

The Piggy in the Middle: The Role of Mediators in PLS-SEM-based Prediction

Nicholas P. Danks

The University of Dublin, Trinity College Dublin, Ireland
nicholasdanks@tcd.ie

Abstract

Partial least squares structural equation modeling (PLS-SEM) is increasingly popular as a joint explanatory predictive approach to modeling complex causal mechanisms. Researchers are becoming cognizant of the value of conducting predictive analysis using PLS-SEM for both the evaluation of overfit and to illustrate the practical value of their models. Mediators are a popular mechanism for adding nuance and greater explanatory power to such causal models. However, mediators pose a special challenge to generating predictions from PLS-SEM models as they serve a dual role of antecedent and outcome. Solutions for generating predictions from mediated PLS-SEM models have not been suitably explored or documented in the literature. Neither has there been sufficient exploration of whether the added model complexity of such mediators is justified in the light of out-of-sample predictive performance. This research note addresses that gap by formally evaluating three methods for generating predictions for mediated models and by proposing a simple metric that quantifies the predictive contribution of the mediator (PCM). We conduct monte-carlo simulations to demonstrate the efficacy of the methods under varying model conditions and then apply the methods in a model popular in the information systems literature. We find that there is no simple best solution, but that all three approaches have strengths and weaknesses. Further, the PCM metric performs well to quantify the predictive qualities of the mediator over-and-above the non-mediated alternative. We present guidelines on selecting the most appropriate method, and applying PCM for additional evidence to support research conclusions.

1 **1. Introduction**

2 Partial least squares structural equation modeling (PLS-SEM) has recently received
3 great attention in the various fields of the social sciences, including information
4 systems (Gefen et al., 2011; Ringle et al., 2012, Petter, 2018). Hair et al. (2017) conducted a
5 literature review of two top outlets for information systems research (namely Management
6 Information Systems Quarterly, MISQ; and Industrial Management and Data Systems, IMDS)
7 and find that for the period 2010 to 2015 10.9 percent of empirical papers in MISQ and 13.0
8 percent in IMDS conduct the primary analysis using PLS-SEM.

9 A fundamental advantage of PLS-SEM is its ability to assess the predictive power of
10 complex cause-effect models. The cause-effect models typically comprise several layers of
11 constructs with multiple mediators that explain the processes through which antecedent
12 constructs influence outcome constructs.

13 Generating predictions from PLS models is a recent and novel addition to the research
14 and practice of structural equation modeling. Shmueli et al. (2016) gave us an explicit
15 understanding of what prediction should entail in the context of PLS. That study also
16 demonstrated how to generate predictions using the measurement indicators and structure of
17 the model, starting with the most antecedent constructs, to predict endogenous construct
18 scores and their measurement indicators. Subsequently, PLS has seen the inclusion of
19 prediction in several new explanatory-predictive methods that seek to complement
20 explanatory modeling with predictive techniques such as the Cross-validated predictive ability
21 test (CVPAT; Liengaard et al., 2021) and predictive model selection criteria (Sharma et al.,
22 2019; Danks et al., 2020). Furthermore, methodologists have also suggested revised model
23 validation criteria in the light of predictive evaluation (Shmueli et al., 2019, Chin et al., 2020).

24 However, these methods have not sufficiently investigated the role of the mediator. The
25 predictive assessment of mediated models poses special challenges as mediators serve as both

1 antecedents and outcomes in PLS path models. Furthermore, the mediator has its own
2 measurement indicators that now compete with the indicators of the antecedent in predicting
3 outcomes. It is therefore an open question how researchers should reconcile the simultaneous
4 predictor role of the antecedent and mediator constructs. Possible strategies for resolving this
5 conflict have not been formally evaluated or explored in depth, researchers have little
6 guidance on how to assess the predictive power of their mediation models in PLS-SEM.

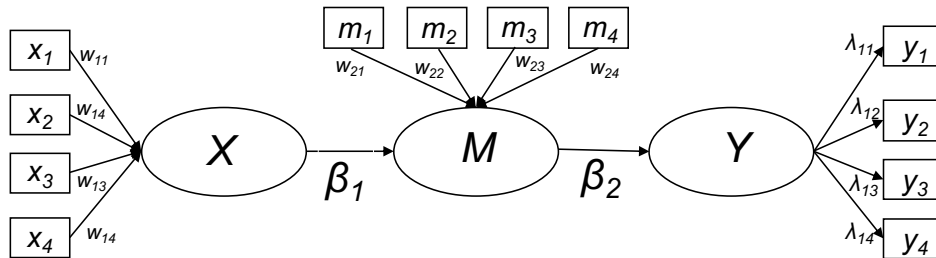
7 Mediators pose an additional risk to models in that they introduce additional
8 complexity, serving as intermediaries in causal paths. Such added complexity might
9 contribute to model fit, at the risk of out-of-sample prediction and thus generalizability. No
10 method for evaluating the predictive role of the mediator has been explored in the extant
11 literature.

12 In this study, we set out to conceptualize each of the three solutions in greater detail and
13 empirically validate their strengths and weaknesses using simulations. We then make use of
14 two of these solutions to generate a metric which quantifies the predictive contribution of the
15 mediating construct. Finally, apply the proposed methods in an empirical model salient to the
16 information systems literature—namely the unified theory of acceptance and use of technology
17 (UTAUT; Venkatesh et al., 2003).

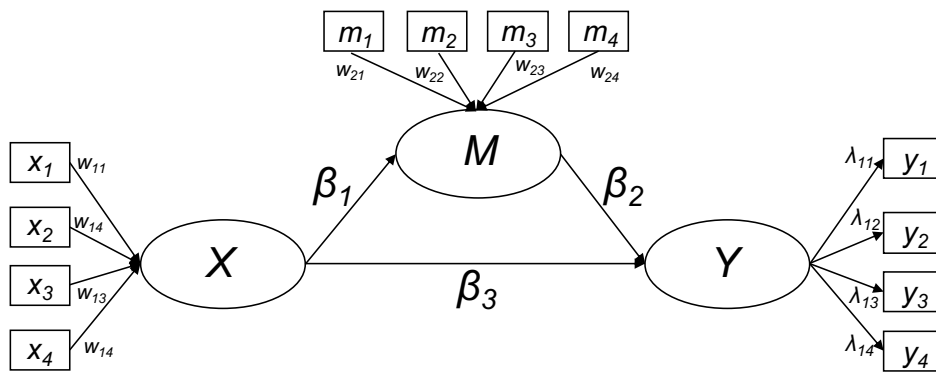
18 **2. Mediation in PLS-SEM**

19 Mediation occurs when the effect of an exogenous construct (X) on an outcome
20 construct (Y) is intermediated through a third mediating construct (M). That is to say that a
21 change in X causes a change in M which is then responsible for a change in Y . The effect of
22 X on Y is said to be fully mediated when there is no direct effect of X on Y , but only through
23 the mediator construct M . This is illustrated in Figure 1. An example of full mediation and the
24 analysis thereof can be found in Ray et al. (2014) where the authors find that engagement
25 fully mediates the influence of identity factors on prosocial intentions.

1 On the other hand, if X is found to have a direct effect on Y, in addition to the indirect
 2 effect via M, the effect of X on M is said to be partially mediated as illustrated in Figure 2.
 3 Dwivedi et al. (2019) conduct meta-analyses of the UTAUT model and find that behavioral
 4 intention partially mediates the relationship between facilitating conditions and use behavior.



5
 6 **Figure 1.** Fully mediated model¹



8
 9 **Figure 2.** Partially mediated model¹

10 In this research note we explore the predictive qualities of the various possible solutions
 11 for generating meaningful predictions from mediated models, and a new evaluation criterion
 12 for evaluating the predictive role of the mediator. For discussions on formal mediation testing
 13 in PLS see Hair et al. (2022), Sarstedt et al. (2020), and Nitzl et al. (2016).

