Faculty of Sciences

Effect size measures for mediation models: a critical evaluation of $\kappa^2$

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Master dissertation submitted to obtain the degree of Master of Statistical Data Analysis

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Academic Year 2014-2015
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Foreword

I would like to thank Lien for the support during this master program, my promotor Tom Loeys for his device, feedback and encouragement during this process of writing a master thesis, the department of data-analysis to give me the opportunity to follow this master in statistical data analysis and all the teachers of the master program for the numerous learning moments during the last two years.
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1 Abstract

Since the paper of Baron & Kenny (1986) mediation analyses are widely used in applied research. Preacher & Kelley (2011) gave an extended overview of effect sizes for mediation models and propose their own effect size for the simple mediation model: $\kappa^2$. In these master thesis we formulate some criticisms on the current estimation method of $\kappa^2$ in addition of Wen & Fan (2015). Next we propose a new estimation method to tackle the current shortcomings. A simulation study was conducted to study the behaviour and the characteristics of the new estimation method. Further we extend our method to more complex models, such as models with exposure-mediator interaction and/or a confounder for mediator-outcome relationship. An R-function $\text{MaxIE}$ was developed such that an applied researcher gets an estimate for $\kappa^2$ with a minimal of input.
2 Introduction

Throughout this section we focus on the key words of the title. First we introduce the term mediation by means of the simple mediation model. After introducing the basic model we consider some more complex models. Next we focus on the term effect size, we give a definition and sum up some desiderata for good effect sizes. Further a short overview of the different effect sizes used in mediation analysis is given. In a third section we consider \( \kappa^2 \) in more detail since this effect size is of primary interest in this master thesis. At the end of this section we formulate our research goals.

2.1 Mediation models

2.1.1 Simple mediation model

When a researcher finds an effect of exposure \( X \) on an outcome \( Y \), the underlying mechanism is often of interest. There could be a third variable \( M \) which is caused by exposure \( X \) and which causes outcome \( Y \). Figure 1 depicts the simple mediation model, where \( a \) denotes the effect of \( X \) on \( M \), \( b \) the effect of \( M \) on \( Y \) and \( c' \) the effect of \( X \) to \( Y \) not going through \( M \). This latter effect is called the direct effect of \( X \) to \( Y \). Further the effect of \( X \) on \( Y \) that goes through \( M \) is called the indirect effect. In simple linear setting the indirect effect is given by the product \( ab \). The widely known causal step approach of Baron and Kenny [1986] relies on three regression equations:

\[
Y_i = \hat{i}_T + cX + \epsilon_T
\]

\[
M_i = \hat{i}_M + aX_i + \epsilon_M
\]

\[
Y_i = \hat{i}_Y + c'X_i + bM_i + \epsilon_Y
\]

where \( \hat{i}_T, \hat{i}_M \) and \( \hat{i}_Y \) denote the intercepts and \( \epsilon_T, \epsilon_M \) and \( \epsilon_Y \) denote the individual error terms where \( \epsilon_M \) and \( \epsilon_Y \) are independent. Estimators of the different paths could be obtained by linear regressions using OLS-estimation [MacKinnon 2008]. The estimators \( \hat{c}' \) and \( \hat{a}\hat{b} \) will be unbiased for the direct and indirect effect if the ignorability assumptions hold [Pearl 2014]:
• (A1) no unmeasured confounders of the $X$-$M$ relationship

• (A2) no unmeasured confounders of the $X$-$Y$ relationship

• (A3) no unmeasured confounders of the $M$-$Y$ relationship

• (A4) no confounders of the $M$-$Y$ relationship are affected by $X$

Note that randomization of exposure $X$ is not enough to conclude that all assumptions hold. It only implies that assumptions (A1) and (A2) are satisfied.

![Diagram of the simple mediation model](image)

**Figure 1:** The simple mediation model

### 2.1.2 More complex mediation models

In practice it is not realistic to assume that the simple mediation model is the correct model. A researcher will add baseline covariates, for instance to control for differences between groups (men vs women), or expects that there is more than one underlying mechanism to explain the effect of $X$ on $Y$, which implies multiple mediators. Another possibility is that researchers add confounders of the $M$-$Y$ relationship to make assumption (A3) more plausible or could be interested in adding interactions, for instance between treatment and mediator. Obviously, there are many extensions of the simple mediation model, but in this section we focus on a model with two mediators, a model with a measured confounder for $M$-$Y$ relationship and a model with $X$-$M$ interaction.

Figure 2 (left) shows the model with a measured confounder $C_1$ for the $M$-$Y$ relationship. We assume that the confounder $C_1$ is independent of treatment $X$ and assumption
(A4) holds. Assumption (A3) will hold if there is no unmeasured \( M-Y \) confounding conditional on \( C_1 \). To make this assumption more plausible, researchers should think about possible confounders for \( M-Y \) relationship and add them to the model. If assumption (A3) holds, the causal parameters of interest could be unbiasedly estimated, i.e. \( c' \) for the direct effect and \( ab \) for the indirect effect. Note that when exposure \( X \) is not randomized, assumptions (A3) and (A4) can not be taken for granted and should be assessed.

Figure 2 (right) depicts the mediation model with two mediators \((M_1 \text{ and } M_2)\). Here we make the assumption that both mediators are independent of each other. In this model we could still make the distinction between the direct effect \((c')\) and the indirect effect \((a_1b_1 + a_2b_2)\). Since we assume independent mediators we could separate the indirect effect in an indirect effect through the first mediator \(M_1\) (i.e. \(a_1b_1\)), and an indirect effect through the second mediator \(M_2\) (i.e. \(a_2b_2\)). Again one should assess the assumptions (A1) to (A4) before estimating and interpreting the parameters of the model. Estimation of these parameters can be done by linear regression using OLS-estimation.

A model with \( X-M \) interaction assumes that the effect of the mediator on outcome depends on treatment. A possible data generating mechanism is:

\[
M_i = aX_i + \epsilon_M \tag{4}
\]

\[
Y_i = c'X_i + bM_i + dX_iM_i + \epsilon_Y \tag{5}
\]

with all variables standardized such that the intercepts are 0 and the regression coefficients
are standardized. In such a model we have to redefine the causal effects. VanderWeele (2013) propose a decomposition of the total effect in a pure direct ($c'$), pure indirect ($ab$) and interactive mediated effect ($ad$). This decomposition is based on the counterfactual framework (Greenland & Robins 1992; Pearl 2001), which is outside the scope of this master thesis.

2.2 Effect sizes

2.2.1 Definition and desiderate of a good effect size

Kelley & Preacher (2012) define effect size as a quantitative reflection of the magnitude of some phenomenon that is used for the purpose of addressing a question of interest. Grissom & Kim (2005) use the term effect size for measures of the degree to which results differ from what is implied for them by a null hypothesis. There are four general categories of effect sizes (Ferguson, 2009): Group difference indices (f.i. Cohen’s d), Strength of association indices (f.i. Pearson r), Corrected estimates (f.i. adjusted $R^2$) and risk estimates (measures compare relative risk for a particular outcome between two or more groups).

What are the important characteristics of a good effect size? Borenstein, Hedges, Higgins, & Rothstein (2009) state that effect sizes should not depend on aspects of study design (i.e. scaled appropriately), have good technical properties (sampling distribution known) and should be interpretable. Kelley & Preacher (2012) extend the latter property by stating that the estimates of the effect size should be unbiased, consistent and efficient. Wen & Fan (2015) consider monotonicity as a basic property of an effect size measure. If the effect becomes larger, the magnitude of the effect size should become larger.

2.2.2 Different effect sizes for mediation analysis

In this section we give a brief overview of effect sizes for mediation analysis. We refer the interested reader to the paper of Preacher & Kelley (2011) for an extensive discussion of each effect size and possible advantages and drawbacks. Here we focus on the capacity of the effect sizes to handle more complex models.
• Verbal descriptors

Two terms are commonly used: complete or partial mediation. The interpretation of these two terms is subjective because these are not expressed in a meaningfully scaled metric (Preacher & Kelley 2011). Despite its limited usefulness these effect size measure can be used in more extended models without any adaptation.

• Ratio measures of relative magnitude

There are different ratios defined in the past. The most common ratio reported, is the proportion mediated which is the ratio of the indirect effect to the total effect. Problem is the misleading name since the effect size is not a proportion. It could be larger than 1 and also negative in case of suppression ($c' < 0$). Shrout & Bolger (2002) recommend to compute this effect size only when there is no strong evidence of suppression. In case of slight empirical suppression which is not statistically significant, they recommend to set the effect size at the upper bound of 1. Another disadvantage of this effect size is that a relatively large sample size is needed (> 500) to have a acceptable small standard error (MacKinnon, Warsi, & Dwyer 1995).

Another ratio is introduced by Sobel (1982) which compares the indirect effect to the direct effect. Both measures could be used in extended models, f.i. with multiple mediators. Fairchild, Mackinnon, Taborga, & Taylor (2009) report that the proportion mediated provides a means to assess the relative contribution of single mediators in multiple mediator models.

