\!\perp X$ or $Z \perp\!\!\!\perp Y$ (but $Z \perp\!\!\!\perp (X, Y)$ is false) and if $\theta_i = \theta_0 \neq 1$, then F must exhibit AMP with respect to θ (Samuels 1981), and, in fact,

$$|\theta_C - 1| < |\theta_0 - 1|. \quad (16)$$

Whittemore (1978) gave necessary and sufficient conditions for (15) to hold.

Theorem 2.4 reveals the quirky nature of the odds ratio. First, note the contrast between (b) and (c). Second, note that each hypothesis in Theorem 2.4 is sufficient to prevent AR, but the hypothesis in (c) guarantees that AMP will occur.

A particularly unsettling consequence of Theorem 2.4(c) is that randomized allocation to levels of X , which prevents AR and prevents AMP for the other measures $\alpha^{(j)}$, $j = 1, 2, 3, 4$, does not prevent AMP for the odds ratio. On the contrary, randomization renders AMP inevitable with respect to any Z that impacts on Y (i.e., any Z such that $Z \perp\!\!\!\perp Y | X$ is false) and for which the odds ratio is constant. We will return to this topic in Section 3.4.

Note that the peculiar relationship between AR and AMP for the odds ratio cannot be expressed in the framework of log-linear models (Bishop et al. 1975) for the $2 \times 2 \times k$ contingency table. The only log-linear models that guarantee

lack of AR are those that satisfy the hypothesis of Theorem 2.4(a), and so cannot exhibit AMP. (The constraint $Z \perp X$ cannot be expressed as a log-linear model.)

Theorem 2.4(c) has the consequence that avoiding AR and avoiding AMP can be incompatible goals. In particular, consider the stratum-matched case-control study, in which controls ($Y = 0$) are matched to randomly sampled cases ($Y = 1$) with respect to Z . The odds ratio is indispensable here because it can be estimated from the data, whereas more straightforward causal parameters, such as $\alpha^{(1)}$, $\alpha^{(2)}$, and $\alpha^{(3)}$, cannot. Because of Corollary 2.8, the matched design guarantees that AR cannot occur in the data. But the design also guarantees that conditions are ripe for AMP, in that (with trivial exceptions) the odds ratio will *not* be collapsible if it is constant. This is a confusing state of affairs, especially if (as some epidemiologists do) one regards noncollapsibility as an indication of “confounding.”

A related difficulty is that the collapsed two-way table from a matched case-control study does not permit estimation of any causally relevant parameters, not even the collapsed odds ratio that would be observed in the population. As a result, Wickramaratne and Holford (1987, p. 763) concluded that (for a nonrare disease) their conditions for “no confounding in the sample” are *not* met by a matched case-control study, even when confounding is absent in the population. Similarly, Holland and Rubin (1988, p. 214), in their analysis of causal inference in case-control studies, concluded that the collapsed two-way table “generally holds no causal interest even for a matched case-control study.” These findings are perhaps too negative and do not give matching the credit it deserves. The common sense view that matching protects against false conclusions due to extraneous variables does have a basis in fact—namely, matching protects against AR, which is a particularly serious form of false conclusion.

3. EXTENSIONS

In this section the notion of AR is extended to the general case where X and Y are real-valued random variables and Z is an arbitrary random variable. It is assumed that X and Z have a joint density with respect to a suitable measure and that $E|Y| < \infty$.

3.1 Definitions

The phenomenon of AR can be defined for any relation, say \mathcal{A} , that indicates directional association between two random variables. We consider four association relations, defined as follows:

- \mathcal{A}_1 : $X \uparrow Y$ [resp. $X \downarrow Y$, $X \perp Y$] if, for all y , $\Pr(Y > y | X = x)$ is strictly increasing [resp. strictly decreasing, constant] in x .
- \mathcal{A}_2 : $X \uparrow Y$ [resp. $X \downarrow Y$, $X \perp Y$] if $E(Y | X = x)$ is strictly increasing [resp. strictly decreasing, constant] in x .
- \mathcal{A}_3 : $X \uparrow Y$ [resp. $X \downarrow Y$, $X \perp Y$] if, for all x and y , $\Pr(X \leq x, Y \leq y) > [\text{resp. } <, =] \Pr(X \leq x)\Pr(Y \leq y)$.
- \mathcal{A}_4 : $X \uparrow Y$ [resp. $X \downarrow Y$, $X \perp Y$] if $\text{cov}(X, Y) > 0$ [resp. < 0 , $= 0$].

