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Rejoinder to Comments on Recent Developments in PLS

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Abstract:

When we were first invited to write an essay on the use of PLS for CAIS, we wanted to focus on recent developments to help applied IS researchers, and the CAIS community of authors, reviewers, and editors make use of the latest research on and methodological advances in PLS. Recognizing that Information Systems is arguably the discipline in which the use of PLS as an alternative to CB-SEM originated and is most widely used, we realized that, pragmatically, our essay must focus on how to use PLS, not whether to use PLS.

We received six interesting responses from researchers active in the PLS community. Their thoughts on our presentation of recent developments in PLS show very different perspectives with many points of differences but also points of agreements in all the responses. In this rejoinder, we briefly respond to the received comments, clarify our position and ideas, and identify points of agreement (and disagreement). We emphasize that none of the responses give us cause to revise or eliminate our recommendations in recent developments.

Overall, we believe this discussion on PLS to be valuable in advancing the use of PLS in Information Systems, which is, as we show in this rejoinder, an urgent issue.

Keywords: Partial Least Squares, PLS, structural equation modeling, prediction, statistics, research methods

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This manuscript underwent [editorial/peer] review. It was received xx/xx/20xx and was with the authors for XX months for XX revisions. [firstname lastname] served as Associate Editor. **or** The Associate Editor chose to remain anonymous.]

1 Introduction

We are happy to see that our paper on “Recent Developments in PLS” (Evermann & Rönkkö, 2021) (hereafter ER21) has attracted significant interest in the form of a large set of responses. These responses comment on various aspects of our paper and provide a range of different perspectives on this topic. We are grateful to the authors of these comments for their in-depth engagement and the often critical, but valuable points they make.

We will next address each response in turn. As the reader can tell from our original paper and the responses to it, research on PLS is a fast-moving field. Between the time we submitted our original paper and the time we write this rejoinder, several special issues and other papers on PLS have been published or are in press. However, to keep the scope of this rejoinder manageable, we focus only on the comments to ER21. We emphasize that none of the responses invalidate our recommendations in recent developments; nothing in the six replies gives us cause to revise or retract any of our original recommendations.

2 Response to Rigdon (2022)

The key question that Rigdon (2022) raises is whether composite-based models are any better or worse than factor models. Rigdon (2022) suggests that ‘data that can be described by a common factor model can also be described by composite-based RCA’ (p. 8). While this is true in principle, the key consideration for researchers is *how well* the data is described by various models. Moreover, factor analysis has traditionally been used for two purposes: Data description and model estimation. When using factor analysis for measurement validation, we are focusing on the latter purpose. If mere description is of interest, using sums or means of indicators is often adequate, as Rigdon (2022) acknowledges.

Rigdon (2022), taking a realist stance, then argues that ‘none of the extant metrics actually quantifies the similarity between empirical proxy and unobserved conceptual variable, so none of them actually assess validity’. By declaring the conceptual variable in principle unobservable yet demanding a metric that measures the similarity of it with some data, Rigdon (2022) asks for the impossible. In reality, the goal of factor analysis is more modest: It can be used to test for the plausibility that observed items have a common cause and factor indeterminacy does not prevent this kind of inference (Haig, 2005, 2013).

While Rigdon (2022) argues that the extant validity metrics need to be replaced, he is unfortunately silent on what they should be replaced with. It is clear that, in light of the unobservable nature of conceptual variables, the validity of a statistical model as a representation of theory of unobservable variables cannot rest only on the similarity between an empirical proxy (i.e. the composite or latent variable) and the unobserved conceptual variable, as a realist would have it.

A way out of this problem is to focus on relationships, instead of proxy scores. Statistical models (should) imply testable relationships among variables, and this is what the inferential use of factor analysis rests on. The degree to which implications of the model agree with observations allows us to also make inferences about the validity, or lack thereof, of the model, and by extension, the nature of its proxy (the composite or factor variable). These inferences are not conclusive but that is a more general problem in the philosophy of science (Haig, 2005, 2013).