¹ It is important to note that we have visualized the model in Figures 1 and 2, and Table 1, as having formative indicators for the antecedent construct X, and as having reflective indicators for the endogenous construct Y. This is done to make the description of the predictive process in Section 3 more clear. When estimating PLS models. Both a loading and a weight are estimated for every construct-indicator relationship (Shmueli et al., 2016). Thus, predictions can be generated for all the various combinations of measurement model specifications.

1 **3. Prediction in PLS-SEM**

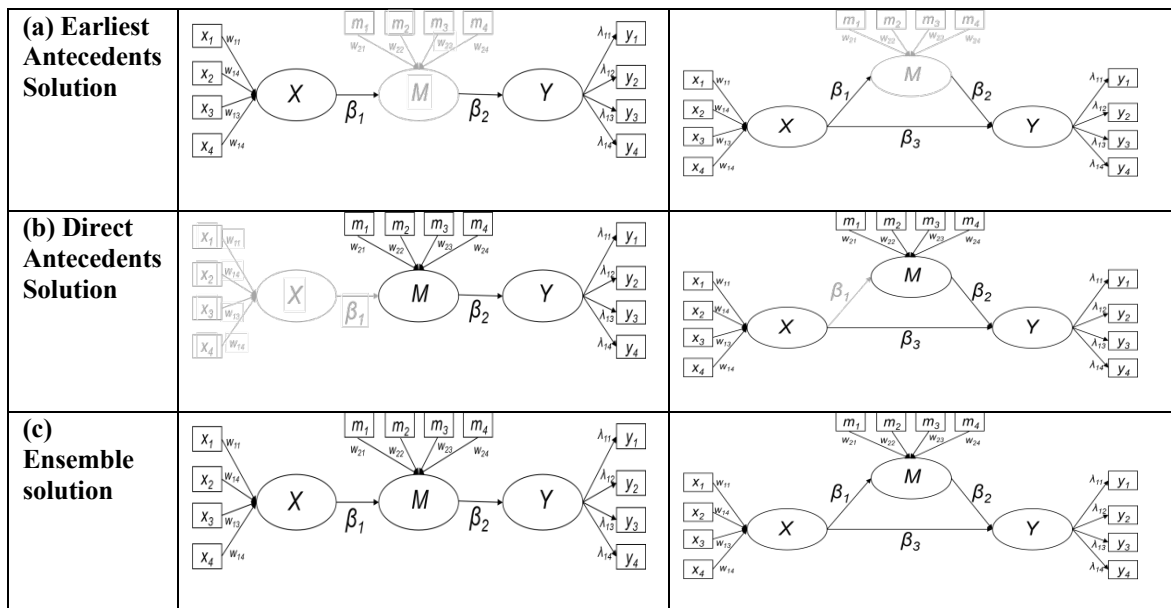
2 Shmueli et al. (2016) provide an explicit algorithm for the generation of both construct-
3 level and indicator-level predictions from PLS-SEM. Specifically, the study demonstrated
4 how to generate predictions using the measurement indicators and structure of the model,
5 starting with the most antecedent constructs, to predict endogenous construct scores and their
6 measurement indicators. This process can be conceptualized for a simple model with a single
7 antecedent construct (X) with measurement indicators x_i and single outcome construct (Y)
8 with indicators y_i : we can use measurement weights (w_{ij}), loadings (λ_{ij}), and structural path
9 (β) to relate the indicators of the antecedent to the indicators of the outcome.

10 However, if we extend this simple model by adding a mediating construct (M), we are
11 presented with a special dilemma in that the mediator is both predictor to the outcome Y and
12 itself the outcome of the antecedent X. Furthermore, the mediator has its own measurement
13 indicators (m_i) that now compete with the indicators of the antecedent in predicting outcomes.

14 **4. The Piggy in the Middle**

15 How should one reconcile the simultaneous predictor role of the antecedent and
16 mediating constructs? Shmueli et al. (2016) and later Danks et al. (2018) describe three
17 alternatives to resolve this dilemma: (a) using only the earliest antecedents as indirect
18 predictors; (b) using mediating constructs (and other direct antecedents of the outcome) as the
19 true predictors; and (c) creating an ensemble of the first two strategies that might surpass both
20 in predictive quality. However, neither Shmueli et al. (2016) nor Danks et al. (2018)
21 investigate the finite sample performance of these methods or how these methods can inform
22 theory development. Table 1 illustrates these three strategies (unused constructs, indicators,
23 and paths are in gray).

| Solution | Full Mediation | Partial Mediation |
|----------|----------------|-------------------|
|----------|----------------|-------------------|



1 **Table 1.** Illustration of the approaches to predicting in a simple mediated model¹

2 We start with the first solution, wherein the earliest antecedents (EA) are used as
3 indirect predictors. If we wish to predict the construct scores and indicators of outcome
4 constructs, we must start with the construct scores of its mediators. But mediators are
5 themselves the immediate outcomes of further antecedent constructs, so we can repeat this
6 process by estimating the mediating constructs using antecedent measures and structures. This
7 process can be repeated until we arrive at ultimate antecedent constructs, from which the
8 prediction process can commence. In this process, the mediator is treated like piggy-in-the-
9 middle, and its measurement indicators are bypassed in the estimation of the construct scores
10 of the mediator and ultimately the outcome construct.

11 Upon reflection, we recognize that this might be a useful solution when generating
12 outcome indicators is itself the goal, and only the indicators of the earliest antecedents are
13 available at the given time. This approach ties in well with the goals of practitioners who need
14 to generate predictions and forecasts for applied purposes. But because only the indirect effect
15 of X on Y is used to predict Y and its indicators, we expect that the more distant the predictor
16 and the outcome, the weaker the prediction. We also caution that it might be erroneous to
17 expect the ultimately antecedent constructs to produce accurate predictions of the outcome

1 when little of the variance of each endogenous construct is explained by its antecedents, a
2 problem that is compounded for increasingly complex models.

3 The second strategy to handling mediators in PLS prediction is to use mediators as the
4 primary predictors of endogenous constructs. This approach entails predicting outcome
5 construct scores and indicators using only the indicators of constructs directly antecedent
6 (DA) to the outcome construct. While the indicators of the mediator are now used in the
7 predictive process, indicators of constructs antecedent to the mediator are not. We argue that
8 this approach is most faithful to the structural model in that it uses only those constructs with
9 a direct causal effect on the outcome in its prediction. In much of the theory-building
10 literature, the mediator is set up to be of focal interest: they are the most fully examined
11 constructs of a model because they are explained by their antecedents and in turn best explain
12 outcomes. We note here that mediators are typically most highly correlated with the outcome
13 constructs and explain much of their variance. And so, we expect the second solution to
14 produce the most accurate predictions of outcome constructs and their indicators, despite
15 omitting major portions of the theorized model. Consequently, if we have measurements of
16 antecedent constructs at hand when making predictions, our predictions will be invariant to
17 those antecedent indicators.

18 The third strategy, though only briefly alluded to by Shmueli et al. (2016), is to combine
19 the predictions of the first two solutions to create an ensemble prediction - an approach often
20 found in purely predictive applications. On the face of it, however, we expect that there will
21 be little or no improvement in accuracy of the predictions generated by ensembles of PLS
22 predictions. Ensembles are known to perform best in situations where different predictive
23 techniques are used and there is negative, near zero, or little correlation between the
24 predictions (Brown et al. 2001). But the two PLS predictive strategies we wish to ensemble
25 use the same predictive technique (PLS) and their predictions should be positively correlated.
26 Despite our pessimism, we note that even if ensembles underperform predictively in our

1 context, they could still be useful to researchers seeking to build theory, compare models, or
2 compare datasets. In such situations, the goal of prediction would be to include information
3 from every part of the PLS model in the predictions, rather than purely generating accurate
4 predictions.