• Unstandardized, partially and completely standardized indirect effects

Unstandardized indirect effects can be used when the original variables are already in a meaningful metric. Partially standardized effect is proposed by MacKinnon (2008) and is the ratio of the indirect effect to the standard deviation of $Y$. These effect size is easy to extend to more complex models because its interpretation remains the same, i.e. the number of standard deviations by which $Y$ is expected to increase/decrease per $a$ change in the mediator. The complete standardized indirect effect is the partially standardized indirect effect multiplied by the standard devia-
tion of $X$. Preacher & Hayes (2008) refer to this effect size as the index of mediation. Different adaptations for more complex models were proposed, for instance Stapleton, Pituch, & Dion (2014) extend this effect size for multilevel designs. But we have to keep in mind that standardization does not make the scaling of the indirect effect any more meaningful if $X$ and $Y$ are arbitrary scales without quantitative meaning (Hayes, 2009).

• Indices of explained variance

MacKinnon (2008) introduces three proportions of explained variance for the mediation context. Preacher & Kelley (2011) conclude that only one of them is an appropriate effect size:

$$R^2 = r_{MX}^2 r_{YM,X}^2$$  \hspace{1cm} (6)

A second one is a rescaled version which is difficult to interpret, while the third effect size is technically not a proportion of variance. Preacher & Kelley (2011) nicely summarize the critics on the indices of explained variance in the literature. The explained variance depends on how much variance there is to explain (Nakagawa & Cuthill, 2007) and this can differ from study to study which implies that this effect size can not be used to compare different studies. Further one assume that the amount of variance to be explained is 100%, but is in practice often less due to measurement error (Sechrest & Yeaton, 1982).

• Other effect sizes

Preacher & Kelley (2011) report some other effect sizes are less frequent, for example the effect size index for two groups Hansen & McNeal (1996). Further they propose two new effect sizes: the residual based index and the $\kappa^2$.

2.3 $\kappa^2$

Preacher & Kelley (2011) introduce and recommend this effect size because it has all desirable properties of a good effect size. The definition is simple: $\kappa^2$ is the magnitude of
the indirect effect relative to the maximum possible indirect effect. The idea behind is quite intuitive: conditional on characteristics of design or variables, there is a range of possible values for each regression coefficient of the indirect effect (i.e. \(a\) and \(b\)). Since the indirect effect in simple linear settings is a product of two regression coefficients, it has a limited range of possible values. More specifically, the maximum possible indirect effect is the product of the maximum possible value of \(a\) and the maximum possible value of \(b\).

Preacher & Kelley (2011) provides closed form expressions for the range of possible values for \(a\) and \(b\) in the simple mediation model. To find the maximum possible indirect effect they start from the linear model with standardized variables which implies that there are no intercepts and that the regression coefficients are the standardized coefficients:

\[
Y_i = cX + \epsilon_T \\
M_i = aX_i + \epsilon_M \\
Y_i = c'X_i + bM_i + \epsilon_Y
\]

with \(\epsilon_T, \epsilon_M\) and \(\epsilon_Y\) error terms which are normally distributed and where \(\epsilon_M\) and \(\epsilon_Y\) are mutually independent. Note that correlation between \(X\) and \(M\), denoted by \(\rho_{XM}\) is given by \(a\) and the correlation between \(X\) and \(Y\), \(\rho_{XY}\), is given by \(c\).

Preacher & Kelley (2011) fix the total effect (i.e. \(c\) in eq. (7)) at a specific value (i.e. \(\hat{c}\)), which does not imply that the indirect effect \(ab\) is bounded because \(b\) is not bounded. The solution they propose, is fixing \(a\) on a specific value, such that \(b\) is bounded and consequently the indirect effect \(ab\). When you have the possible range of values for \(b\), given \(a\), you choose the most extreme value, \(\mathcal{R}(b)\), of the range with the same sign as the point estimate \(\hat{b}\). On the other hand, if you fix \(b\) at a specific value, you find the range of possible values for \(a\) and you can select the most extreme value, \(\mathcal{R}(a)\), with the same sign as the point estimate \(\hat{a}\) to obtain the maximum possible value for \(a\). Now you have for the two coefficients of the indirect effect the maximum possible value. Multiplying both values yields the maximum possible indirect effect, \(\mathcal{R}(a)\mathcal{R}(b)\). \(\kappa^2\) is than given by:

\[
\kappa^2 = \frac{\hat{a}\hat{b}}{\mathcal{R}(a)\mathcal{R}(b)}
\]
The closed form expressions of the upper and lower bounds are based on the covariance matrix of \(X, M\) and \(Y\). This covariance matrix \(S\) should be nonnegative defined (Hubert, 1972 in Preacher & Kelley (2011)). More specifically:

\[
S = \begin{pmatrix}
A & G \\
G' & \text{var}(Y)
\end{pmatrix} = \begin{pmatrix}
\sigma_X^2 & \sigma_{XM} & \sigma_{XY} \\
\sigma_{XM} & \sigma_M^2 & \sigma_{MY} \\
\sigma_{XY} & \sigma_{MY} & \sigma_Y^2
\end{pmatrix}
\]

with \(S\) is nonnegative definite if \(G'A^{-1}G \leq \text{var}(Y)\). Working out the latter equality leads to an allowed range of \(a\) values:

\[
a \in \sigma_Y \sigma_M \pm \sqrt{\sigma_Y^2 \sigma_M^2 - \sigma_{XY}^2} \left/ \sqrt{\sigma_X^2 \sigma_Y^2 - \sigma_{XY}^2} \right. \tag{11}
\]

with \(b\) and \(c\) fixed. Preacher & Kelley (2011) define \(\Re(a)\) as the most extreme value of \(a\) with the same sign, when \(b\) and \(c\) are hold fixed. For example if \(\hat{a} = -0.5\) than \(\Re(a)\) equals the bound found by (11) which is negative. Following the same reasoning they found the range for parameter \(b\) given \(a\) and \(c\) fixed:

\[
b \in \left\{ \pm \sqrt{\sigma_X^2 \sigma_Y^2 - \sigma_{XY}^2} / \sqrt{\sigma_X^2 \sigma_M^2 - \sigma_{XM}^2} \right\} \tag{12}
\]

\(\Re(b)\) denotes now the most extreme value of \(b\) found by equation (12) with the same sign as \(\hat{b}\), when \(a\) and \(c\) are hold fixed. The maximum possible indirect effect is defined as \(\Re(a)\Re(b)\). The derivations of the ranges of \(a\) and \(b\) can be found in appendix A of Preacher & Kelley (2011).

### 2.4 Research goals

Throughout this section we introduced the key conceptions of our research: mediation, effect size and \(\kappa^2\). The goal of this master thesis is to make some critical remarks on the work of Preacher & Kelley (2011) and the critics on this paper by Wen & Fan (2015). Further we propose a new method which is easy to implement. Moreover the extension of this method to more complex models is very straightforward. A third and most important research goal is to formulate some critical remarks about the effect size measure \(\kappa^2\), even after the introduction of our new estimation method.
3 Method

3.1 The problems of $\kappa^2$

The idea of a maximum possible indirect effect seems attractive, but from our point of view there are some shortcomings in the way it is calculated.

To determine the maximum possible value for $a$ or $b$ we take the most extreme value with the same sign. This implies an underlying assumption that we have unbiased estimators and standard errors, which is not mentioned by Preacher & Kelley (2011). Small differences in point estimates $\hat{a}$ and $\hat{b}$ when these are near 0 and/or the confidence interval contains 0, could yield large differences in $\kappa^2$. More specifically, for $\hat{b}$ makes this no difference in absolute value, since the possible range of values is symmetric, only the sign of the maximum value would change. In contrast the range of possible values for $a$ is asymmetric and a large asymmetry can lead to large difference in the most extreme value for $a$ depending on the sign of $\hat{a}$. Consequently large difference can be introduced for the maximum possible indirect effect and thus for $\hat{\kappa}^2$.

Secondly, considering $\kappa^2$ in his current form learns us that Preacher & Kelley (2011) condition on the total effect, $c$, to determine the maximum possible value for $a$ and $b$. In the simple linear setting we know that the total effect $c$ can be written as the sum of the direct effect $c'$ and the indirect effect $ab$, i.e. $c = c' + ab$. The latter expression shows us that if you search for the maximum value of $a$, conditional on $b$ and $c$ implies that you search the maximum value of $a$ conditional on $a$. This seems contradictory and to obtain correct expressions for maximum $a$ and $b$, we think that one should condition on $c'$ instead of $c$.

A third remark is whether it makes sense that you only obtain the maximum value for each path of the indirect effect separately while holding the other path constant? Shouldn’t it be the case that you search immediately for the maximum possible indirect effect? From our point of view and confirmed by the development of an alternative strategy (see further) the maximum possible indirect effect is always finite if you let vary $a$ and $b$ together,
conditional on $c'$, while this is not guaranteed if you condition on $c$.

The concern of infinity was recently reported by Wen & Fan (2015). Further the researchers consider monotonicity as a basic property of an effect size measure, which implies that when the effect becomes larger, the magnitude of the effect size becomes larger. They argue that this does not hold for $\kappa^2$, because the equation $\Re(ab) = \Re(a)\Re(b)$ is generally not true. Further they argue that $\kappa^2$ is incorrectly defined because the maximum value of the indirect effect $ab$ could be infinite (Wen & Fan, 2015). Their conclusion is that $\kappa^2$ can not be used as an effect size.