We will write $X \uparrow Y(\mathcal{A})$, $X \downarrow Y(\mathcal{A})$, and $X \perp Y(\mathcal{A})$ to indicate which relation is meant. The relations $X \uparrow Y(\mathcal{A}_1)$

and $X \uparrow Y(\mathcal{A}_3)$ are stricter forms of the relations *Y stochastically increasing in X and X and Y positively quadrant-dependent* (Barlow and Proschan 1975). The four relations are connected by the implications $\mathcal{A}_1 \Rightarrow \mathcal{A}_2 \Rightarrow \mathcal{A}_4$ and $\mathcal{A}_1 \Rightarrow \mathcal{A}_3 \Rightarrow \mathcal{A}_4$. Note that $X \perp Y(\mathcal{A})$ is equivalent to $X \perp Y$ for \mathcal{A}_1 and \mathcal{A}_3 , but is weaker than $X \perp Y$ for \mathcal{A}_2 and weaker still for \mathcal{A}_4 .

For a given relation \mathcal{A} , we consider two reversal phenomena: AR and *association distortion*, written as $\text{AR}(\mathcal{A})$ and $\text{AD}(\mathcal{A})$. The concepts *F is a candidate for positive [negative] AR(\mathcal{A})* and *F exhibits positive [negative AR(\mathcal{A})* are defined as in Section 1.1, but with the relations \uparrow , \downarrow , and \perp understood to be in the sense of \mathcal{A} and with “for all z ” understood to mean “for almost all (F) z .” We will say that *F exhibits AD(\mathcal{A})* if *F* is a candidate for positive [negative] AR(\mathcal{A}) and either (a) H_0 is false and $X \downarrow Y(\mathcal{A})$ [$X \uparrow Y(\mathcal{A})$] is false or (b) H_0 is true but $X \perp Y(\mathcal{A})$ is false. Informally, AD occurs if the relation that holds conditionally does not hold unconditionally. For \mathcal{A}_1 , \mathcal{A}_2 , and \mathcal{A}_3 , we have $\text{AR}(\mathcal{A}) \Rightarrow \text{AD}(\mathcal{A})$ but not vice versa; for \mathcal{A}_4 , $\text{AR}(\mathcal{A}) \Leftrightarrow \text{AD}(\mathcal{A})$. If X and Y are both dichotomous, as in Section 2, then all forms of AR and AD are equivalent.

The concept of AMP is readily extended to general F . Let α be a measure of association between X and Y , and let $\alpha(z)$ and α_C be the values of α conditional on $Z = z$ and unconditionally. We will say that *F exhibits AMP with respect to α* if

$$\alpha_C < \inf_z \alpha(z) \quad \text{or} \quad \alpha_C > \sup_z \alpha(z).$$

3.2 General Results

We first consider the relations \mathcal{A}_3 and \mathcal{A}_4 , which are symmetric in X and Y , and ask whether $\text{AR}(\mathcal{A})$ or $\text{AD}(\mathcal{A})$ can occur if Z is not doubly linked to (X, Y) , where double linkage is still defined as in (4) in terms of independence. The answer is no for \mathcal{A}_3 but yes for \mathcal{A}_4 . The following theorem (proved in Appendix A) is an extension of Corollary 2.4.

Theorem 3.1. F cannot exhibit $\text{AR}(\mathcal{A}_3)$ or $\text{AD}(\mathcal{A}_3)$ if Z is not doubly linked to (X, Y) .

For the covariance relation \mathcal{A}_4 , Theorem 3.1 is not true; the unlinkage condition $Z \perp Y | X$ is not sufficient to prevent $\text{AR}(\mathcal{A}_4)$. (A counterexample is given in Appendix B.)

Conditions symmetric in X and Y can be given that are necessary and sufficient for $\text{AR}(\mathcal{A}_4)$. Let

$$\begin{aligned} q(z) &= E(X | Z = z) \\ \tilde{q}(z) &= E(Y | Z = z) \\ \eta(z) &= \text{cov}(X, Y | Z = z). \end{aligned} \tag{17}$$

It is straightforward to show that η_i as defined in (12) is in fact $\eta_i = \text{cov}(X, Y | Z = i)$. Thus the following two theorems (proved in Appendix A) generalize Theorems 2.2 and 2.3(b).