Rigdon (2022) suggests that it is unknown (and unknowable!) whether unobserved conceptual variables are best approximated by factors or composites. This is not true. If the interest is in rank-ordering of observations, then composites are preferable because latent variables cannot be used for this purpose as they do not have case values. However, if the purpose is to make inferences about the relationships between unobservable, conceptual variables, the situation is different. The realist perspective assumes that the conceptual variable is a common cause for the items of a scale that measures the variable. As such, a common factor model seems to be a reasonable starting point for modeling the relationship between two unobservable variables. Indeed, it seems to us it would be a very special coincidence if the conceptual causes of observables could be best approximated by the very specific linear combination *of just those observables they are causing*. Applying Occam’s razor, this is a very strong assumption, and it appears to us that, in the absence of our ability in principle to verify this, we would be well advised to make less specific or weaker assumptions. Of course, this does not mean that using a simple common factor model is always better than using composites (Rhemtulla et al., 2020). If a factor model is misspecified (e.g. there are unmodeled correlations between indicators) a composite model might produce estimates that are less erroneous. But this argument has nothing to do with factor indeterminacy.

Besides this main issue, there are other passages in Rigdon's (2022) response that give us pause. After describing iterative composite-based estimation (p. 5), Rigdon suggests that 'modelers could gain the benefit of flexibility without switching between factor model and composite model'. This last sentence is to us a puzzling non-sequitur, and, indeed, Rigdon does not further define 'the benefit of flexibility'. Rigdon (2022) also suggests that ER21 embraces the outdated notion that 'statistically significant' results are qualitatively different'. Yet, we have made no such claim. In contrast, we recommend that t-tests should be avoided and researchers should use confidence intervals instead (Recommendation 2). Finally, in describing Schönemann and Steiger's (1976) regression component analysis, Rigdon (2022) notes that the loading matrix in a composite description 'could very well be the same loading matrix' as in the factor description. We agree with the 'could', but more interesting is whether it 'should' be the same, or 'will' be the same.

3 Response to Kock (2022)

Kock is the author of the software tool WarpPLS. Kock (2022) presents three recently added features to his software product in a paper that does not engage with the issues in "Recent Developments". These features have a number of methodological problems. We therefore take the opportunity to critically evaluate the ideas mentioned by Kock (2022).

The first feature in Kock (2022) is that of 'lateral collinearity' and common method bias: Kock and Lynn (2012) introduce 'lateral collinearity' claiming that "two or more variables are said to be collinear when they measure the same attribute of an object" (p. 547). However, the statistical literature simply uses the term 'collinearity' to refer to two or more variables being linearly dependent without attributing this dependency to any specific cause. In fact, the problem that Kock and Lynn (2012) explain already has an established term in the methodological literature: lack of discriminant validity (Rönkkö & Cho, 2022) . In fact, Kock and Lynn (2012) themselves note that 'the strong association is due to both latent variables essentially measuring the same "thing" (i.e., the same construct)' (p. 552).

Kock and Lynn (2012) continue by proposing an adoption of traditional VIF cutoff guidelines to this new concept. They present no simulation study with synthetic data to support their recommendations, but only an illustrative example with a real data set where the ground truth is unknown. It is also unclear why VIF would be the best way to quantify the phenomenon. In the context of multicollinearity between predictors, VIF is useful because it presents the factor with which the variance of estimates inflates compared to uncorrelated predictors (hence Variance Inflation Factor; Wooldridge, 2013, p. 98). But, in a more general context, the R^2 statistic provides the same information and is easier to interpret because VIF = $1/(1-R^2)$.