The problem of this article is that it copies the method of Preacher and Kelley (2015), and thus also the conditioning on the total effect, $c$. Table 1 (left) shows the results for the example they use to show the non-monotonicity of $\kappa^2$, while conditioning on $c$. On right hand side we report our results conditional on $c'$ instead of $c$. Because the mathematical derivation is complex, we use a self-writed R function to calculate the maximum possible values of paths $a$ and $b$ (see further). We see that results are contradictory and that the example given in the article of Wen & Fan (2015) does not show the non-monotonicity of $\kappa^2$ if you condition on $c'$.

Next to the fact that the closed-form expressions proposed by Preacher & Kelley (2011) are wrong, they also only are correct for the simple mediation setting with one mediator and with no covariates considered in the model. Wen & Fan (2015) want to show the paradoxical behaviour of $\kappa^2$ in multiple mediator models. They start with the correlation matrix between $X$, $M_1$, $M_2$ and $Y$, whereby there is no correlation between the 2 mediators ($\rho_{M_1, M_2} = 0$). Like Preacher & Kelley (2011) they use mathematical derivations to obtain maximum possible effects, which become complex. Moreover they follow the same strategy as in the previous example by conditioning on $c$. We have the same critics as before, that you let vary $a$, conditional on $c$ which depends on $a$ since $c = c' + ab$. Again we doubt if the obtained results are correct.

It is clear that a simple setting with no covariates is very unlikely to be correct in practice. Implicitly one makes the assumption that there are no confounders for mediator-outcome relationship. Since randomization of the exposure only excludes unmeasured
### Situation 1: $ab = .1390, a = .291, b = .478, c = .19$ and $c' = .051$

<table>
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<th>Conditional on $c$</th>
<th>Conditional on $c'$</th>
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</thead>
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<tr>
<td>$#a$</td>
<td>.948</td>
<td>1</td>
</tr>
<tr>
<td>$#b$</td>
<td>1.026</td>
<td>.983</td>
</tr>
<tr>
<td>$#ab$</td>
<td>.973</td>
<td>.983</td>
</tr>
<tr>
<td>$\kappa^2$</td>
<td>.143</td>
<td>.1415</td>
</tr>
</tbody>
</table>

### Situation 2: $ab = .13625, a = .25, b = .545, c = .19$ and $c' = .054$

<table>
<thead>
<tr>
<th></th>
<th>Conditional on $c$</th>
<th>Conditional on $c'$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$#a$</td>
<td>.921</td>
<td>1</td>
</tr>
<tr>
<td>$#b$</td>
<td>1.014</td>
<td>.985</td>
</tr>
<tr>
<td>$#ab$</td>
<td>.934</td>
<td>.985</td>
</tr>
<tr>
<td>$\kappa^2$</td>
<td>.146</td>
<td>.138</td>
</tr>
</tbody>
</table>

**Table 1:** Comparison of the results of theoretical example given in Wen & Fan (2015), left conditional on $c$, right conditional on $c'$.  

...confounders for $X-M$ and $X-Y$ relationship, this will not exclude unmeasured confounders for $M-Y$ relationship.

Further it is easy to see for extended models with covariates and/or multiple mediators it will be hard to find closed-form expressions because the S matrix becomes large and consequently solving the expression $G' A^{-1} G \leq \text{var}(Y)$ with respect to $a$ or $b$ is no longer straightforward. A possible alternative will be proposed in the next section.

### 3.2 Alternative method to obtain $R(a)R(b)$

Instead of starting from the covariance matrix, we start from the correlation matrix where correlations are expressed in terms of regression coefficients.
3.2.1 Simple mediation model

The equations of the simple mediation model are given before (unstandardized: (1) to (3), standardized: (7) to (9)). The $S$-matrix is alternatively formulated in terms of the correlation matrix:

$$
\begin{pmatrix}
1 & \rho_{XM} & \rho_{XY} \\
\rho_{XM} & 1 & \rho_{MY} \\
\rho_{XY} & \rho_{MY} & 1
\end{pmatrix}
$$

Rewrite the correlations in terms of **standardized** effects:

$$
\begin{pmatrix}
1 & a & c \\
a & 1 & b + a(c - ab) \\
c & b + a(c - ab) & 1
\end{pmatrix}
$$

(13)

Following Preacher & Kelley (2011) we have to condition on $a, b$ and $c$, but since $c$ depends on $a$ and $b$, it seems more appropriate to express $c$ in terms of $c', a$ and $b$, i.e. $c = c' + ab$ and consequently condition on $a, b$ and $c'$.

$$
\begin{pmatrix}
1 & a & c' + ab \\
a & 1 & b + ac' \\
c' + ab & b + ac' & 1
\end{pmatrix}
$$

(14)

This correlation matrix can be used in a similar way as in Preacher & Kelley (2011) to obtain the closed form expressions. Using the latter matrix yields different expressions since we condition on $c'$ instead of $c$. We already argued that these derivations are relatively simple in the simple mediation model, but that for more complex model this are no longer straightforward. For this reason we wrote a function (in R), $MaxIE$ that gives us immediately the maximum possible indirect effect based on the same criterium, but without mathematical derivations (see further). The idea behind is that we can do a grid-search over possible values of $a$ and $b$ respectively (for given values of $b$ and $c$, or $a$ and $c$, resp.), and check whether the above correlation matrix is nonnegative definite. Moreover, we can let vary $a$ and $b$ together and search for the combination which has the highest product (i.e. indirect effect) and for which the covariance matrix is non negative definite.
3.2.2 Mediation model with confounder for M-Y relationship

Let us assume that we start from the next data generating mechanism:

\[
\begin{align*}
X &\sim N(0, 1) \\
C &\sim N(0, 1) \\
M &= 0 + aX + \delta_1 C + \epsilon_M \\
Y &= 0 + c'X + bM + \delta_2 C + \epsilon_Y
\end{align*}
\]

With \(X\) is a randomized exposure and where \(C\) denotes a baseline confounder for \(M-Y\) relationship which is independent of exposure \(X\). The \(S\)-matrix (expressed in correlations) becomes then:

\[
S = \begin{pmatrix}
1 & \rho_{XM} & \rho_{XC} & \rho_{XY} \\
\rho_{XM} & 1 & \rho_{MC} & \rho_{MY} \\
\rho_{XC} & \rho_{MC} & 1 & \rho_{CY} \\
\rho_{XY} & \rho_{MY} & \rho_{CY} & 1
\end{pmatrix}
\]

Because treatment is randomized \(\sigma_{XC} = \rho_{XC} = 0\). Further if we standardize all variables we could again rewrite the correlations in terms of the (standardized) regression coefficients:

\[
\begin{pmatrix}
1 & a & 0 & c' + ab \\
a & 1 & \delta_1 & b + ac' + \delta_1 \delta_2 \\
0 & \delta_1 & 1 & b\delta_1 + \delta_2 \\
c' + ab & b + ac' + \delta_1 \delta_2 & b\delta_1 + \delta_2 & 1
\end{pmatrix}
\]  

(15)

To find the maximum possible values for \(a\) and \(b\), we now have to condition on \(\delta_1, \delta_2\) and \(c'\). The idea of Preacher & Kelley (2011) is that the matrix \(S\) should be nonnegative definite.

If we use the same reasoning as in the previous section, we rewrite the function \(\text{MaxIE}\). The correlation matrix is changed since we add an extra predictor. This implies that the input is no longer only the parameter estimate for \(c'\), but also the parameter estimates for \(\delta_1\) and \(\delta_2\), the effect of the covariate \(C\) on mediator and outcome respectively. One could use the function for a grid of values for \(a\), while keeping \(\delta_1, \delta_2, c'\) and \(b\) fixed, to find the
maximum possible value for $a$. In a similar way we find the maximum possible value for $b$, conditional on $\delta_1, \delta_2, c'$ and $a$. Note that also the range of possible values for $a$ should be larger than $-1$ and $1$, since the equation for the mediator is a multiple regression. Again this is the method proposed by Preacher & Kelley (2011), but it seems more appropriate to find the maximum values for $a$ and $b$ simultaneously. The code you find in appendix (A2) starts from this point of view and so you have only to give the values for $c', \delta_1$ and $\delta_2$. The function returns the maximum possible indirect effect and $\kappa^2$.

Since in this model the equation for the mediator contains multiple predictors, it raises the question if we have to check the nonnegative definiteness of the correlation matrix for treatment $X$, mediator $M$ and confounder $C$. Based on a property of semi-positive definiteness we can conclude that this extra step is unnecessary: matrix $A$ is positive (semi)definite if and only if all of its principal submatrices are positive (semi)definite (Zhang, 2011). Since the correlation matrix of $X, M$ and $C$ is a submatrix of matrix (15), searching for the maximum value of $a$ for which this matrix is nonnegative definite will yield the same maximum possible value for $a$ as found based on matrix (15). Maybe it can help computationally, because you can limit the range of possible $a$ values and thus $ab$ values, but it will not change the estimate of the maximum possible indirect effect.