Theorem 3.2. Suppose that F is a candidate for positive [negative] $\text{AR}(\mathcal{A}_4)$. Then F exhibits positive [negative] $\text{AR}(\mathcal{A}_4)$ if and only if $\psi > 0$ [$\psi < 0$] and $|\psi| \geq |\eta|$, where $\psi = \text{cov}[q(Z), \tilde{q}(Z)]$ and $\eta = E[\eta(Z)]$.

Corollary 3.1. If $Z \perp X(\mathcal{A}_2)$ or $Z \perp Y(\mathcal{A}_2)$, then F cannot exhibit any form of AR.

Theorem 3.3. If $\psi = 0$, then F cannot exhibit AMP with respect to covariance.

For the relations \mathcal{A}_1 and \mathcal{A}_2 , which are not symmetric in X and Y , the following asymmetric version of Theorem 3.1 holds. (See Appendix A for proof.)

Theorem 3.4. For $\mathcal{A} = \mathcal{A}_1$ or \mathcal{A}_2 , F cannot exhibit AR(\mathcal{A}) or AD(\mathcal{A}) if either (a) $Z \perp X$ or (b) $Z \perp Y(\mathcal{A})|X$.

Note that Theorems 3.1, 3.2, and 3.4 together show that the condition $Z \perp X$ prevents all forms of AR and AD.

3.3 AR and AMP When X is Dichotomous

In this section X is assumed dichotomous, and two of the results given in Section 2 for the $2 \times 2 \times k$ contingency table are generalized to the case of real-valued Y and arbitrary Z . We consider only AR(\mathcal{A}_2), which here is equivalent to AR(\mathcal{A}_4), AD(\mathcal{A}_2), and AD(\mathcal{A}_4).

Assume that $X = 0$ or 1. Then $q(z)$ as defined in (17) is $q(z) = \Pr(X = 1|Z = z)$.

Define

$$\begin{aligned}\mu(z) &= E(Y|X = 0, Z = z) \\ \mu'(z) &= E(Y|X = 1, Z = z) \\ \delta(z) &= \mu'(z) - \mu(z).\end{aligned}\quad (18)$$

As in Section 2, one may visualize a population of individuals, with $X = 0, 1$ representing no treatment and treatment, Y representing a response variable, and Z representing a covariate. Then $q(z)$ is the probability that an individual with $Z = z$ receives the treatment and $\mu'(z)$ and $\mu(z)$ are the expected responses among treated and untreated individuals with $Z = z$.

Let

$$\begin{aligned}q &= E[q(Z)] \\ \phi &= \text{cov}[\mu(Z), q(Z)] \\ \delta &= q^{-1}E[\delta(Z)q(Z)].\end{aligned}\quad (19)$$

The following theorems (proved in Appendix A) generalize Theorem 2.1 and part of Theorem 2.3.

Theorem 3.5. Suppose that X is dichotomous and F is a candidate for positive [negative] AR(\mathcal{A}_2). Then F exhibits positive [negative] AR(\mathcal{A}_2) if and only if $\phi > 0$ [$\phi < 0$] and $|\phi| \geq |\delta|q(1 - q)$.

Theorem 3.6. Suppose that X is dichotomous and $\phi = 0$. Then F cannot exhibit AMP with respect to the association measure $\delta(z)$.

As in Section 2, the parameters ϕ and δ are easily interpreted in statistical terms. Using causal language as in Section 2.1, the condition $\phi > 0$ means that individuals more likely to receive the treatment also tend to be those whose expected response would be relatively high even without treatment; positive AR occurs if this tendency outweighs the treatment effect parameter δ .

3.4 AR and AMP in the Linear Regression Model

In the linear regression setting specified by

$$E(Y|X, Z) = \beta_0 + \beta_1 X + \beta_2 Z, \quad (20)$$

F is always a candidate for AR(\mathcal{A}_2) and AR(\mathcal{A}_4). Two well-known results are stated here in terms that highlight the parallels with previous sections; proofs are in Appendix A.

Theorem 3.7. Suppose that F satisfies (20) with $\beta_1 \leq 0$ [≥ 0]. Then F exhibits positive [negative] AR(\mathcal{A}_4) if and only if $\phi^* > 0$ [$\phi^* < 0$] and $|\phi^*| \geq |\beta_1| \text{var}(X)$, where

$$\phi^* = \beta_2 \text{cov}(X, Z). \quad (21)$$

Corollary 3.2. Theorem 3.7 holds for AR(\mathcal{A}_2).