Kock (2015b) extends this idea to suggest that lateral collinearity may be useful to identify common-method bias and suggests using 3.3 as a cutoff for the VIF. Presented in the form of R^2, this rule says that if the R^2 of a regression of a variable on all others exceeds 0.7, common method variance is a problem and otherwise it is not. This rule is problematic in at least three different ways: First, it practically never indicates the existence of a method variance problem when the latent variables are uncorrelated, which may lead to incorrect conclusions about the existence of relationships where none exists. On the other hand, it always indicates the existence of a method variance problem for constructs that are genuinely highly correlated, and essentially prevents research on highly correlated constructs. Second, a high R^2 may also be caused by other problems, such as a lack of discriminant validity. Third, Kock (2015b) ignores decades of existing research on the subject of common method bias (e.g. the debate in Organizational Research Methods 13(3)). Identifying whether correlation caused by one shared method factor or multiple correlated minor factors is a hard problem that is often impossible to solve (Eid et al., 2018) and it may be more productive to try to measure and model the causes of method variance (Spector et al., 2019).

Kock and Hadaya (2018) present two rules for calculating required sample sizes for PLS analyses. The first rule assumes that the sampling distribution of PLS estimates is normal. Kock and Hadaya (2018) invoke the central limit theorem to justify this assumption, but it is difficult to see how the conclusion would follow[1] and there is ample evidence that the distribution of PLS estimates is not generally normal, even in moderately sized samples (Aguirre-Urreta & Rönkkö, 2018; Goodhue et al., 2007; Rönkkö & Evermann, 2013). Kock and Hadaya (2018) then assume that the standard error of PLS estimates can be estimated by $1/\sqrt{N}$, which resembles a well-known estimator of standard error of mean. In reality, the standard error depends at least on model complexity, collinearity between predictors, measurement quality, and whether Mode A and Mode B indicator weights are used. Using these unsubstantiated and incorrect assumptions, Kock and Hadaya present that minimum sample size for PLS can be estimated by $(2.486/|\beta|_{min})^2$. The second rule is simply a bias-corrected variant of the first one. Both rules happen to perform well in the simulation performed by Kock and Hadaya (2018), but this could be a chance occurrence and more rigorous testing of the rules is needed before they can be recommended to applied researchers.

PLSF ("Factor-based PLS") is the final theme in Kock (2022). We focus on the most recent iteration (Kock, 2019) that consists of four stages. The first stage is PLSc, which was discussed in ER21 and is not unique to PLSF. The second stage consists of a novel composite estimation technique and the third stage involves estimation of factor scores so that their correlations match the consistent factor correlation estimates from the first stage. In the fourth stage, these factor scores are used to estimate the model parameters.

We see two main problems with this algorithm. First, the purpose of the three final stages is unclear: A first step in estimating a regression model in Stage 4 is to calculate cross-product matrices of the variables (Wooldridge, 2013, Appendix E), which, because of standardization, equals correlations. In other words, as far as parameter estimation is concerned, Stage 2, Stage 3, and the first step in Stage 4 simply recalculate a matrix that was already available from Stage 1. It appears that the PLSF algorithm will simply reproduce the PLSc estimates from Stage 1 while having a nontrivial computational cost because of the iterative nature of Stages 2 and 3. In summary, as far as parameter estimation is concerned, PLSF is simply PLSc but slower and more difficult to understand.

Second, the selling point of PLSF appears to be the factor scores. But it is not clear why a new iterative factor score calculation technique is needed, considering the existence of non-iterative correlation preserving factor scores (Grice, 2001), or what advantages the PLSF factor scores would have over those of traditional techniques. Moreover, we do not recall any example where composites from a PLS analysis are used for purposes other than parameter estimation, a case that PLSc already handles. Finally, if the factor scores were used for something other than estimating model parameters, their usefulness would be limited because of factor score indeterminacy. That is, while correlation preserving factor scores do reproduce the estimated factor correlations, they do not generally reproduce any other features of the true factors. Hence, the factor scores cannot be productively used to e.g. estimate nonlinear models, contrary to Kock's (2019) claims.