3.2.3 Mediation model with two mediators

A possible data generating mechanism for such a model is:

\[
X \sim N(0, 1) \\
M_1 = 0 + a_1 X + \epsilon_{M_1} \\
M_2 = 0 + a_2 X + \epsilon_{M_2} \\
Y = 0 + c' X + b_1 M_1 + b_2 M_2 + \epsilon_Y
\]

Note that we assume that the mediators are independent of each other conditional on $X$. The $S$-matrix (expressed in correlations) for this model is:
which we could we rewrite in function of standardized regression coefficients:

\[
S = \begin{pmatrix}
1 & \rho_{XM_1} & \rho_{XM_2} & \rho_{XY} \\
\rho_{XM_1} & 1 & \rho_{M_1M_2} & \rho_{MY} \\
\rho_{XM_2} & \rho_{M_1M_2} & 1 & \rho_{MY} \\
\rho_{XY} & \rho_{M_1Y} & \rho_{M_2Y} & 1 \\
\end{pmatrix}
\]

In line with the previous models, we have to condition on \(c'\). Now we have four parameters which we let vary: \(a_1, a_2, b_1\) and \(b_2\). It is clear the this becomes computational very intensive. The function \(MaxIE\) could be rewritten similar as in previous examples. we redefine the correlation matrix and we have now two different effect size estimates, one for each indirect effect.

### 3.2.4 Simple mediation model with \(X-M\) interaction

We could assume a data generating mechanism under equation (4) and (5). With an interaction term included in the model, one should be careful when using standardized regression coefficients. Friedrich (1982) concludes that it makes the most sense to standardize the variables which form the interaction term (here \(X\) and \(M\)) and then take the product of these two standardized variables to form the standardized interaction term. The procedures for calculating unstandardized coefficients, can than be used to obtain standardized regression coefficients. The \(S\)-matrix (expressed in correlations) for this model is:

\[
S = \begin{pmatrix}
1 & \rho_{XM_1} & \rho_{XM_2} & \rho_{XY} \\
\rho_{XM_1} & 1 & \rho_{M_1M_2} & \rho_{MY} \\
\rho_{XM_2} & \rho_{M_1M_2} & 1 & \rho_{MY} \\
\rho_{XY} & \rho_{M_1Y} & \rho_{M_2Y} & 1 \\
\end{pmatrix}
\]
which we could we rewrite in function of standardized regression coefficients:

\[
\begin{pmatrix}
1 & a & 0 & c' + ab \\
a & 1 & 0 & ac' + b \\
0 & 0 & 1 & d \\
c' + ab & ac' + b & d & 1
\end{pmatrix}
\]

If we focus on the indirect effect \(ab\) we can condition on \(c'\) and \(d\). Additionally one could let vary regression coefficient \(d\) freely, by rewriting the function such that only \(c'\) is fixed.

### 3.2.5 Generalisation

Based on the criterium that the covariance (correlation) matrix should be non negative definite, it is easy to extend the current method to more complex models following the next steps:

1. Standardize the variables

2. Write down the model for the standardized variables using regression equations (i.e. without intercept).

3. Set up the \(S\) matrix for the equation of the outcome with (at least) the exposure and a mediator as predictors.

4. Rewrite the \(S\) matrix in terms of standardized regression coefficients, i.e. replace every covariance by an expression in terms of standardized regression coefficients.

5. Determine a realistic range of possible values for the parameters of interest, those who are relevant for estimating the indirect effect.

6. Check for which values of \(a\) and \(b\) the covariance matrix of step 4 is non negative definite, find the maximum possible effect and the estimator for \(\kappa^2\).
3.2.6 R-function: MaxIE

The steps described in the previous section are easy to implement in R. You can do this for each model by adapting the covariance matrix and the range of values for \( a \) and \( b \).

To help researchers which are not familiar with covariance matrices and calculations we provide the R-function \textit{MaxIE}. It automatically returns the maximum possible indirect effect and an estimate of \( \kappa^2 \). The function combines the different models proposed in this section: simple mediation model, model with \( X-M \) interaction and model with measured confounder for \( M-Y \) relationship. The multiple mediator model is not considered since we assume that both mediators are independent. In this case we can estimate \( \kappa^2 \) for each indirect effect by a simple mediation model. The R-code of the function can be found in Appendix A1. The function \textit{MaxIE} is based on the covariance matrices given above and will check its non negative definiteness for different values for \( a \) and \( b \). Therefore we use the R-function \texttt{is.positive.semi.definite}, which gives a logical output (TRUE/FALSE).

In the simple mediation model, with or without \( X-M \) interaction, the equation for the mediator containing \( a \) (eq. 8) has only one predictor, \( X \). To obtain an estimate for \( a \) a univariate simple regression can be used. Since it are standardized regression coefficients, this implies that the possible values for \( a \) lay between \(-1\) and \(1\). The equation of the outcome containing the parameters \( b \) (for mediator) and \( d \) (for interaction) has several predictors. To obtain estimates for the parameters of interest a multiple regression is needed. Consequently, the possible values for the regression coefficients are not bounded between \(-1\) and \(1\) (Deegan, 1978). Although in practice this will be rarely the case, we choose here a maximum possible range which is broader (i.e. from \(-2\) to \(2\)). When we add a confounder for the \( M-Y \) relationship the equation for the mediator involves that multiple regression is needed to obtain estimators for the different parameters. The range of possible values for \( a \) is then also set from \(-2\) to \(2\).

One of our critics on the estimation method of Preacher & Kelley (2011) is that they search for the maximum possible values of \( a \) (with \( b \) and \( c' \) fixed) and \( b \) (with \( a \) and \( c' \) fixed) separately and then take the product to obtain the maximum possible indirect effect.
\Re(a) \Re(b)$. In contrast to the method of Preacher & Kelley (2011) we can simultaneously vary $a$ and $b$. Note that by varying $a$ and $b$ simultaneously, the number of possible values in the grid increases highly, since every value for $a$ is combined with every value for $b$. If we have 200 possible values for $a$ and 200 for $b$ than we have 40000 combinations of $a$ and $b$. The calculation time is thus a bit longer than the method of Preacher & Kelley (2011).

The function works as follows. For every combination of possible values for $a$ and $b$ the function checks if the covariance matrix is non negative definite, such that we have a collection of combinations for which this condition is fulfilled. In a second step we search for the most extreme value of the indirect effect with the same sign as the point estimate of the indirect effect. If the estimate of $ab$ is negative (positive), the function takes the combination of $a$ and $b$ for which the product is minimal (maximal).

The input of the function depends on the mediation model. For the simple mediation model the input is only the point estimate of the standardized regression coefficient for the direct ($\hat{c}'$) and indirect effect ($\hat{ab}$). If we model an $X$-$M$ interaction we need to add the point estimate for the standardized regression coefficient of the interaction ($\hat{d}_{xm}$). For a measured confounder for the $M$-$Y$ relationship two extra arguments should be add, more specifically the point estimates of the standardized effect of the confounder on mediator ($\hat{d}_1$) and outcome ($\hat{d}_2$). The default values for $\hat{d}_{xm}, \hat{d}_1$ and $\hat{d}_2$ is 0. If the arguments are left empty, the function assumes the simple mediation model is used to obtain point estimates of the different parameters.

In conclusion, the function \textit{MaxIE} immediately returns the maximum possible value for the indirect effect and an estimate for $\kappa^2$. The applied researcher needs only point estimates of the standardized regression coefficients which can be obtained by linear regression techniques using standardized variables. A confidence interval for $\kappa^2$ could be obtained by bootstrap methods.
3.2.7 Simulation study

A simulation study was conducted to check the behaviour of $\kappa^2$ in different mediation settings. More specifically, we focus on the simple mediation model and on the model with measured $M-Y$ confounding.

A first goal of the simulation study is to compare the results of the two estimating methods for the maximum possible indirect effect. The first method is the one proposed by Preacher & Kelley (2011) which estimates the maximum possible values for the parameters of the indirect effect separately (i.e. estimating $\mathcal{R}(a)$, keeping $b$ and $c'$ constant and estimating $\mathcal{R}(b)$, keeping $a$ and $c'$ constant). The product $\mathcal{R}(a)\mathcal{R}(b)$ is then used to obtain an estimate for $\kappa^2$. The second method is the method proposed in the previous section, i.e. let vary $a$ and $b$ together, condition on $c'$. We denote the estimate of the maximum possible indirect effect obtained by this second method as $\mathcal{R}(ab)$.

For this part of the simulation study we start from the simple mediation model and let vary $c, c'$ and $a$. Since the total effect $c$ could be estimated by simple linear regression the value lies in a range between $-1$ and $1$. In this simulation study $c$ could take the values $-.4, -.2, 0, .2$ and $.4$. Further we fix $c'$ at the values $-.5, -.25, 0, .25$ and $.5$. In total we get 25 combinations and for each combination we can calculate the indirect effect $ab$ by $c' - c$ (Baron & Kenny, 1986). We fix $a$ at some value ($.5, .2, -.2$ or $-.5$) and calculate the value for $b$. Note that we limit the value for $b$ to the range $[-1.3, 1.3]$, since the point estimate for this parameter is obtained by multiple regression of standardized variables. Each combination for which the absolute value for $b$ larger than $1.3$ is removed, and we keep 20 (10) combinations if $a = .5$ or $-.5$ ($a = .2$ or $-.2$). For each combination of $c, c', a$ and $b$ we estimate $\mathcal{R}(a)\mathcal{R}(b)$ and $\mathcal{R}(ab)$. Note that the absolute value of $b$ rarely be larger than 1 and thus the range of possible maximum values of $b$ should be sufficiently wide, therefore we choose a range of $[-2, 2]$. Both ranges (for $a$ and $b$) increase by 0.01 which implies that we have 80601 combinations of $a$ and $b$ for the latter method.