Corollary 3.3. Suppose that, in addition to (20), $E(Y|X)$ is a monotone function of X . Then Theorem 3.7 holds for AD(\mathcal{A}_2).

Theorem 3.7 is analogous to Theorem 3.5. The coefficient β_1 is analogous to δ ; moreover, in the context of Theorem 3.5, we have $\text{var}(X) = q(1 - q)$. The parameters ϕ and ϕ^* have similar interpretations. For instance, $\phi^* > 0$ means that individuals who tend to have larger X also tend to have higher expected response Y for fixed X .

Define the regression coefficient of Y on X as

$$\beta_{1C} = \frac{\text{cov}(X, Y)}{\text{var}(X)}.$$

Now, (20) implies that

$$\beta_1 = \frac{\text{cov}(X, Y|Z)}{\text{var}(X|Z)}.$$

Consequently, AMP with respect to the regression coefficient occurs if $\beta_1 \neq \beta_{1C}$. The following theorem is analogous to Theorem 3.6.

Theorem 3.8. Suppose that F satisfies (20) and $\phi^* = 0$. Then F cannot exhibit AMP with respect to the regression coefficient.

The analogies between Theorems 3.5 and 3.7 and Theorems 3.6 and 3.8 can be made even closer. Let $\mu_x(z) = E(Y|X = x, Z = z)$ in analogy to the definition of $\mu(z)$ in (18). If it is now assumed, in addition to (20), that $q(z)$ as defined in (17) is a linear function of z , then it is straightforward (see Appendix A) to show that

$$\phi^* = \text{cov}[\mu_x(Z), q(Z)], \quad (22)$$

which is exactly analogous to ϕ as defined in (19).

3.4 AR and AMP in the Logistic Regression Model

Assume that Y takes values 0 and 1 and consider the logistic regression model given by

$$\log\{p(X, Z)/[1 - p(X, Z)]\} = \gamma_0 + \gamma_1 X + \gamma_2 Z, \quad (23)$$

where $p(X, Z) = \Pr(Y = 1|X, Z)$. In this model AR(\mathcal{A}_1) \Leftrightarrow AR(\mathcal{A}_2), and F is always a candidate for all forms of AR. If $Z \perp X$ or $\gamma_2 = 0$, then F cannot exhibit any form of AR or AD.

Model (23) is similar to the linear regression model (20) but differs in an important respect. For linear regression, the condition $Z \perp X$ not only prevents AR, but also prevents AMP with respect to the regression coefficient. The situation is quite different for logistic regression. In particular, suppose that X in (23) takes values 0 and 1. Then the condition $Z \perp X$ prevents AR but (unless $\gamma_1 = 0$ or $\gamma_2 = 0$) it guarantees that AMP will occur—that is, $\gamma_1 \neq \gamma_{1C}$, where γ_{1C} is defined by the unconditional model

$$\log \{p(X)/[1 - p(X)]\} = \gamma_{0C} + \gamma_{1C}X, \quad (24)$$

where $p(X) = \Pr(Y = 1 | X)$. This result is a simple extension of Theorem 2.4(c); both γ_1 and γ_{1C} are logarithms of odds ratios. Note that the model (24) does not constrain the joint distribution of X and Y , and so cannot fail to hold.

This counterintuitive result for dichotomous X in the model (23) is especially perplexing, because it means that randomized allocation to levels of X makes AMP inevitable. How should one view this situation? Gail, Wieand, and Piantadosi (1984), in discussing the randomized experiment, regarded γ_1 as the “true” measure of treatment effect and, by implication, regarded γ_{1C} as “false.” This view seems to lead to an infinite regress, because there is always another covariate lurking somewhere. A more even-handed view would be that γ_1 and γ_{1C} are equally valid, although different, measures of treatment effect. This appears to be the view taken by Holland and Rubin (1988, p. 217), who described γ_{1C} (actually, $e^{\gamma_{1C}}$) as a “population-level causal parameter.”

4. CONCLUSIONS

Simpson's paradox is actually no more paradoxical than the reversal or distortion of association in other settings, no more, for instance, than the familiar fact that a partial regression coefficient can have a different sign from a simple regression coefficient. Among the AR and AD phenomena studied in this article, all but one can occur only if the covariate Z is doubly linked to X and Y . (The exception is reversal of covariance, which can occur even without double linkage; see Sec. 3.2.)