5 **5. Predictive contribution of the mediator**

6 When hypothesizing the addition of further complexity to a model—such as a mediating
7 construct—it is important to consider whether such additional complexity contributes not only
8 to increased model fit quality, but also to the predictive accuracy of the model. That is, one
9 should consider the potential of such complexity to lead to overfit. Overfit is particularly a
10 concern in the evaluation of PLS models, which is often conducted using model fit criteria
11 which favor overly complex models (Sharma et al. 2019). Models that are overfit suffer poor
12 generalizability when applied to out-of-sample cases (Danks et al., 2020). Thus, it is of great
13 importance to evaluate the out-of-sample performance of any such additions to complexity to
14 ensure that the performance on out-of-sample prediction is commensurate with model fit.

15 Shmueli et al. (2016) describe such an evaluation when they propose the following
16 regarding mediation and prediction:

17 “Full mediators (such as Y1) should produce better predictions (lower out-of-sample
18 RMSE or narrower prediction intervals) than antecedents. But if antecedents produce
19 better-quality predictions, then researchers might want to reconsider the theoretical
20 efficacy of their proposed mediators or acknowledge the shortcomings of their theory
21 in terms of predictive performance. In this way, the alternative prediction schemes can
22 be used to refine theorized models and augment traditional mediation tests such as
23 Baron and Kenny's (1986) classical test of mediation and the Sobel test.”

24 We propose that such a predictive evaluation of mediation should evaluate the
25 additional predictive accuracy which is contributed to the model over-and-above the

1 antecedent construct—as conceptualized by Shmueli et al. (2016). That is, in order to justify
2 the addition of a mediating construct, the mediating construct should yield an improved
3 predictive accuracy of the outcome construct. Such an evaluation should be conducted in
4 parallel to traditional mediation testing in order to provide additional evidence for the
5 generalizability of the mediator.

6 When testing for mediation, the direct path should always be estimated (Carrión, Nitzl,
7 & Roldán, 2017; Nitzl, Roldán, & Cepeda, 2016). When conducting such mediation testing,
8 the resultant model estimated is equivalent to the partial mediation model in column 2 of
9 Table 1 (including only the focal antecedent, mediator, and outcome for clarity and
10 simplicity). The EA approach when applied to such a model results in the use of the total
11 effect of X on Y (which is equivalent to the direct effect of X on Y) in predicting Y (column 2
12 row 1 of Table 1). On the other hand, the DA approach makes use of both the mediator (M)
13 and antecedent (X) constructs when predicting Y (column 2 row 2 of Table 1).

14 A direct comparison of the additive predictive accuracy of the model including both
15 antecedent and mediator constructs versus the predictive accuracy of the model including the
16 antecedent construct alone will provide an indication of the additive contribution of the
17 mediator construct to the predictive accuracy of the model. Thus, if we wish to know the
18 contribution of the mediator to the predictive accuracy of the model on the outcome construct,
19 we can compare the results of the DA and EA approaches applied in a partial mediation
20 context. Such an evaluation will provide additional evidence of the predictive contribution of
21 the mediator, rather than simply serving to increase model complexity.

22 We propose calculating this predictive contribution of the mediator (PCM) by first
23 taking the difference of the out-of-sample predictive metrics (such as RMSE, or MAE,
24 Shmueli et al., 2019) calculated for each of the DA and EA approaches (equation 1). This
25 simple difference would vary greatly depending on the magnitude of the predictive metrics
26 analyzed and the scale of the underlying data and thus might be difficult to interpret across

1 models. Thus, we recommend that difference then be divided by the predictive metric for the
2 EA approach to yield a percentage (equation 2). The resultant percentage then represents the
3 increase in predictive accuracy due to the addition of the mediator.

$$4 \quad \Delta METRIC = METRIC_{EA} - METRIC_{DA} \quad (1)$$

$$5 \quad PCM = \frac{\Delta METRIC}{METRIC_{EA}} \quad (2)$$

6 We recommend the use of cross-validated predictive metrics such as RMSE and MAE
7 as described by Shmueli et al. (2019) in calculating PCM. Since it is formulated as a
8 percentage, this metric should have a range approximately from -1 to 1, with a negative value
9 indicating that the mediator has damaged the predictive accuracy of the model on the outcome
10 construct and a positive value indicating that the mediator has a positive impact on the
11 predictive accuracy of the outcome construct. In the context of a more complex model (such
12 as the UTAUT model), with multiple additional antecedents to the focal outcome the
13 predictive contribution of the mediator might be attenuated. Thus, we recommend conducting
14 the estimation of PCM on the focal mediation model in isolation. It is not initially clear what
15 constitutes a low, moderate, or high value for the PCM metric, and thus we conduct a monte-
16 carlo simulation to explore the performance of the metric.

17 **6. Monte-carlo simulations**

18 **6.1. Simulation experiment I**

19 **6.1.1. Design, data, and estimation**

20 To investigate the performance of these three solutions and the PCM metric, we
21 conducted a monte-carlo simulation in the R statistical environment (R Core Team, 2021).
22 We specify three structural models, one fully mediated, one partially mediated (see Table 1),
23 and a third model excluding the mediator and specifying only a direct effect of the antecedent
24 construct (X) on the outcome (Y). All constructs are specified as having reflective
25 measurement models. Using these three structural models, we manipulated the following

1 experimental conditions, which correspond to the conditions commonly encountered in
 2 applied research (e.g., Hair, Hollingsworth, et al., 2017; Nitzl, 2016; Ringle et al., 2020):

- 3 • Four conditions of sample size (100, 200, 300, and 500),
- 4 • Five conditions of effect sizes on the structural paths (0.1, 0.2, 0.3, 0.4, and 0.5),
- 5 • Three indicator loading patterns with different levels of average variance extracted

6 (AVE): – High AVE with loadings: (0.9, 0.9, 0.9, and 0.9), – Moderate AVE with loadings:
 7 (0.8, 0.8, 0.8, and 0.8), and – Low AVE with loadings: (0.7, 0.7, 0.7, and 0.7),

- 8 • Three conditions of simulated mediation (full, partial, and no).

9 The data were generated using Schlittgen’s procedure available in the cbsem package
 10 for the R statistical software (Schlittgen, 2019). Specifically, we generate 1,800 simulated
 11 datasets for each of the fully mediated, partially mediated, and no mediation models. We then
 12 apply the three proposed predictive strategies for a model with mediator described in Table 1
 13 and conduct the estimation and prediction using the SEMinR package in R (Ray et al., 2021).
 14 We calculate the out-of-sample RMSE for each method across the simulation factors, as well
 15 as PCM, and evaluate the predictive performance.

16 **6.1.2. Results**

| Data generation type | Full mediated model | | Partial mediated model | | Ensemble prediction | Direct effect model |
|----------------------|---------------------|-------------|------------------------|-------------|---------------------|---------------------|
| | DA | EA | DA | EA | | |
| Full mediation | 1050 (58.3%) | 195 (10.8%) | 183 (10.2%) | 16 (1.5%) | 305 (16.9%) | 51 (2.8%) |
| Partial mediation | 104 (5.8%) | 96 (5.3%) | 1187 (65.9%) | 49 (2.7%) | 274 (15.2%) | 90 (5%) |
| No mediation | 59 (3.3%) | 154 (8.6%) | 225 (12.5%) | 493 (27.4%) | 302 (16.8%) | 567 (31.5%) |

17 **Table 2.** Number of times the approach generates the highest predictive accuracy in terms of
 18 out-of-sample RMSE.