The same values were used for the parameters in the second model with the measured confounder for the $M-Y$ relationship. The influence of confounder $C$ on mediator and
outcome is fixed at .25 and .15 respectively. Further the regression to obtain an estimate for $a$ is a multiple regression (on $X$ and $C$) which implies that the range of values for $a$ should be larger. We take the same range for possible values as $b$, i.e. $[-2, 2]$.

Next we want to check if the new estimation method of $\kappa^2$ implies that the characteristic of monotonicity is fulfilled. Wen & Fan (2015) argued that this is problematic for the effect size proposed by Preacher & Kelley (2011). In the simulation study we will compute $\kappa^2$ by our method for a range of values for the indirect effect. We expect that when the deviation from the indirect effect to 0 increases, the estimate of $\kappa^2$ increases. We fix the total effect $c$ in the simple mediation model at $-.5$ and .25, for the model with the measured confounder $c$ is fixed at $-.2$ and .4. Further we let vary $c'$ from $-1$ to 1 and thus the indirect effect $ab$ since $c' - c = ab$. For the second model the effect of the confounder is fixed at .2 and .4 for the first simulation and .3 and .1 for the second simulation, on mediator and outcome respectively. Results are shown by graphs which can be used to assess the monotonicity of the function. For comparison we estimate $\kappa^2$ for some fixed values in the simple mediation setting by the method of Preacher & Kelley (2011). We let vary the total effect $c$ from $-.75$ to .75. Further the parameter $c'$ is fixed at $-.15$ and .25 respectively. We estimate the maximum possible value for each path separately and thus we need to let vary the values for $a$ between $-.5$ and $-.4$. The value of $b$ can then be obtained by $(c - c')/a$, such that we have a range for $ab$ from $-.6$ to .9 and from $-1$ to .5 respectively.

In a third part we want to compare results of our method if we condition on $c'$ and $c$ respectively. We already argue that conditioning on $c$ is not correct, but here we want to check if this implies large differences in the estimation of $\Re(ab)$ and thus also $\kappa^2$. We fix $c$ at $-.4, -.3, -.2, -.1, 0, .1, .2, .3, .4$ and $a$ at .5. Further $c'$ can take the values $-.1$ and .2. For every combination of these parameters we found another value for $b$. We only retain the combinations of parameters for which $b$ is smaller than 1.3. For both methods we estimate the maximum possible indirect effect $\Re(ab)$ with the same combinations of $a$ and $b$. The difference lies in the correlation matrix that is used to estimate $\Re(ab)$. For the method conditional on $c'$ we express each term in function of $a, b$ and $c'$ (see [14]), for the method conditional on $c$ we do this for each term in function of $a, b$ and $c$ (see [13]).
4 Results

4.1 Comparison of estimating $\mathcal{R}(a)$ and $\mathcal{R}(b)$ separately with estimating $\mathcal{R}(a)\mathcal{R}(b)$ immediately.

Tables 2-3 and 5 summarize the results. For ease of notation and formulation we will refer to the $\mathcal{R}(a)\mathcal{R}(b)$-method when both parts of the indirect effect are separately maximized. When we estimate immediately the maximum possible indirect effect $\mathcal{R}(ab)$ we will refer to the $\mathcal{R}(ab)$-method. The corresponding effect sizes are denoted as $\kappa_{ab}$ and $\kappa_{a|b}$ respectively.

Table 2: Results for simple mediation model with $a = .5$.

<table>
<thead>
<tr>
<th>$ab$</th>
<th>.10</th>
<th>-.15</th>
<th>-.40</th>
<th>-.65</th>
<th>.30</th>
<th>.05</th>
<th>-.20</th>
<th>-.45</th>
<th>.50</th>
<th>.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b$</td>
<td>.20</td>
<td>-.30</td>
<td>-.80</td>
<td>-1.30</td>
<td>.60</td>
<td>.10</td>
<td>-.40</td>
<td>-.90</td>
<td>1</td>
<td>.50</td>
</tr>
<tr>
<td>$c'$</td>
<td>-.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>-.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>-.50</td>
<td>-.250</td>
</tr>
<tr>
<td>$\mathcal{R}(a)$</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>-Inf</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>$\mathcal{R}(b)$</td>
<td>1.15</td>
<td>-.85</td>
<td>-1</td>
<td>-1.10</td>
<td>1.15</td>
<td>1.10</td>
<td>-1</td>
<td>-1.10</td>
<td>1.15</td>
<td>1.10</td>
</tr>
<tr>
<td>$\mathcal{R}(a)\mathcal{R}(b)$</td>
<td>1.15</td>
<td>-.85</td>
<td>-1</td>
<td>Inf</td>
<td>1.15</td>
<td>1.10</td>
<td>-1</td>
<td>-1.10</td>
<td>1.15</td>
<td>1.10</td>
</tr>
<tr>
<td>$\kappa_{a</td>
<td>b}$</td>
<td>.09</td>
<td>.18</td>
<td>.40</td>
<td>-.00</td>
<td>.26</td>
<td>.05</td>
<td>.20</td>
<td>.41</td>
<td>.43</td>
</tr>
<tr>
<td>$\mathcal{R}(ab)$</td>
<td>1.50</td>
<td>-.75</td>
<td>-1</td>
<td>-1.25</td>
<td>.50</td>
<td>1.50</td>
<td>-.75</td>
<td>-1</td>
<td>.75</td>
<td>.50</td>
</tr>
<tr>
<td>$\kappa_{ab}$</td>
<td>.07</td>
<td>.20</td>
<td>.40</td>
<td>.52</td>
<td>.60</td>
<td>.03</td>
<td>.27</td>
<td>.45</td>
<td>.67</td>
<td>.50</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>$ab$</th>
<th>-.25</th>
<th>-.50</th>
<th>.45</th>
<th>.20</th>
<th>-.05</th>
<th>-.30</th>
<th>.65</th>
<th>.40</th>
<th>.15</th>
<th>-.10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$b$</td>
<td>-.50</td>
<td>-1.00</td>
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<td>-.10</td>
<td>-.60</td>
<td>1.30</td>
<td>.80</td>
<td>.30</td>
<td>-.20</td>
</tr>
<tr>
<td>$c'$</td>
<td>.25</td>
<td>.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>.50</td>
</tr>
<tr>
<td>$\mathcal{R}(a)$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>-Inf</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\mathcal{R}(b)$</td>
<td>-1.10</td>
<td>-1.15</td>
<td>1.10</td>
<td>1.00</td>
<td>-1.10</td>
<td>-1.15</td>
<td>1.10</td>
<td>1.00</td>
<td>.85</td>
<td>-1.15</td>
</tr>
<tr>
<td>$\mathcal{R}(a)\mathcal{R}(b)$</td>
<td>-1.10</td>
<td>-1.15</td>
<td>1.10</td>
<td>1.00</td>
<td>-1.10</td>
<td>-1.15</td>
<td>-Inf</td>
<td>1.00</td>
<td>.85</td>
<td>-1.15</td>
</tr>
<tr>
<td>$\kappa_{a</td>
<td>b}$</td>
<td>.23</td>
<td>.43</td>
<td>.41</td>
<td>.20</td>
<td>.05</td>
<td>.26</td>
<td>-.00</td>
<td>.40</td>
<td>.18</td>
</tr>
<tr>
<td>$\mathcal{R}(ab)$</td>
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<td>.75</td>
<td>.50</td>
<td>-.50</td>
<td>-.75</td>
<td>1.00</td>
<td>.75</td>
<td>.50</td>
<td>-.50</td>
</tr>
<tr>
<td>$\kappa_{ab}$</td>
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<td>.50</td>
<td>.60</td>
<td>.40</td>
<td>.10</td>
<td>.40</td>
<td>.65</td>
<td>.53</td>
<td>.30</td>
<td>.20</td>
</tr>
</tbody>
</table>
Table 3: Results for simple mediation model for \( a = -0.5 \)