Finally, Kock (2022) concludes by mentioning other "methodological innovations". We want to address one of them, Simpson's paradox, which Kock (p. 128) defines as 'path coefficients associated with links and the corresponding correlations have different signs (a very odd and counterintuitive phenomenon).' This phenomenon is referred to as suppression in the methodological literature and explanations can be found in introductory texts on regression (e.g., Cohen et al., 2003, pp. 77–78) and SEM (e.g., Kline, 2011, pp. 26–27) and a number of articles (Friedman & Wall, 2005; Shieh, 2006) and even on YouTube (Rönkkö, 2019). Suppression is a feature of how correlation and causation work and not a threat to causal inference as Kock (2022) implies. A classic example is that increasing the number of firefighters decreases the amount of fire damage. Yet, the number of firefighters is positively correlated with the amount of fire damage because both depend on the size of the fire (Singleton & Straits, 2018, p. 100). Simpson's paradox typically refers to a different phenomenon: the sign difference between population and subgroup associations (Kievit et al., 2013).

[1] Koch and Hadaya (2018) write: "The assumption that path coefficients are normally distributed generally holds for PLS-SEM, because coefficients calculated based on sample sets taken randomly from a population tend to be distributed in conformity with the central limit theorem". Yet, this is not what central limit theorem states. It states that the sampling distribution of the *sample mean* tends to follow normal distribution in fairly general conditions. That is, central limit theorem is not a general theory about any coefficient or estimate but about sample mean. Many other commonly used statistics (e.g. sample correlation) have non-normal sampling distribution.

In summary, Kock's (2022) response does not engage with our recommendations and the response does not cause us to revise or retract any of our original recommendations.

4 Response to Goodhue, Lewis, and Thompson (2022)

We thank Goodhue, Lewis, and Thompson (GLT) (2022) for the very clear, step-by-step illustration of the PLS weighting algorithm. Their article explains in diagrams how the regression of indicators on the connected composite proxy causes a bias in the estimated beta regression coefficient away from 0, as described in Rönkkö and Evermann (2013). From their illustrations, it is also clear how idiosyncratic chance correlations between indicators of adjacent latent variables are capitalized on, as shown by Rönkkö (2014). Importantly, in addition to confirming and explaining our earlier results, GLT (2022) have demonstrated that the PLS algorithm assumes a non-zero relationship between adjacent latent variables, and this assumption renders any subsequent statistical test of such a relationship as biased. We agree with those authors that 'this is actually a pretty big deal!' (p. 8)

We appreciate that GLT (2022) have laid out so clearly the options available to the research community and are advocating for their options 1 and 2 (stopping the use of PLS and using CB-SEM or summed scales). Unfortunately, to this we reply that the proverbial horse has left the barn. Or, reflecting on the effect that uncritical use of PLS has had on our research community, Pandora's box has been opened.

They further claimed that in ER21 we advocated for option 3. However, the reality is more nuanced. Consider the two final recommendations in ER21: 'PLS composites should be compared to unweighted composites to demonstrate any possible advantage that the PLS composites might have.' (Recommendation 13) and 'Faced with multiple, equivalent methodological options, the simplest method should be preferred.' (Recommendation 14). In practice PLS often tends to produce composites that are nearly identical with unit weighted ones (Rönkkö et al., 2022) and following these rules would thus lead to the use of unit weights or GLT's options 1 and 2 most of the time.

We do not think that a categorical ban of PLS or any analysis or inference technique is useful because it invites pushback without forcing researchers to consider the methodological issues involved in their choice of technique. Instead, we advocate that editors and reviewers should always press authors to justify their choices based on methodological grounds instead of appeals to expert opinions (Guide & Ketokivi, 2015). Particularly, we recently introduced the composite equivalence index (CEI), a measure of correlation between PLS composites and unweighted composites (Rönkkö et al., 2022). We suggest that journal editors (a) require the reporting of this index because it clearly shows whether PLS makes a difference compared to simpler regression analysis with unit weights and (b) require the interpretation and theoretical justification of PLS weights if they are used instead of the simpler unit weights. These requirements do not seem too onerous to us.