19 **Notes:** Bolded values show the method with highest accuracy across mediation and model
 20 types. The first column distinguishes between the data simulated to contain a fully mediated
 21 relationship, partially mediated relationship, or no mediated relationship.

| Data generation type | Full mediated model | | Partial mediated model | | Ensemble prediction | Direct effect model | Correlation DA vs EA |
|----------------------|---------------------|-------|------------------------|-------|---------------------|---------------------|----------------------|
| | DA | EA | DA | EA | | | |
| Full mediation | 0.973 | 0.997 | 0.976 | 1.000 | 0.983 | 1.001 | 0.91 |

| | | | | | | | |
|--------------------------|-------|-------|--------------|-------|-------|--------------|------|
| Partial mediation | 0.938 | 0.963 | 0.905 | 0.938 | 0.921 | 0.938 | 0.77 |
| No mediation | 1.008 | 1.002 | 0.977 | 0.974 | 0.982 | 0.974 | 0.29 |

1 **Table 3.** Average RMSE for the approach

2 **Notes:** Bolded values show the method with highest accuracy across mediation and model
3 types. The first column distinguishes between the data simulated to contain a fully mediated
4 relationship, partially mediated relationship, or no mediated relationship.

5 The results demonstrate that the direct-antecedents solution generates predictions with
6 the highest accuracy for both full and partial mediation (58.3% and 65.9% respectively), far
7 beyond the ensemble solution (16.9% and 15.2% respectively), and the earliest-antecedents
8 solution (10.8% and 2.7%) as illustrated in Table 2. When no mediation is present, that is
9 there is only a direct effect of X on Y, then unsurprisingly the direct effect model generates
10 the highest levels of predictive accuracy (31.5%). These results are mirrored by the mean
11 RMSEs reported in Table 3.

12 The ensemble approach consistently outperforms the EA approach, but fails to improve
13 upon the DA approach. As predicted, this is due to the high correlation between the
14 predictions generated by the DA and EA approaches ($\rho=0.77$ and $\rho=0.91$ for partial and full
15 mediation respectively).

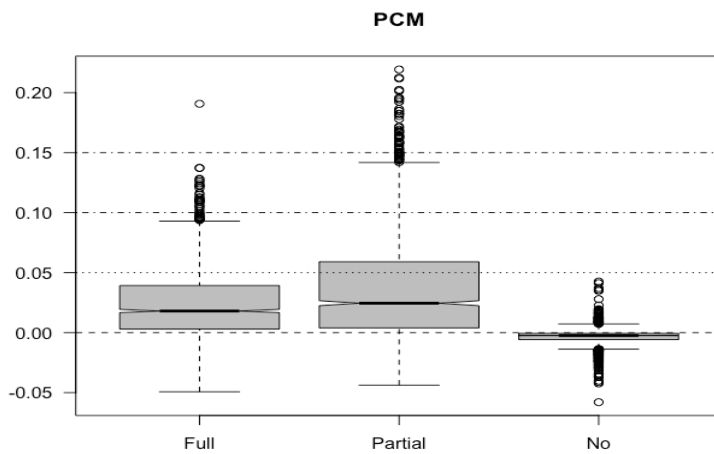
16 An interesting result to note is that the RMSE yielded by the EA approach in the partial
17 mediation model is almost identical to that yielded by the direct effect model for all three
18 simulated mediation types. This is because the EA approach when applied to the case of
19 partial mediation is in essence the total effect of X on Y and neglects any contribution by the
20 mediating construct. This reinforces our formulation of the PCM as the difference between
21 EA and DA approaches (equation 1).

| Data generation type | PCM positive | PCM negative |
|-----------------------------|---------------------|---------------------|
| Full mediation | 1477 (82.1%) | 323 (17.9%) |
| Partial mediation | 1497 (83.2%) | 303 (16.8%) |
| No mediation | 356 (19.8%) | 1444 (80.2%) |

1 **Table 4.** Number of times the PCM is positive indicating improved predictive power of
 2 mediated model in terms of out-of-sample RMSE.

| Data generation type | Descriptive Statistics | | | | | | Max |
|----------------------|------------------------|--------------------|--------------|--------|--------------------|-----------------|-------|
| | Min | 1st Quartile (25%) | Median (50%) | Mean | 3rd Quartile (75%) | 90th Percentile | |
| Full mediation | -0.049 | 0.003 | 0.021 | 0.031 | 0.049 | 0.064 | 0.219 |
| Partial mediation | -0.044 | 0.004 | 0.025 | 0.038 | 0.059 | 0.102 | 0.219 |
| No mediation | -0.058 | -0.006 | -0.002 | -0.003 | -0.006 | 0.002 | 0.042 |

3 **Table 5.** Descriptive statistics describing the PCM ratio performance on the simulated data in
 4 terms of out-of-sample RMSE.



5
 6 **Figure 3.** Distribution of the PCM metric on Full mediation, Partial mediation, and No
 7 mediation conditions of simulation

8 The simulation brings to light some indications of the performance of the PCM metric
 9 on evaluating the predictive contributions of the mediator in Tables 4 and 5. The PCM metric
 10 is positive indicating additional predictive contribution of the mediator over-and-above the
 11 antecedent construct in more than 80% of the cases in which mediation was designed in the
 12 data generation model. Similarly, the PCM metric is negative indicating no additional
 13 predictive contribution of the mediator in over 80% of the cases in which no mediation was
 14 designed in the data generation model. These results indicate that the metric is robust at
 15 identifying when the mediator has predictive contribution.

1 We further analyze the distribution of the metric under the various mediation conditions
2 in the data generation model – partial mediation, full mediation, and no mediation (Table 5).
3 Under conditions of mediation (partial and full), the PCM metric ranges from approximately 0
4 to 0.05 for the lower 75% of cases. Indicating that a value of 0 to 0.05 represents that
5 mediation is present, and the mediator has a mild contribution to predictive accuracy. The
6 PCM metric ranges from 0.05 to 0.10 in the 75th to 90th percentile of the partially mediated
7 models. This represents a strong contribution to predictive power by the mediator. After this
8 point, the two distributions diverge, but we expect that a PCM value of greater than 0.10 (90th
9 percentile for partial mediation) should represent a strong contribution to predictive power by
10 the mediator. The PCM distributions under the three data generation models can be inspected
11 in figure 3.

12 **6.2. Simulation Experiment II**

13 **6.2.1. Design, data, and estimation**

14 Next, we investigate the performance of PCM metric by means of a further monte-carlo
15 simulation in the R statistical environment (R Core Team, 2021). From the perspective of this
16 simulation, we wish to explore the values that the PCM metric can take under varying levels
17 of strength of mediation.

18 The Variance Accounted For (VAF) is often used to determine the proportion of the
19 mediation effect (Hair et al., 2014). This criterion is not without criticism but can be seen as a
20 “rule-of-thumb” when describing the size of the mediation effect (Ramayah et al., 2018). A
21 VAF value of less than 0.2 is seen as indicating no mediation, a value larger than 0.2 but less
22 than 0.8 as indicating partial mediation, and value greater than 0.8 as indicating full mediation
23 (Ramayah et al., 2018).

24 We use this a base from which to describe varying levels of mediation, however we
25 believe that the absolute magnitude of the paths plays a greater role than the proportion of

1 indirect to total effects. Thus, we specify five conditions of effect size that relate to mediation
 2 size—specifically we allocate values to β_1 , β_2 , and β_3 such that the mediation in the data
 3 generation model indicates VAF of 0.1, 0.3, 0.5, 0.7, 0.9 respectively. Additionally, we
 4 include a sixth condition of effect size with a higher direct effect of 0.3 to inspect how the
 5 magnitude of the path effects the PCM metric.