<table>
<thead>
<tr>
<th>( ab )</th>
<th>.10</th>
<th>-.15</th>
<th>-.40</th>
<th>-.65</th>
<th>.30</th>
<th>.05</th>
<th>-.20</th>
<th>-.45</th>
<th>.50</th>
<th>.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>( b )</td>
<td>-.20</td>
<td>.30</td>
<td>.80</td>
<td>1.30</td>
<td>-.60</td>
<td>-.10</td>
<td>.40</td>
<td>.90</td>
<td>-1.00</td>
<td>-.50</td>
</tr>
<tr>
<td>( c' )</td>
<td>-.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>-.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>-.50</td>
<td>-.25</td>
</tr>
<tr>
<td>( \Re(a) )</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>Inf</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
<td>-1</td>
</tr>
<tr>
<td>( \Re(b) )</td>
<td>-1.15</td>
<td>.85</td>
<td>1.00</td>
<td>1.10</td>
<td>-.115</td>
<td>-1.10</td>
<td>1.00</td>
<td>1.10</td>
<td>-1.15</td>
<td>-1.10</td>
</tr>
<tr>
<td>( \Re(a)\Re(b) )</td>
<td>1.15</td>
<td>-.85</td>
<td>-1.00</td>
<td>Inf</td>
<td>1.15</td>
<td>1.10</td>
<td>-1.00</td>
<td>-1.10</td>
<td>1.15</td>
<td>1.10</td>
</tr>
<tr>
<td>( \kappa_{ab} )</td>
<td>.09</td>
<td>.18</td>
<td>.40</td>
<td>-.00</td>
<td>.26</td>
<td>.05</td>
<td>.20</td>
<td>.41</td>
<td>.43</td>
<td>.23</td>
</tr>
<tr>
<td>( \Re(ab) )</td>
<td>1.50</td>
<td>-.75</td>
<td>-1.00</td>
<td>-1.25</td>
<td>.50</td>
<td>1.50</td>
<td>-.75</td>
<td>1.00</td>
<td>.75</td>
<td>.50</td>
</tr>
<tr>
<td>( \kappa_{ab} )</td>
<td>.07</td>
<td>.20</td>
<td>.40</td>
<td>.52</td>
<td>.60</td>
<td>.03</td>
<td>.27</td>
<td>.45</td>
<td>.67</td>
<td>.50</td>
</tr>
</tbody>
</table>

The two estimation methods for \( \kappa^2 \) yield different results. The differences are not consistent, sometimes \( \hat{\kappa}^2 \) obtained by the \( \Re(ab) \)-method is larger, sometimes smaller in comparison with \( \Re(a)\Re(b) \)-method.

First we focus on the \( \Re(ab) \)-method. When the indirect effect \( ab \) is the same, this method leads to the same estimator for \( \kappa^2 \), independent of the values of \( \hat{a} \) and \( \hat{b} \). This can be observed if you compare estimates of \( \Re(ab) \) in table\[2\] and table\[3\]. An extra simulation was conducted where all the indirect effects are the same but the values of \( a \) and \( b \) differ. Results are summarized in table\[4\] and confirm our findings. Each possible combination
of $a$ and $b$, for which $ab$ equals $-.04$, yield the same estimate for $\kappa^2$ obtained by the $\Re(ab)$-method.

**Table 4:** Results for the same indirect effect but different values for $a$ and $b$

<table>
<thead>
<tr>
<th>$a$</th>
<th>$b$</th>
<th>$ab$</th>
<th>$\Re(a)$</th>
<th>$\Re(b)$</th>
<th>$\frac{ab}{\Re(a)\Re(b)}$</th>
<th>$\frac{ab}{\Re(ab)}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>-.1</td>
<td>.4</td>
<td>-.040</td>
<td>-10</td>
<td>.890</td>
<td>.045</td>
<td>.027</td>
</tr>
<tr>
<td>.1</td>
<td>-.4</td>
<td>-.040</td>
<td>10</td>
<td>-.890</td>
<td>.045</td>
<td>.027</td>
</tr>
<tr>
<td>.4</td>
<td>-.1</td>
<td>-.040</td>
<td>10</td>
<td>-1.080</td>
<td>.037</td>
<td>.027</td>
</tr>
<tr>
<td>-.4</td>
<td>.1</td>
<td>-.040</td>
<td>-10</td>
<td>1.080</td>
<td>.037</td>
<td>.027</td>
</tr>
<tr>
<td>-.2</td>
<td>.2</td>
<td>-.040</td>
<td>-10</td>
<td>.950</td>
<td>.042</td>
<td>.027</td>
</tr>
<tr>
<td>.2</td>
<td>-.2</td>
<td>-.040</td>
<td>10</td>
<td>-.950</td>
<td>.042</td>
<td>.027</td>
</tr>
</tbody>
</table>

Further inspection of tables 2 and 3 learn us that the largest estimate of the maximum possible indirect effect equals 1.5 or $-1.5$ for $\Re(ab)$. Remember that we condition on $c'$ instead of $c$ which implies that when $c'$ and $ab$ have opposite signs, the maximum possible indirect effect could be infinite, as concluded by [Wen & Fan (2015)](http://example.com). However, the results do not show evidence for this statement since none of estimators of the maximum possible indirect effect $\Re(ab)$ equals the most extreme value of $-2/2$.

Considering the results of the $\Re(a)\Re(b)$-method in more detail we see that the maximum possible indirect effect is the same when the absolute values for $a$ and $b$ are the same, but that their signs are interchanged. Table 4 shows that identical estimates of the indirect effect $ab$ does not imply identical estimates for $\kappa^2$. Further we see that when we do not limit the value of $b$ to the range of $[-1, 1]$, we get sometimes the problem that we do not obtain an estimate for $\Re(a)$. For every possible value of $a$ the $S$-matrix is then not non-negative definite. Since in the simple mediator model we use simple linear regression to obtain an estimate for $a$, the possible range is bounded to $[-1, 1]$. The results for the model with the measured confounder can be found in the appendix (table 7 ($a = .5$) and 8 ($a = -.5$)). The conclusions about $\Re(ab)$ are the same as these in the simple mediation model. For the $\Re(a)\Re(b)$-method we now see small differences in the estimates for $\kappa^2$, when the absolute
values for $a$ and $b$ are the same, but that their signs are interchanged (in contrast to the results of the simple mediation model).

Table 5: Results for the simple mediation setting with $c' = \ldots$

<table>
<thead>
<tr>
<th>$ab$</th>
<th>.10</th>
<th>-.15</th>
<th>.05</th>
<th>-.20</th>
<th>.25</th>
<th>-.25</th>
<th>.20</th>
<th>-.05</th>
<th>.15</th>
<th>-.10</th>
</tr>
</thead>
<tbody>
<tr>
<td>$a = .2$</td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$b$</td>
<td>0.50</td>
<td>-0.75</td>
<td>0.25</td>
<td>-1.00</td>
<td>1.25</td>
<td>-1.25</td>
<td>1.00</td>
<td>-0.25</td>
<td>0.75</td>
<td>-0.50</td>
</tr>
<tr>
<td>$\mathbb{R}(a)$</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
<td>1.00</td>
</tr>
<tr>
<td>$\mathbb{R}(b)$</td>
<td>0.97</td>
<td>-0.91</td>
<td>1.01</td>
<td>-1.00</td>
<td>1.01</td>
<td>-1.01</td>
<td>1.00</td>
<td>-1.01</td>
<td>0.91</td>
<td>-0.97</td>
</tr>
<tr>
<td>$\mathbb{R}(a)\mathbb{R}(b)$</td>
<td>0.97</td>
<td>-0.91</td>
<td>1.01</td>
<td>-1.00</td>
<td>1.01</td>
<td>-1.01</td>
<td>1.00</td>
<td>-1.01</td>
<td>0.91</td>
<td>-0.97</td>
</tr>
<tr>
<td>$\kappa_{a</td>
<td>b}$</td>
<td>0.10</td>
<td>0.16</td>
<td>0.05</td>
<td>0.20</td>
<td>0.25</td>
<td>0.25</td>
<td>0.20</td>
<td>0.05</td>
<td>0.16</td>
</tr>
<tr>
<td>$\mathbb{R}(ab)$</td>
<td>1.50</td>
<td>-0.75</td>
<td>1.00</td>
<td>-1.25</td>
<td>0.50</td>
<td>-0.75</td>
<td>1.00</td>
<td>-1.25</td>
<td>0.50</td>
<td>-0.50</td>
</tr>
<tr>
<td>$\kappa_{ab}$</td>
<td>0.07</td>
<td>0.20</td>
<td>0.05</td>
<td>0.16</td>
<td>0.50</td>
<td>0.33</td>
<td>0.20</td>
<td>0.04</td>
<td>0.30</td>
<td>0.20</td>
</tr>
</tbody>
</table>

| $a = -0.2$ | | | | | | | | | | |
| $b$ | -0.50 | 0.75 | -0.25 | 1.00 | -1.25 | 1.25 | -1.00 | 0.25 | -0.75 | 0.50 |
| $\mathbb{R}(a)$ | -1.00 | -1.00 | -1.00 | -1.00 | -1.00 | -1.00 | -1.00 | -1.00 | -1.00 | -1.00 |
| $\mathbb{R}(b)$ | -0.97 | 0.91 | -1.01 | 1.00 | -1.01 | 1.01 | -1.00 | 1.01 | -0.91 | 0.97 |
| $\mathbb{R}(a)\mathbb{R}(b)$ | 0.97 | -0.91 | 1.01 | -1.00 | 1.01 | -1.01 | 1.00 | -1.01 | 0.91 | -0.97 |
| $\kappa_{a|b}$ | 0.10 | 0.16 | 0.05 | 0.20 | 0.25 | 0.25 | 0.20 | 0.05 | 0.16 | 0.10 |
| $\mathbb{R}(ab)$ | 1.50 | -0.75 | 1.00 | -1.25 | 0.50 | -0.75 | 1.00 | -1.25 | 0.50 | -0.50 |
| $\kappa_{ab}$ | 0.07 | 0.20 | 0.05 | 0.16 | 0.50 | 0.33 | 0.20 | 0.04 | 0.30 | 0.20 |

4.2 Monotonicity of $\kappa^2$ by $\mathbb{R}(ab)$-method

To check the monotonicity of $\kappa^2$ obtained by our estimation method, we estimate $\kappa^2$ for combinations of $ab$ and $c'$, for a fixed value of $c$. In contrast to the method of Preacher & Kelley (2011), demonstrated by Wen & Fan (2015), our estimation of $\kappa^2$ implies that this effect size is monotone. Indeed, figure 3 (left) shows that if the indirect effect lies further away from 0 in the simple mediation setting, the estimate for the effect size $\kappa^2$ increases.
Figure 3 (right) shows the results for the method of Preacher & Kelley (2011). When we fix the value of $c'$ on .25, the function of $\kappa^2$ is monotone (not shown). In contrast, when $c'$ is $-.15$ we see some values of $ab$ where the function is non monotone (see Figure 3). In each graph we see that the estimate of $\kappa^2$ is 0 if the indirect effect is 0 and increases when the absolute value of the indirect effect increases. As earlier mentioned, the difference with Preacher & Kelley (2011) lie in conditioning on $c'$ instead of $c$ and the fact that we estimate the maximum possible indirect effect directly instead of the maximum possible values for each path ($a$ and $b$) separately. We also check the monotonicity of our method for the model with a measured confounder for $M-Y$ relationship. The graphs in the appendix show monotonicity.