5 Response to Russo and Stol (2022)

We appreciate Russo and Stol's comments on the larger discussion around PLS and on our own part within this debate.

Russo and Stol (2022) suggest that our article falls short of its promise on two accounts, first by ignoring recent work on PLS by Kock and colleagues and, second, by taking an overly critical and polarizing position toward PLS. While Kock and colleagues have published extensively on PLS, it is unconvincing to us, as our detailed reply to Kock (2022) above shows. It is for this reason that we have not recommended Kock's work to the CAIS community.

Russo and Stol (2022) suggest that both CB-SEM and PLS have a place in the methodological toolbox. Composite models and prediction from plausible theoretical models, as proposed by Schuberth, Zaza, and Henseler (2022) and Sharma, Liengaard, Sarstedt, Hair, and Ringle (2022) (see below), may well be appropriate areas of application for PLS. However, there are two issues: First, we have seen only initial work on this and many open questions remain, and second, this is unfortunately not the reality of PLS use (cf. Section 8 below). It is clear from our literature survey below that the shortcomings and limitations of PLS need to be pointed out, if anything, even more clearly to applied researchers.

Russo and Stol (2022) proceed to make four points: (1) towards a more balanced debate, (2) knowing the audience, (3) being mindful of philosophical and practical differences, and (4) on flawed evidence. We briefly address these points in turn.

First, Russo and Stol (2022) call for a more balanced debate of PLS. They start by suggesting that our position with respect to whether we consider PLS to be a SEM technique is inconsistent, pointing to the "highlight" of Rönkkö et al. (2015) 'Partial least squares (PLS) is simply an indicator weighting system and not SEM' on the ScienceDirect website[2]. Yet, the article itself presents a much more nuanced view that is consistent through our work (Rönkkö et al., 2022; Rönkkö, McIntosh, Antonakis, et al., 2016; Rönkkö & Evermann, 2013): We do not think that debating whether PLS is or is not SEM is useful because this boils down to differences in definitions. Indeed, in Rönkkö and Everman (2013) we explain that as 'the argument that PLS is an SEM estimator is technically true, it is as correct to state that OLS regression is an SEM estimator.' (p.433) Rönkkö et al. (2015, Footnote 1) point out tongue-in-cheek that with a sufficiently broad interpretation of the term SEM, even a random number generator qualifies as a SEM estimator. Importantly, labeling PLS as a SEM technique matters insofar as it signals certain characteristics. Applied researchers may assume that all techniques labeled as 'SEM' are equally appropriate, are interchangeable, and yield very similar results, which is not the case. We caution that the labeling of PLS path modeling as PLS-SEM has contributed, intentionally or not, to applied researchers making inappropriate methodological choices.

For an applied researcher, the labeling issue has two important implications when choosing methods: First, the PLS literature often presents the choice of technique as one between PLS-SEM and CB-SEM within the set of so-called "second generation techniques" (Panel A in Figure 1). However, researchers should first make a choice between modeling with latent variables or with scale scores (Panel B in Figure 1), and then make an informed choice between different indicator weighting systems. Both choices should be justified (Rönkkö et al., 2022). Second, using PLS is not an all or nothing decision. It is entirely possible to use PLS for main hypothesis testing while assessing measures with exploratory factor analysis and Cronbach's alpha. Moreover it is possible to mix composites and latent variables in analysis. For example, a researcher could use SmartPLS to calculate a set of composite scores, export them and use them as data in AMOS. Introductory texts on PLS unfortunately omit these possibilities.

[2] So why did we have the highlight that we did if it does not accurately represent what the article says? Indeed, we originally wanted the first highlight of the Rönkkö et al. (2015) to be "Partial least squares (PLS) is simply an indicator weighting system and calling it as SEM is misleading" but were forced to leave the end out because of the 85 character length limitation of highlights in the journal.