6 We now only specify a partially mediated (see Table 1) data generation model and
 7 commensurate with simulation experiment I. All constructs are specified as having reflective
 8 measurement models. We manipulated the following experimental conditions, which
 9 correspond to the conditions commonly encountered in applied research:

- 10 • Four conditions of sample size (100, 200, 300, and 500),
- 11 • Six conditions of effect sizes on the structural paths:

| Condition | β_1 | β_2 | β_3 | VAF |
|-----------|-----------|-----------|-----------|------|
| 1 | 0.1 | 0.1 | 0.09 | 0.10 |
| 2 | 0.23 | 0.23 | 0.1 | 0.31 |
| 3 | 0.32 | 0.32 | 0.1 | 0.51 |
| 4 | 0.6 | 0.6 | 0.15 | 0.71 |
| 5 | 0.6 | 0.6 | 0.05 | 0.88 |
| 6* | 0.6 | 0.6 | 0.3 | 0.55 |

12 **Table 6.** Six conditions of effect sizes and resultant VAF

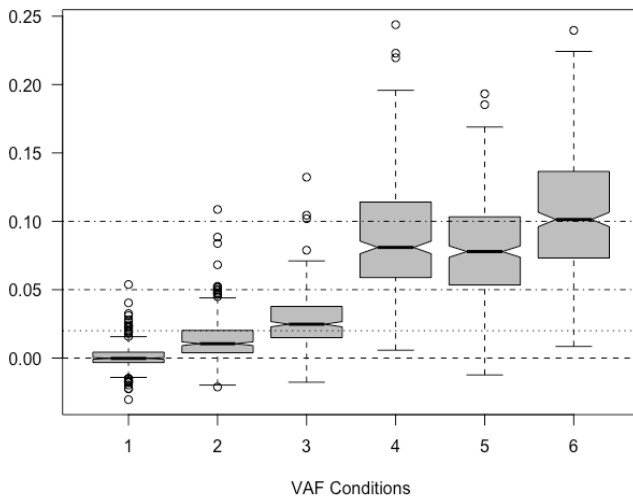
- 13 • Three indicator loading patterns with different levels of average variance extracted
 14 (AVE): – High AVE with loadings: (0.9, 0.9, 0.9, and 0.9), – Moderate AVE with loadings:
 15 (0.8, 0.8, 0.8, and 0.8), and – Low AVE with loadings: (0.7, 0.7, 0.7, and 0.7).

16 The data were generated using Schlittgen’s procedure available in the cbsem package
 17 for the R statistical software (Schlittgen, 2019). Specifically, we generate 2,160 simulated
 18 datasets. We then apply the proposed approach for calculating PCM, and evaluate the

1 performance of the PCM metric. We conduct the estimation and prediction using the SEMinR
 2 package in R (Ray et al., 2021).

3 **6.2.2. Results**

4 The simulation provides further evidence of the performance of the PCM metric on
 5 evaluating the predictive contributions of the mediator. When inspecting the boxplots in
 6 Figure 4 there is a clear positive relationship between VAF and PCM. We find that the PCM
 7 metric increases with an increase in VAF, but is also directly related to the absolute
 8 magnitude of the paths.



9

10 **Figure 4.** Distribution of the PCM metric on varying conditions of VAF

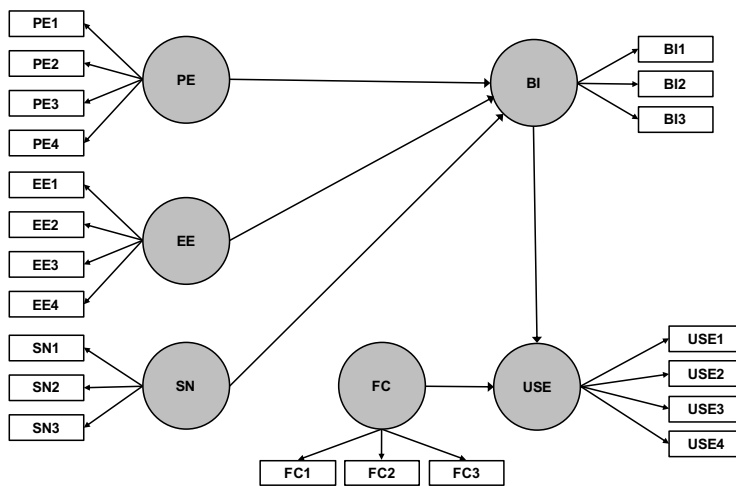
11 The approximate boundaries of 0 – 0.5 for small, 0.05 – 0.1 for moderate, and greater
 12 than 0.1 for strong predictive contribution of the mediator can be observed in the results of
 13 these simulations (Figure 4). These findings are supported by the descriptive statistics of these
 14 simulation conditions in Table 7, providing further evidence for this rule-of-thumb for
 15 evaluating the predictive contribution of the mediator. We now apply the three approaches to
 16 generating predictions from mediated models and the proposed PCM metric to an extant
 17 example from the literature.

| Simulated VAF condition | Descriptive Statistics | | | | | | |
|-------------------------|------------------------|--------------------|--------------|------|--------------------|-----------------|-----|
| | Min | 1st Quartile (25%) | Median (50%) | Mean | 3rd Quartile (75%) | 90th Percentile | Max |
| | | | | | | | |

| | | | | | | | |
|---|--------|--------|--------|-------|-------|-------|-------|
| 1: 0.1 | -0.030 | -0.003 | -0.000 | 0.001 | 0.004 | 0.011 | 0.054 |
| 2: 0.3 | -0.021 | 0.004 | 0.010 | 0.013 | 0.020 | 0.032 | 0.109 |
| 3: 0.5 | -0.018 | 0.015 | 0.0248 | 0.027 | 0.038 | 0.051 | 0.132 |
| 4: 0.7 | 0.006 | 0.059 | 0.081 | 0.086 | 0.114 | 0.133 | 0.244 |
| 5: 0.9 | -0.012 | 0.054 | 0.078 | 0.079 | 0.103 | 0.125 | 0.193 |
| 6*: 0.55 higher β_3 | 0.008 | 0.073 | 0.101 | 0.106 | 0.137 | 0.164 | 0.240 |

1 **Table 7.** Descriptive statistics describing the PCM ratio performance on the simulated data in
2 terms of out-of-sample RMSE.