**Figure 3:** The evolution of $\kappa^2$ in the simple mediation setting. Two left: our method for $c$ equals $-.5$ and .25. Two right: method of Preacher & Kelley (2011) for $c'$ equals $-.15$, right an enlargement to show non-monotonicity.
4.3 Comparison conditioning on $c'$ and $c$

The third goal of the simulation study is to compare the estimators of $\kappa^2$ if you condition on $c'$, like we propose, and $c$, like Preacher & Kelley (2011) propose. Note that for both methods we estimate the maximum possible indirect effect $\mathcal{R}(ab)$ immediately instead of estimating the maximum possible values for path $a$ and $b$ separately. Results are summarized in table 6.

**Table 6:** Results $\kappa^2$ conditional on $c$ and $c'$ in simple mediation model

<table>
<thead>
<tr>
<th></th>
<th>$c' = -.1$</th>
<th></th>
<th>$c' = .2$</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$ab$</td>
<td>$\mathcal{R}(ab)_{c'}$</td>
<td>$\mathcal{R}(ab)_{c}$</td>
</tr>
<tr>
<td>$c$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>-.4</td>
<td>-.30</td>
<td>-.90</td>
<td>-2.00</td>
</tr>
<tr>
<td>-.3</td>
<td>-.20</td>
<td>-.90</td>
<td>-2.00</td>
</tr>
<tr>
<td>-.2</td>
<td>-.10</td>
<td>-.90</td>
<td>-2.00</td>
</tr>
<tr>
<td>-.1</td>
<td>.00</td>
<td>1.10</td>
<td>2.00</td>
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<tr>
<td>.0</td>
<td>.10</td>
<td>1.10</td>
<td>2.00</td>
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<tr>
<td>.1</td>
<td>.20</td>
<td>1.10</td>
<td>2.00</td>
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<tr>
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<td>1.10</td>
<td>2.00</td>
</tr>
<tr>
<td>.3</td>
<td>.40</td>
<td>1.10</td>
<td>2.00</td>
</tr>
<tr>
<td>.4</td>
<td>.50</td>
<td>1.10</td>
<td>2.00</td>
</tr>
</tbody>
</table>

The results conditional on the total effect $c$ shows us that the maximum possible value of the indirect effect is each time the minimum or maximum of the range of possible values depending on the sign of the indirect effect (i.e. -2 if $ab < 0$ and 2 if $ab > 0$). In contrast if we condition on $c'$, we never obtain an extreme of the range as maximum possible value, but values close to 1 which is in practice often the maximum bound. Consequently the estimates of $\kappa^2$ are larger and more realistic then if one condition on $c$. Further we remark that there is no much variation in $\mathcal{R}(ab)_{c'}$, nor in $\mathcal{R}(ab)_{c}$ for a broad range of values for the indirect effect.
5 Illustration

We now illustrate our estimation method for $\kappa^2$ with a study by De Ruddere et al. (2013). Interest lies in whether priming with social deception affects responses towards others’ pain. In this randomized study participants ($n=55$) read a text about the use of the health care system (neutral, $X=0$) or a text about its misuse (social deception, $X = 1$). Next they were asked to rate patients’ pain on a numeric scale of 0 to 10 ($Y$, $0 = \text{'no pain at all'}, 10 = \text{'pain as bad as could be'}$) based on videos where pain patients perform pain-inducing activities. The rating of the overall valence of a patient (based on a picture) was considered as mediator. A 21-point scale was used for this variable (-10 = very negative, 0 = neutral, 10 = very positive). Researchers expect that the priming effect on pain rating is mediated by the valence of the patients. Further we assume that the valence of the patient depends on the condition to which the participant is assigned (i.e. $X$-$M$ interaction) and that effects are homogeneous. We consider (4) and (5) as the model for mediator and outcome respectively. Since the goal of this illustration is to show how to obtain an estimate for $\kappa^2$, we assume that assumptions (A1) to (A4) are fulfilled. Note that assumptions (A1) and (A2) are automatically fulfilled since $X$ is randomized. Assumption (A3) will be violated if there is an unmeasured variable which effects mediator and outcome. In practice this is often a hard assumption to make. In our example it is not unlikely that the disease history of the rater may impact valence and pain. Since only a few baseline characteristics were measured which are all time-invariant, assumption (A4) seems to hold for the measured variables. There could of course be an unmeasured confounder for $M$-$Y$ relationship which is influenced by $X$.

By using OLS regression we obtain the standardized point estimates for each parameter: $\hat{a} = -.255, \hat{c'} = .054, \hat{b} = .392$ and $\hat{d} = .325$. The pure indirect effect is then estimated by $\hat{a}\hat{b} = -.100$ (VanderWeele, 2013). Priming with social deceptions leads to lower pain rating through changes in valence in comparison with people in a hypothetical world where everyone were the neutral condition. But how large is this effect? For this issue we can estimate $\kappa^2$ by the function MaxIE. The input for this function is the estimated indirect
effect ($\hat{a}b$), direct effect ($\hat{c}'$) and the estimate $\hat{d}$ for the regression coefficient $d$. As output we get the maximum possible indirect effect with the same sign as the estimated indirect effect (here $\Re(ab) = -0.99$) and an estimate of $\kappa^2$ (here $\hat{\kappa}^2 = 0.101$, 95% percentile bootstrap CI: [0.005, 0.206]). Following the guideline of Preacher & Kelley (2011), based on the similarities with proportion of the variance accounted for in one variable by another (i.e., $r_{xy}^2$) and on Cohen’s guidelines Cohen (1988) (small effect size: .01, medium = .09 and large .25), this can be considered as a medium effect.

If we rewrite the correlation matrix in function of $c$ instead of $c'$, like Preacher & Kelley (2011), we get $-2$ as the maximum possible indirect effect and an estimate of $0.05$ for $\kappa^2$. Than the effect can be considered between small (.01) and medium (.09).
6 Discussion

In this master thesis we propose a new method to estimate the effect size measure $\kappa^2$ which incorporates some improvement in comparison with the closed-form expressions proposed by Preacher & Kelley (2011).

First our proposed method is computational instead of mathematical derivations. The advantage of finding the maximum possible indirect effect by our method is that it is very easy to extend to new and more complex models without advanced mathematical knowledge. A researcher only needs to know the rules of correlation and variance such that they can rewrite the correlation matrix in terms of standardized coefficients. In addition, some function in R are given, such that the interested researcher can calculate the $\kappa^2$ if he or she knows the point estimates for the regression coefficients. This can be seen as a second advantage in comparison with Preacher & Kelley (2011).

Further we condition on $c'$ instead of $c$. Because in our opinion it is contradictory to fix $a$ in one part of the matrix (if $c$ appears in a term, without $a$) and let it vary in another part of the matrix (terms with $a$, but without $c$). This seems also the reason why Wen & Fan (2015) found that $\kappa^2$ conditional on $c$ is non-monotone. In our simulation study we did not found evidence of non-monotonicity if you condition on $c'$ and we invalidate the example of Wen & Fan (2015).

Although our method is mathematically correct, one could argue that it is a drawback to condition on $c'$ instead of $c$. Since $c$ denotes the total effect of exposure on outcome, the assumption for identification $c$ are less stringent than for the direct and indirect effects in the simple mediation model. Moreover, if the exposure is randomized, the assumptions (A1) and (A2) hold and the total effect of exposure on outcome is identified ($c$). This total effect can be unbiasedly estimated by regression of $Y$ on $X$. On the other hand the direct effect is identified if assumptions (A1) to (A4) hold. Since $c'$ is the direct effect of $X$ on $Y$ after controlling for mediator(s) or covariates, randomization of exposure is not sufficient to identify $c'$. So while $c$ can be unbiasedly estimated if exposure $X$ is randomized, we can not guarantee that this is the case for $c'$. However, for identification of the indirect effect
ab, assumptions (A1) to (A4) need to be satisfied. In that case the indirect effect can be unbiasedly estimated and the question raises if it is interesting to have an effect size for a biased estimate of the indirect effect.