The paradox of AR for linear regression is readily “explained” graphically by displaying a scatterplot of Y versus X for several values of Z . The covariance parameter ϕ provides an equally simple explanation of Simpson's paradox for the $2 \times 2 \times k$ contingency table and, more generally, of AR(\mathcal{A}_2) in the more general case of dichotomous X and real-valued Y (Theorem 3.5); moreover, the parameter ϕ has a natural analog ϕ^* in the linear regression setting. The symmetric covariance parameter ψ is also available for explanation of Simpson's paradox and, more generally, of reversal of covariance (Theorem 3.2). In many cases, however, ϕ may be more useful heuristically than ψ , especially when X is explanatory or causal and Y is a response.

Amalgamation paradoxes are closely tied to AR phenomena, and sufficient conditions for preventing AR will often prevent AMP also. The odds ratio is an exception to this pattern, however; its peculiar behavior (Secs. 2.4 and 3.4), which has confusing implications both for design and analysis, may itself deserve to be called “paradoxical.”

APPENDIX A: PROOFS

A.1 Proofs of Theorems 2.1, 2.3(a), 3.1, 3.4, 3.5, and 3.6

Lemma 1. Let X and Z have a joint density with respect to a suitable measure and let $f_{X|Z}(x|z)$, $f_X(x)$, and $G(z)$ denote the conditional density of X given Z , the marginal density of X , and the distribution function of Z . Let $k(x, z)$ be any function such that $E|k(X, Z)| < \infty$. Then for any x_1 and x_2 with $f_X(x_1)f_X(x_2) > 0$, we can write

$$\begin{aligned} E[k(X, Z)|X = x_2] - E[k(X, Z)|X = x_1] \\ = [f_X(x_2)]^{-1} \int [k(x_2, z) - k(x_1, z)] f_{X|Z}(x_2|z) dG(z) \\ + [f_X(x_1)f_X(x_2)]^{-1} \int k(x_1, z) [f_X(x_1)f_{X|Z}(x_2|z)] \\ - f_X(x_2)f_{X|Z}(x_1|z)] dG(z). \quad (A.1) \end{aligned}$$

Proof. Using Bayes's theorem to invert the conditional distribution of Z given X , we can write $E[k(X, Z)|X = x] = [f_X(x)]^{-1} \int k(x, z) f_{X|Z}(x|z) dG(z)$.

Therefore,

$$\begin{aligned} E[k(X, Z)|X = x_2] - E[k(X, Z)|X = x_1] \\ = [f_X(x_2)]^{-1} \int k(x_2, z) f_{X|Z}(x_2|z) dG(z) \\ - [f_X(x_1)]^{-1} \int k(x_1, z) f_{X|Z}(x_1|z) dG(z). \quad (A.2) \end{aligned}$$

It is straightforward to rewrite (A.2) as (A.1), and Lemma 1 is proved.

To prove Theorem 3.5, let $x_1 = 0$ and $x_2 = 1$. Then $f_X(x_1) = 1 - q$ and $f_X(x_2) = q$. Set $k(x, z) = E(Y|X = x, Z = z)$ in Lemma 1. Using the notation (19) and letting $\delta_C = E(Y|X = 1) - E(Y|X = 0)$, Equation (A.1) becomes

$$\delta_C = \delta + \phi/[q(1 - q)]. \quad (A.3)$$

Theorem 3.5 is immediate from (A.3). Theorem 2.1 is a special case of Theorem 3.5.

Theorem 3.6 follows from (A.3) on noting from (19) that $\inf_z \delta(z) \leq \delta \leq \sup_z \delta(z)$. Theorem 2.3(a) for $\alpha^{(1)}$ is a special case of Theorem 3.6.

To prove Theorem 2.3(a) for $\alpha^{(2)}$, note that $\phi = 0 \Rightarrow \Pr(Y = 1 | X = 0) = p$. Using (A.3), this implies that $\alpha_C^{(2)} = \sum \alpha_i^{(2)} w_i$, where $w_i = p_i q_i r_i / pq$. If $\phi = 0$, then $\sum w_i = 1$, so that AMP cannot occur, and the result is proved. Theorem 2.3(a) for $\alpha^{(3)}$ follows by symmetry.

To prove Theorem 3.1, fix x and y , let X^* and Y^* be indicators of the events $[X \leq x]$ and $[Y \leq y]$, and apply Corollary 2.4 to X^* and Y^* .