3 **7. Empirical example**



4
5 **Figure 5.** Empirical example conceptual model

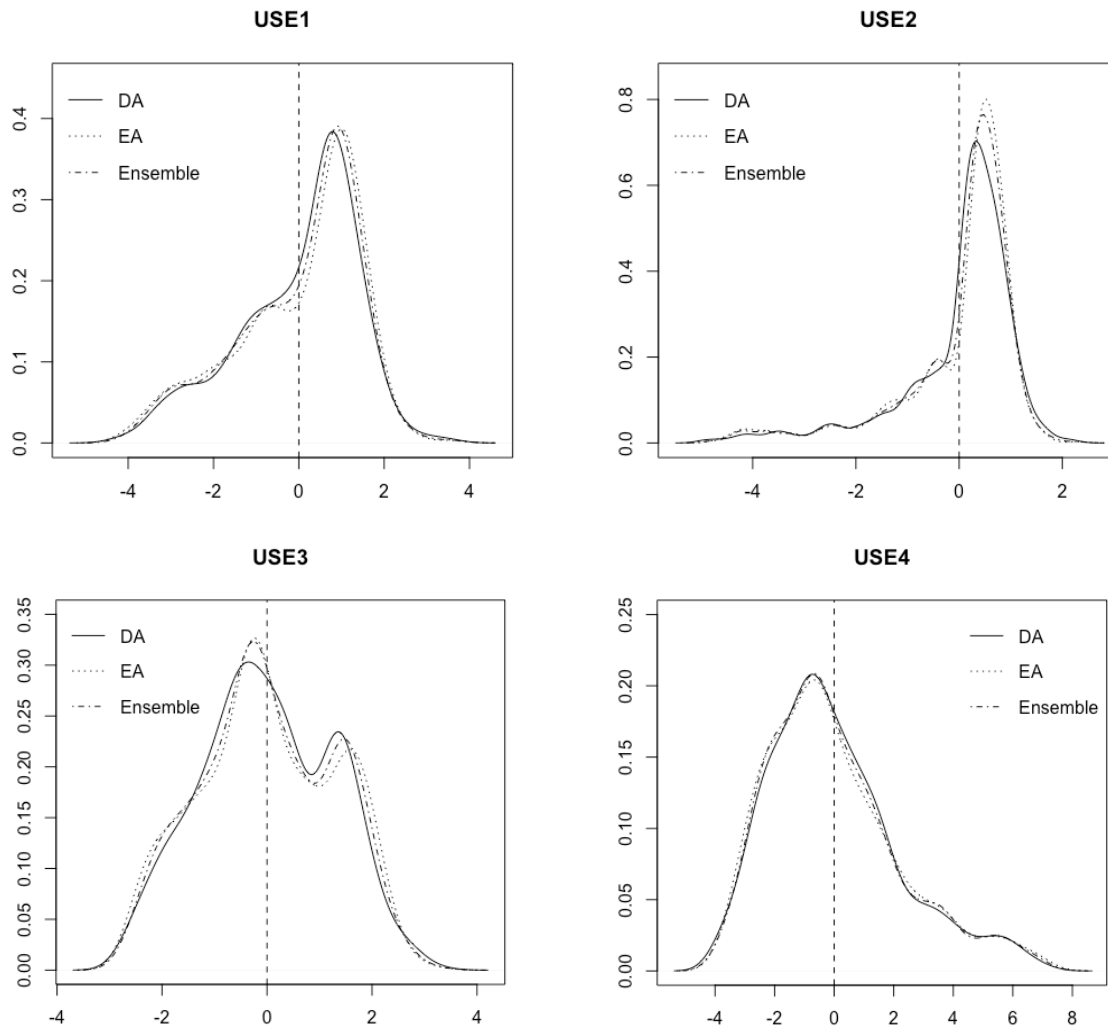
6 In our empirical example we will compare the application of these approaches and the
7 PCM metric to a well-established and widely used model from the information systems
8 literature—the unified theory of acceptance and use of technology (Venkatesh, 2003).
9 Specifically, we use the data and model of Al-Gahtani et al. (2007). Figure 5 illustrates the
10 conceptual model of the empirical demonstration. The primary antecedent constructs are
11 Performance Expectancy (PE), Effort Expectancy (EE), Social Norms (SN), and Facilitating
12 Conditions (FC) which collectively explain the Behavioral Intention (BI) and ultimately the
13 Use (USE) of the software. The model includes three mediated paths: (1) PE via BI to USE,
14 (2) EE via BI to USE, and (3) SN via BI to USE. According to the original study, these three
15 paths are modeled (and by implication hypothesized) as fully mediated paths.

1 We employed the SEMinR package (Ray et al., 2021) to both estimate and generate
2 predictions from the PLS-SEM model in the R statistical Environment (R Core Team, 2021).
3 The estimated model meets the criteria necessary to validate a PLS-SEM model (Hair et al.
4 2020, Henseler et al. 2016). We will not discuss these validations in detail but will instead
5 proceed directly to the results generated by applying the EA, DA, and ensemble predictive
6 approaches to the model.

7 First, we consider the general model evaluation criteria for predictive model assessment
8 as described by Shmueli et al. (2019). We focus our attention on the indicators of the USE
9 construct as our focal construct of interest. The reason is two-fold. First, analyzing the
10 predictions of the indicators of USE allows us to make a direct comparison between the
11 predictions generated by the EA approach (which would use the Earliest Antecedent
12 constructs PE, EE, SN, and FC to predict USE) and the DA approach (which would use only
13 the direct antecedent constructs BI and FC to predict USE). Second, USE is the construct of
14 primary interest to practitioners seeking to make useful and actionable predictions from such
15 PLS-SEM models.

16 We first compare the prediction errors from the three techniques and find that the three
17 methods generate highly comparable distributions of prediction errors (figure 6). Generally,
18 the ensemble approach falls somewhere between the EA and DA approaches in the error
19 distribution echoing our results in the monte-carlo simulation.

20



1 **Figure 6.** Distribution of out-of-sample prediction residuals generated from competing
 2 approaches for USE1, USE2, USE3, and USE4

3 Next, we consider the prediction metrics generated by the three metrics – we primarily
 4 consider RMSE but include MAE in addition as the distributions of prediction error are non-
 5 symmetrical (Shmueli et al., 2019).

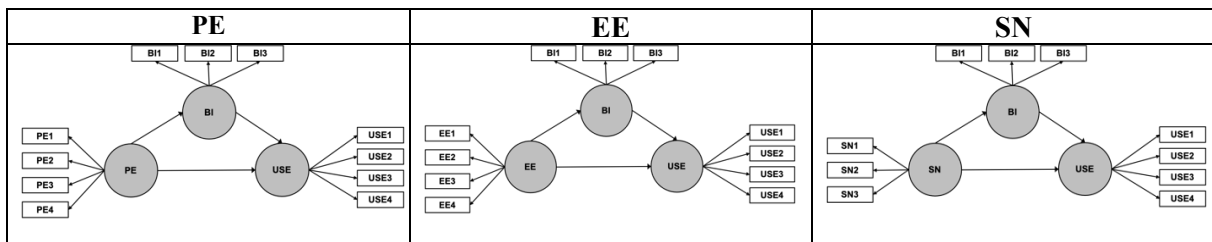
| Indicator | DA Approach | | EA Approach | | Ensemble Approach | |
|-----------|-------------|-------|-------------|-------|-------------------|-------|
| | RMSE | MAE | RMSE | MAE | RMSE | MAE |
| USE1 | 1.409 | 1.145 | 1.481 | 1.234 | 1.436 | 1.184 |
| USE2 | 1.127 | 0.788 | 1.161 | 0.841 | 1.137 | 0.812 |
| USE3 | 1.253 | 1.036 | 1.295 | 1.070 | 1.266 | 1.047 |
| USE4 | 2.201 | 1.720 | 2.257 | 1.775 | 2.220 | 1.738 |

6 **Table 8.** Results from three approaches

7 When considering the predictive metrics from the three approaches, it is clear that the
 8 DA approach consistently performs the best in terms of predictive power. In addition, the

1 Ensemble approach seems to average the better DA prediction and worse EA prediction to
 2 generate results somewhere between the two.

3 We now consider the predictive contribution of the three mediators (PE, EE, and SN) in
 4 terms of the PCM metric. We thus isolate the three focal mediation relationships (visualized
 5 in Table 9) and estimate the PCM for each of the indicators USE1, USE2, USE3, and USE4
 6 (Table 10).



7 **Table 9.** Models for the estimation of PCM for empirical example

| Indicator | PE PCM | Conclusion | EE PCM | Conclusion | SN PCM | Conclusion |
|-----------|-----------|------------|-----------|------------|-----------|------------|
| USE1 | 0.080 | Moderate | 0.068 | Moderate | 0.096 | Moderate |
| USE2 | 0.054 | Moderate | 0.046 | Weak | 0.069 | Moderate |
| USE3 | 0.059 | Moderate | 0.045 | Weak | 0.087 | Moderate |
| USE4 | 0.039 | Weak | 0.039 | Weak | 0.070 | Moderate |

8 **Table 10.** PCM results for empirical example

9 We estimate PCM of 0.080, 0.054, 0.059, and 0.039 for USE1, USE2, USE3, and USE4
 10 respectively, in the context of the mediated path of PE via BI to USE. These PCM values are
 11 largely moderate, and we thus conclude that BI has an overall moderate improvement of
 12 predictive power when considering this mediation relationship. Similarly, we calculate PCM
 13 of 0.068, 0.046, 0.045, 0.039 for USE1, USE2, USE3, and USE4 respectively, in the context
 14 of the mediated path of EE via BI to USE. These values fall within the weak category and
 15 thus we conclude that BI has an overall weak improvement of predictive power when
 16 considering this mediation relationship.

17 Interestingly, when we analyze the mediated effect of SN via BI on USE, we find that
 18 the PCM estimates are higher at 0.096, 0.069, 0.087, and 0.070 for USE1, USE2, USE3, and
 19 USE4 respectively. These values fall firmly within the strong category and suggest that there

1 might be more to this relationship than full mediation. Our re-estimation of the model
2 (Appendix B) finds that for this dataset, SN indeed has an indirect effect on USE. However,
3 we caution that it is important to re-consider the hypotheses underlying the model—such a
4 partial mediation might not make sense from a theoretical perspective. It is important,
5 however, to note that the PCM metric gave evidence to support such a finding from a data-
6 driven perspective.