Despite the improvements proposed in this master thesis for the estimation method of $\kappa^2$, we still have our doubts about the usefulness of this effect size measure. A question that raises is if the non negative definiteness of the correlation matrix is a sufficient reason to derive the maximum possible indirect effect. Are there no other data features that we need to take in account?

Further the estimate of the maximum possible indirect effect is often the same for the different values of $c'$. For a range of values around 0 the maximum possible indirect effect differs, but outside that range it has the same value, i.e. the maximum possible value of the range. This implies that the different estimates for $\kappa^2$, for different values of $c'$ holding $c$ constant, lie closely together on a line. Taking this in account it makes it difficult to determine when an effect is large, based on the $\kappa^2$. From our point of view this conclusion limits the usefulness of $\kappa^2$.

Future research can try to extend the current method to more complex models. The current method is already worked out for linear models with interactions and/or founders, but focus on a continuous outcome. In practice the outcome will often be binary and logistic regression should be applied. Also multilevel models which are frequently used in educational research could not use $\kappa^2$ in his current form.

However, given the limitations and the doubt about the usefulness of $\kappa^2$ mentioned above, we do not think that further research for this effect size in its current form is appropriate. The idea of finding the maximum possible indirect effect is still intuitive and attractive and could form a base to ameliorate or create a new effect size. More specifically, it would be interesting to think about other conditions which should be fulfilled to find the maximum possible indirect effect. Combining these conditions with the current estimation method could lead to an effect size which is more appropriate and useful than $\kappa^2$ in his current form.
7 Conclusion

In this master thesis we considered effect sizes for mediation models with a focus on \( \kappa^2 \) proposed by Preacher & Kelley (2011) for the simple mediation model and criticized by Wen & Fan (2015). In line with the latter authors we have some serious questions about the effect size and how it was estimated by Preacher & Kelley (2011). Therefore we proposed a new estimation method for \( \kappa^2 \) conditional on \( c' \) instead of \( c \). This new estimation method offers an answer to the criticisms of Wen & Fan (2015). For instance, we do not find evidence for non-monotonicity of \( \kappa^2 \). While Preacher & Kelley (2011) search the maximum possible values for each path of the indirect effect seperately and multiply them, we immediately search for the maximum possible indirect effect. The current estimation method has several advantages in comparison with the method of Preacher & Kelley (2011). Because we do a search over a grid of possible values for the regression coefficients of the indirect effect, there is no need to do some complex mathematical derivations. The method can be applied to more complex models such as models with X-M-interactions and/or with confounder for M-Y-relationship and it is easy to extend to new models. Moreover, we developed a R-function \textit{MaxIE} which automatically returns an estimate of \( \kappa^2 \) for the applied researcher.

However, despite these advantages of the new estimation method we are not convinced that \( \kappa^2 \) in his current form is the perfect effect size. Probably there are conditions, other than the semi positive definiteness of a matrix, that should be taken in account to estimate the maximum possible indirect effect and thus \( \kappa^2 \). More research to find these conditions is needed.
References


Appendix

R-function MaxIE

MaxIE <- function(ab, cacc, dxm = 0, d1=0, d2=0){
  vala0 <- seq(-2,2,by=0.01)
  valb0 <- seq(-2,2,by=0.01)
  vala <- rep(vala0,each=length(valb0))
  valb <- rep(valb0,length(vala0))
  AABB <- as.matrix(cbind(vala, valb))
  AABBs <- AABB[vala <= 1 & vala >= -1 , ]
  AB <- AABB[,1] * AABB[,2]
  ABs <- AABBs[,1] * AABBs[,2]

  if (cacc*dxm == 0)
    if ((d1==0) | (d2==0)) {
      aabb <- apply(AABBs, 1 , function(AABBs) {
        is.positive.semi.definite(matrix(
          c(1, AABBs[1], cacc + AABBs[1]*AABBs[2],
          AABBs[1] ,1, AABBs[2] + AABBs[1]* cacc,
          cacc + AABBs[1]*AABBs[2], AABBs[2] + AABBs[1]*cacc,1),nrow=3,byrow=T))
        pos <- which(aabb == TRUE)
        ABextreme <- ifelse(ab < 0, min(ABs[pos]), max(ABs[pos]))
        result <- c(ABextreme, ab/ABextreme)
        return(result)
      })
    } else { aabb <- apply(AABB, 1 , function(AABB) {
      is.positive.semi.definite(matrix(
        c(1, AABB[1], 0, cacc + AABB[1]*AABB[2],
        AABB[1] ,1, d1, AABB[2] + AABB[1]* cacc + d1*d2,
        0, d1, 1, AABB[2] + d1 + d2,
        cacc + AABB[1]*AABB[2], AABB[2] + AABB[1]*cacc + d1*d2, AABB[2]*d1 + d2, 1),
        nrow=4,byrow=T)))
    }
  } else {
    aabb <- apply(AABBs, 1 , function(AABBs) {
      is.positive.semi.definite(matrix(
        c(1, AABBs[1], cacc + AABBs[1]*AABBs[2],
        AABBs[1] ,1, d1, AABBs[2] + AABBs[1]* cacc + d1*d2,
        0, d1, 1, AABB[2] + d1 + d2,
        cacc + AABB[1]*AABB[2], AABB[2] + AABB[1]*cacc + d1*d2, AABB[2]*d1 + d2, 1),
        nrow=4,byrow=T)))
    }
  }
}


pos <- which(aabb == TRUE)
ABextreme <- ifelse(ab < 0, min(AB[pos]), max(AB[pos]))
result <- c(ABextreme, ab/ABextreme)
return(result)
}
else if ((d1 == 0) | (d2 == 0)) {
aabb <- apply(AABBs, 1 , function(AABBs) {
  is.positive.semi.definite(matrix(
    c(1, AABBs[1], 0, cacc + AABBs[1]*AABBs[2],
    AABBs[1], 1, d1, AABBs[1]*cacc + AABBs[2],
    0, 0, 1, dxm,
    cacc + AABBs[1]*AABBs[2], AABBs[1]*cacc + AABBs[2],dxm, 1),
    nrow=4,byrow=T))})
pos <- which(aabb == TRUE)
ABextreme <- ifelse(ab < 0, min(ABs[pos]), max(ABs[pos]))
result <- c(ABextreme, ab/ABextreme)
return(result)
}
else {
aabb <- apply(AABB, 1 , function(AABB) {
  is.positive.semi.definite(matrix(
    c(1, ABB[1], 0, 0, cacc + ABB[1]*AABB[2],
    ABB[1], 1, 0, d1, ABB[1]*cacc + AABB[2] + d1*d2,
    0, 0, 1, 0, dxm,
    0, d1, 0, 1, d2 + AABB[2]*d1,
    cacc + ABB[1]*AABB[2], ABB[1]*cacc + AABB[2] + d1*d2, dxm, d2 + AABB[2]*d1, 1),
    nrow=5,byrow=T))})
pos <- which(aabb == TRUE)
ABextreme <- ifelse(ab < 0, min(AB[pos]), max(AB[pos]))
result <- c(ABextreme, ab/ABextreme)
return(result)
}
B. Monotonicity of $\kappa^2$ estimated by our method for the model with the measured confounder for M-Y relationship.

Figure 4: The evolution of $\kappa^2$ in the mediation setting with measured M-Y confounding by our estimation method for $c'$ equals $-0.5$ and $0.25$. 
C. Results for the model with the measured confounder for M-Y relationship.

Table 7: Results for the model with the measured confounder, \( a = .5 \)

<table>
<thead>
<tr>
<th>( ab )</th>
<th>.10</th>
<th>.15</th>
<th>.40</th>
<th>.65</th>
<th>.30</th>
<th>.05</th>
<th>.20</th>
<th>.45</th>
<th>.50</th>
<th>.25</th>
</tr>
</thead>
<tbody>
<tr>
<td>( b )</td>
<td>.20</td>
<td>-.30</td>
<td>-.80</td>
<td>-1.30</td>
<td>.60</td>
<td>.10</td>
<td>-.40</td>
<td>-.90</td>
<td>1.00</td>
<td>.50</td>
</tr>
<tr>
<td>( c' )</td>
<td>-.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>-.50</td>
<td>-.25</td>
<td>.00</td>
<td>.25</td>
<td>-.50</td>
<td>-.25</td>
</tr>
<tr>
<td>( \mathcal{R}(a) )</td>
<td>.98</td>
<td>.98</td>
<td>.98</td>
<td>-Inf</td>
<td>.98</td>
<td>.98</td>
<td>.98</td>
<td>.98</td>
<td>.98</td>
<td>.98</td>
</tr>
<tr>
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<td>-1.00</td>
<td>-1.11</td>
<td>1.06</td>
<td>1.02</td>
<td>-1.00</td>
<td>-1.11</td>
<td>1.06</td>
<td>1.02</td>
</tr>
<tr>
<td>( \mathcal{R}(a)\mathcal{R}(b) )</td>
<td>1.04</td>
<td>-.83</td>
<td>-.98</td>
<td>Inf</td>
<td>1.04</td>
<td>1.00</td>
<td>-.98</td>
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Table 8: Results for the model with the measured confounder, $a = -0.5$

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