To prove Theorem 3.4 for \mathcal{A}_1 , fix y and set $k(x, z) = \Pr(Y > y | X = x, Z = z)$ in Lemma 1. If either condition (a) or (b) of Theorem 3.4 holds, then the second term in (A.1) vanishes. First, suppose that F is a candidate for positive AR and H_0 is false. Then, for any $x_1 < x_2$, we have $\Pr(Y > y | X = x_2, Z = z) \leq \Pr(Y > y | X = x_1, Z = z)$ for all z , with strict inequality for a Z set of positive probability, so (A.1) implies that $\Pr(Y > y | X = x_2) < \Pr(Y > y | X = x_1)$.

Table A.1. Counterexamples Concerning ϕ , $\tilde{\phi}$ and ψ

Example	p_1	p'_1	p_2	p'_2	q_1	q_2	r_1	r_2
1	.8	.3	.7	.4	.3	.4	.5	.5
2	.8	.3	.7	.6	.3	.4	.5	.5

Table A.2. Counterexample Concerning AR(\mathcal{A}_4)

X	Y	Z	Prob.	X	Y	Z	Prob.
0	1	1	.24	0	1	2	.01
1	2	1	.24	1	2	2	.01
2	0	1	.01	2	0	2	.24
3	1	1	.01	3	1	2	.24

$= x_1$); thus F does not exhibit AD. The arguments for negative AD and for AD when H_0 is true are similar. To prove Theorem 3.4 for \mathcal{A}_2 , set $k(x, z) = E(Y|X = x, Z = z)$ in Lemma 1 and proceed as for \mathcal{A}_1 .

A.2 Proofs of Theorems 2.2, 2.3(b), 3.2, and 3.3

Theorems 3.2 and 3.3 are immediate from the well-known identity

$$\text{cov}(X, Y) = E[\text{cov}(X, Y|Z)] + \text{cov}[E(X|Z), E(Y|Z)].$$

Theorems 2.2 and 2.3(b) are special cases of Theorems 3.2 and 3.3.

A.3 Proofs of Theorems 3.7 and 3.8 and Equation (22)

It follows from (20) that $\text{cov}(X, Y) = \beta_1 \text{var}(X) + \beta_2 \text{cov}(X, Z)$; therefore, $\beta_{1C} = \beta_1 + \phi^*/\text{var}(X)$, and Theorems 3.7 and 3.8 follow immediately. If, in addition, $q(z)$ is a linear function of z , then $q(z) = \kappa_0 + \kappa_1 z$, where $\kappa_1 = \text{cov}(X, Z)/\text{var}(Z)$ and κ_0 is a constant. It then follows that

$$\begin{aligned} \text{cov}[\mu_x(Z), q(Z)] &= \text{cov}(\beta_0 + \beta_1 x + \beta_2 Z, \kappa_0 + \kappa_1 Z) \\ &= \beta_2 \kappa_1 \text{var}(Z) = \beta_2 \text{cov}(X, Z) \\ &= \phi^*, \end{aligned}$$

as claimed in Equation (22).

APPENDIX B: COUNTEREXAMPLES

B.1 Counterexamples Concerning ϕ , $\tilde{\phi}$, and ψ

In Section 2.2 it was stated that ϕ , $\tilde{\phi}$, and ψ need not agree in sign. The examples in Table A.1 illustrate this point. For Example 1, $\phi < 0$ and $\psi < 0$ but $\tilde{\phi} > 0$; for Example 2, $\phi < 0$ and $\tilde{\phi} < 0$ but $\psi > 0$. (Notation is defined in equations (5), (6), and (8), in the first paragraph of Section 2.2, and in Theorem 2.2.) For both examples, F is a candidate for positive AR.

B.2 Counterexample Concerning AR(\mathcal{A}_4)

In Section 3.2 it was stated that the unlinkage condition $Z \perp\!\!\!\perp Y|X$ is not sufficient to prevent AR(\mathcal{A}_4), as defined in Sec-

tion 3.1. Table A.2 shows an F that exhibits AR(\mathcal{A}_4) even though $Z \perp\!\!\!\perp Y|X$. For Table A.2, $\text{cov}(X, Y|Z = 1) = \text{cov}(X, Y|Z = 2) = .1732$, but $\text{cov}(X, Y) = -.25$. (In Table A.2 the conditional distribution of Y given X is degenerate, but it is easy to construct a lengthier example for which this is not the case.)

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