7 The results from this empirical study confirm those observed in the monte-carlo
8 experiment and provide little evidence for employing either the EA or ensemble approaches
9 when the goal of the model is to maximize predictive accuracy. However, the PCM metric
10 performs well in providing additional post-hoc evidence to support the generalizability of a
11 mediation relationship after traditional mediation testing has been applied.

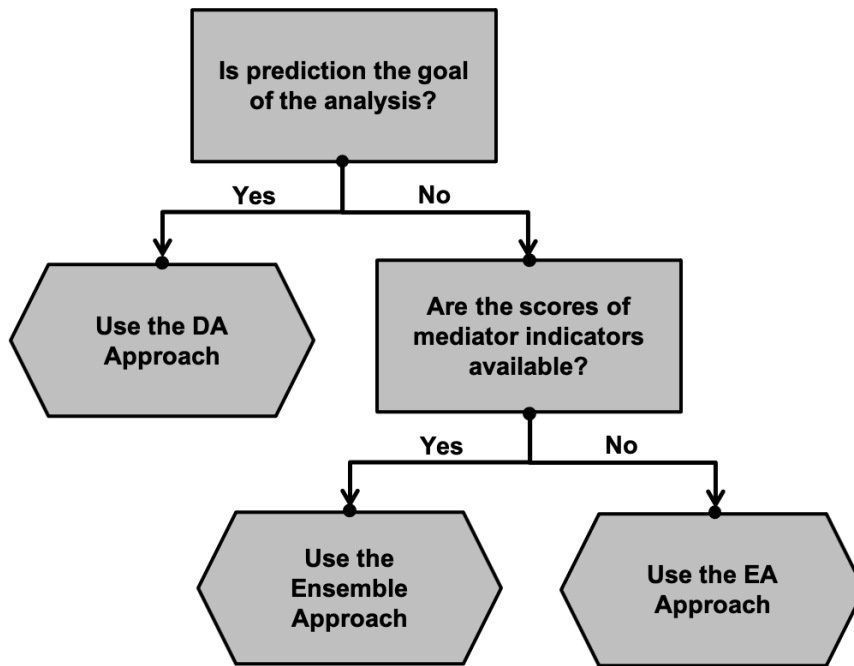
12 **7. Conclusion**

13 **7.1. Discussion**

14 This research note investigated the performance of three proposed solutions for
15 generating predictions from PLS-SEM models and provided a predictive method for
16 providing evidence of the generalizability of a mediated relationship. We developed a variety
17 of simulations in the R statistical environment, generated three structural models, one fully
18 mediated, one partially mediated (see Table 1), and a non-mediated model, considered
19 different predictive approaches for models of varying complexity. In addition to simulated
20 data using Schlittgen's (2019) method, we tested the relative performance of the three
21 solutions and the PCM metric on actual likert data collected from an empirical study.

22 Our findings suggest that many of our expectations and concerns are valid. For
23 example, the overwhelming predictive superiority of the direct-antecedents solution that we
24 expected was verified by both the monte-carlo simulation and empirical example. We find
25 that the direct antecedents solution generates predictions with the highest accuracy, well

1 beyond both the ensemble and earliest-antecedents solutions. Overall, we demonstrated that
2 although alternative strategies exist to incorporating mediators in PLS prediction, and
3 although each strategy has its role in research and practice, that their predictive qualities differ
4 greatly.



5

6 **Figure 5.** Decision tree for selecting the prediction approach

7 When the goal of PLS-SEM modeling is generating predictions or maximizing accuracy
8 of predictions, then researchers would be best served by using the DA approach. However, if
9 predictions were sought for a model for which mediating construct indicator data were not
10 available, the EA approach would prove highly suitable. An example of such is when archival
11 data is used to generate predictions in a mediated model, but no data was collected for the
12 hypothesized mediator at that time. When researchers wish to omit no portion of the model
13 and generate predictions that take into account all indicators and weights, then they would be
14 best suited by the Ensemble approach.

15 We demonstrated that the PCM metric can be used to provide additional evidence as to
16 whether the added complexity of a mediation relationship in a PLS model is justified by the
17 predictive performance. We suggest that researchers routinely conduct such an analysis in

1 parallel to traditional mediation testing in order to present evidence of predictive validity of
2 mediated relationships. High levels of predictive validity would reassure researchers and
3 practitioners alike that results could generalize to further datasets and potentially similar
4 contexts, and increase confidence in the inferential findings.

5 **7.2. Limitations and further research**

6 We suggest that future researchers pay particular attention to the ensemble strategy,
7 which offers a fruitful direction for theory building, despite its predictive nature differing
8 greatly from its use in purely predictive disciplines where it originates. In particular, we
9 suspect that ensemble predictions might yield greater advantages when disparate methods are
10 used – such as a linear model or regression tree. An alternative might be to seek some
11 weighting scheme that might yield an optimal combination of EA and DA predictions.

12 We acknowledge that our proposed initial rule-of-thumb for classifying the predictive
13 contribution of the mediator as weak, moderate, or strong has not been sufficiently tested. We
14 suggest that researchers publish the results of their PCM analysis, and that through meta-
15 analysis the rules-of-thumb for this metric can be refined in later research. We additionally
16 suggest that the PCM be re-evaluated considering the effect size for mediation proposed by
17 Lachowicz et al. (2018). This is a particularly promising line of research.

18 Predictive validation of mediating constructs might have relevance to the broader topic
19 of external validation of construct measures in a nomological network in PLS-SEM (Hair,
20 Howard, & Nitzl, 2020). We believe that more investigation in this field of research might
21 yield promising results.

22

23

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38

1 Appendix A

2 Code to replicate the Empirical Example

```
library(semnr)
data <- read.csv(file = "UTAUT-722.csv")
meas_model <- constructs(
  composite("PE", multi_items("PE", 1:4), weights = mode_A),
  composite("EE", multi_items("EE", 1:4), weights = mode_A),
  composite("SN", multi_items("SN", 1:3), weights = mode_A),
  composite("FC", multi_items("FC", 1:3), weights = mode_A),
  composite("BI", multi_items("BI", 1:3), weights = mode_A),
  composite("USE", multi_items("USE", 1:4), weights = mode_A)
)
struc_model <- relationships(
  paths(from = c("PE", "EE", "SN"), to = "BI"),
  paths(from = c("FC", "BI"), to = "USE")
)
utaut_model <- estimate_pls(data,
  measurement_model = meas_model,
  structural_model = struc_model)
sum_utaut_model <- summary(utaut_model)
utaut_DA <- predict_pls(utaut_model,
  technique = predict_DA,
  noFolds = 10,
  reps = 10)
utaut_EA <- predict_pls(utaut_model,
  technique = predict_EA,
  noFolds = 10,
  reps = 10)

sum_utaut_DA <- summary(utaut_DA)
sum_utaut_EA <- summary(utaut_EA)
sum_utaut_DA
sum_utaut_EA
ensemble_USE1 <- (utaut_DA$PLS_out_of_sample_residuals[, "USE1"] +
  utaut_EA$PLS_out_of_sample_residuals[, "USE1"])/2
ensemble_USE2 <- (utaut_DA$PLS_out_of_sample_residuals[, "USE2"] +
  utaut_EA$PLS_out_of_sample_residuals[, "USE2"])/2
ensemble_USE3 <- (utaut_DA$PLS_out_of_sample_residuals[, "USE3"] +
  utaut_EA$PLS_out_of_sample_residuals[, "USE3"])/2
```

```

ensemble_USE4 <- (utaut_DA$PLS_out_of_sample_residuals[,"USE4"] +
utaut_EA$PLS_out_of_sample_residuals[,"USE4"])/2

plot(density(utaut_DA$PLS_out_of_sample_residuals[,"USE1"]),
      main = "USE1", lwd = 1, ylim = c(0, 0.45))
abline(v = c(0),lty = 2)
lines(density(utaut_EA$PLS_out_of_sample_residuals[,"USE1"]),
      lwd = 1, lty = 3)
lines(density(ensemble_USE1), lwd = 1, lty = 4)
legend("topleft",
      legend = c("DA", "EA", "Ensemble"),
      lwd = c(1,1,1),
      lty = c(1,3,4),
      bty = "n",
      text.col = "black",
      horiz = F )

plot(density(utaut_DA$PLS_out_of_sample_residuals[,"USE2"]),
      main = "USE2", lwd = 1, ylim = c(0,0.85))
abline(v = c(0),lty = 2)
lines(density(utaut_EA$PLS_out_of_sample_residuals[,"USE2"]),
      lwd = 1, lty = 3)
lines(density(ensemble_USE2), lwd = 1, lty = 4)
legend("topleft",
      legend = c("DA", "EA", "Ensemble"),
      lwd = c(1,1,1),
      lty = c(1,3,4),
      bty = "n",
      text.col = "black",
      horiz = F )

plot(density(utaut_DA$PLS_out_of_sample_residuals[,"USE3"]),
      main = "USE3", lwd = 1, ylim = c(0,0.35))
abline(v = c(0),lty = 2)
lines(density(utaut_EA$PLS_out_of_sample_residuals[,"USE3"]),
      lwd = 1, lty = 3)
lines(density(ensemble_USE3), lwd = 1, lty = 4)
legend("topleft",
      legend = c("DA", "EA", "Ensemble"),
      lwd = c(1,1,1),

```

```

    lty = c(1,3,4),
    bty = "n",
    text.col = "black",
    horiz = F )

plot(density(utaut_DA$PLS_out_of_sample_residuals[, "USE4"]),
     main = "USE4", lwd = 1, ylim = c(0,0.25))
abline(v = c(0), lty = 2)
lines(density(utaut_EA$PLS_out_of_sample_residuals[, "USE4"]),
      lwd = 1, lty = 3)
lines(density(ensemble_USE4), lwd = 1, lty = 4)
legend("topright",
      legend = c("DA", "EA", "Ensemble"),
      lwd = c(1,1,1),
      lty = c(1,3,4),
      bty = "n",
      text.col = "black",
      horiz = F )

ensemble_use1_rmse <- sqrt(mean(ensemble_USE1^2))
ensemble_use1_mae <- mean(abs(ensemble_USE1))
ensemble_use2_rmse <- sqrt(mean(ensemble_USE2^2))
ensemble_use2_mae <- mean(abs(ensemble_USE2))
ensemble_use3_rmse <- sqrt(mean(ensemble_USE3^2))
ensemble_use3_mae <- mean(abs(ensemble_USE3))
ensemble_use4_rmse <- sqrt(mean(ensemble_USE4^2))
ensemble_use4_mae <- mean(abs(ensemble_USE4))

## PCM metric
## Mediator 1 PE
utaut_data <- read.csv(file = "UTAUT-722.csv")

meas_model <- constructs(
  composite("PE", multi_items("PE", 1:4), weights = mode_A),
  composite("EE", multi_items("EE", 1:4), weights = mode_A),
  composite("SN", multi_items("SN", 1:3), weights = mode_A),
  composite("FC", multi_items("FC", 1:3), weights = mode_A),
  composite("BI", multi_items("BI", 1:3), weights = mode_A),

```

```

composite("USE", multi_items("USE", 1:4), weights = mode_A)
)

struc_model <- relationships(
  paths(from = c("PE"), to = c("BI", "USE")),
  paths(from = c("BI"), to = "USE")
)

utaut_model <- estimate_pls(utaut_data,
  measurement_model = meas_model,
  structural_model = struc_model)

utaut_DA <- predict_pls(utaut_model,
  technique = predict_DA,
  noFolds = 10,
  reps = 10)

utaut_EA <- predict_pls(utaut_model,
  technique = predict_EA,
  noFolds = 10,
  reps = 10)

sum_utaut_DA <- summary(utaut_DA)
sum_utaut_EA <- summary(utaut_EA)

(sum_utaut_EA$PLS_out_of_sample[1,4:7] -
sum_utaut_DA$PLS_out_of_sample[1,4:7])/sum_utaut_EA$PLS_out_of_sample[1,4:7]

## Mediator 2 EE
struc_model <- relationships(
  paths(from = c("EE"), to = c("BI", "USE")),
  paths(from = c("BI"), to = "USE")
)

utaut_model <- estimate_pls(utaut_data,
  measurement_model = meas_model,
  structural_model = struc_model)

utaut_DA <- predict_pls(utaut_model,
  technique = predict_DA,

```

```

        noFolds = 10,
        reps = 10)

utaut_EA <- predict_pls(utaut_model,
                        technique = predict_EA,
                        noFolds = 10,
                        reps = 10)

sum_utaut_DA <- summary(utaut_DA)
sum_utaut_EA <- summary(utaut_EA)

(sum_utaut_EA$PLS_out_of_sample[1,4:7] -
sum_utaut_DA$PLS_out_of_sample[1,4:7])/sum_utaut_EA$PLS_out_of_sample[1,4:7]

## Mediator 3 SN
struc_model <- relationships(
  paths(from = c("SN"), to = c("BI", "USE")),
  paths(from = c("BI"), to = "USE")
)

utaut_model <- estimate_pls(utaut_data,
                            measurement_model = meas_model,
                            structural_model = struc_model)

utaut_DA <- predict_pls(utaut_model,
                        technique = predict_DA,
                        noFolds = 10,
                        reps = 10)

utaut_EA <- predict_pls(utaut_model,
                        technique = predict_EA,
                        noFolds = 10,
                        reps = 10)

sum_utaut_DA <- summary(utaut_DA)
sum_utaut_EA <- summary(utaut_EA)

(sum_utaut_EA$PLS_out_of_sample[1,4:7] -
sum_utaut_DA$PLS_out_of_sample[1,4:7])/sum_utaut_EA$PLS_out_of_sample[1,4:7]

```

1 **Appendix B**

2 We first estimate the Al-Gahtani et al. (2007) model excluding direct relationships to
 3 demonstrate that we have reproduced the findings from Figure 3 in Al-Gahtani et al. (2007).
 4 These results are shown in Table B1.

| Exogenous | Endogenous | |
|----------------|------------|--------|
| | BI | USE |
| PE | 0.214* | - |
| EE | 0.363* | - |
| SN | 0.208* | - |
| FC | - | 0.199* |
| BI | - | 0.376* |
| R ² | 0.353 | 0.251 |

5 Table B1. Original Al-Gahtani et al. (2007) estimates excluding direct effects

6 Note: * Significant at P < 0.001

7 We then turn to the evaluation of the mediated relationships PE, EE, and SN via BI on
 8 USE. We re-estimate the Al-Gahtani et al. (2007) model including the direct effects of PE,
 9 EE, and SN on USE (Table B2). We find that according to the criteria set out by Nitzl et al.
 10 (2016) and find that the relationships of both PE and EE on USE are fully mediated, while SN
 11 displays competitive mediation as evidenced by the significant and negative path of SN on
 12 USE.

| Exogenous | Endogenous | |
|----------------|------------|----------------------|
| | BI | USE |
| PE | 0.214* | -0.008 ^{NS} |
| EE | 0.363* | 0.032 ^{NS} |
| SN | 0.208* | -0.173* |
| FC | - | 0.207* |
| BI | - | 0.422* |
| R ² | 0.353 | 0.278 |

13 Table B2. Original Al-Gahtani et al. (2007) estimates including direct effects

14 Note: * Significant at P < 0.001, NS not significant at P > 0.10