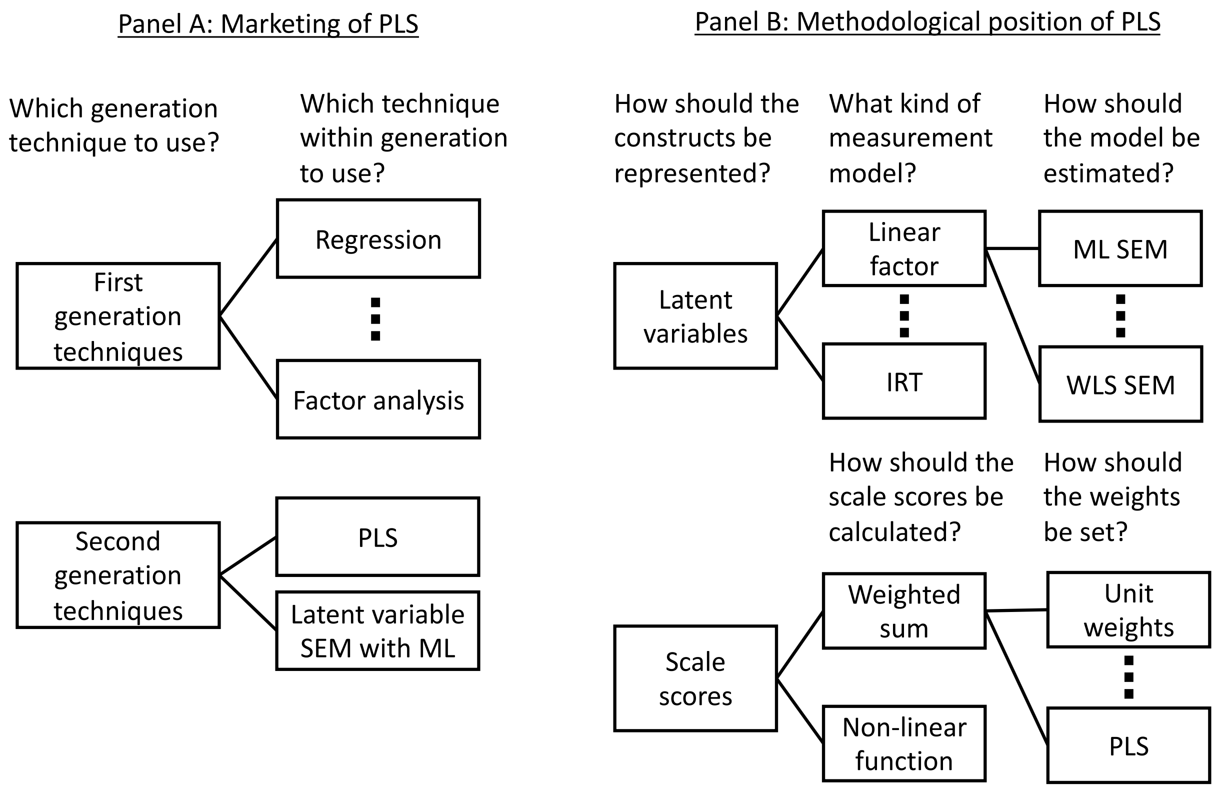

Figure 1. Comparison of how PLS is marketed and how it is positioned methodologically (Rönkkö et al., 2022)

In the remainder of their first comment, Russo and Stol (2022) criticize us for not addressing Rigdon's views on factors and composites (Rigdon, 2016; Rigdon et al., 2014). We do so in ER21 (Sections 4.7 and 4.8) but we focus more on estimating factor models as this remains the main application area in Information Systems and other disciplines (cf. Section 8 below). Russo and Stol (2022) criticize that our presentation in ER21 with 'formulas, deductions, and results of simulation studies' are overwhelming due its technical nature. We are surprised, as ER21 contains only 10 formulas, no deductions, and no simulation studies. We suggest that a researcher who does not understand the statistical techniques embodied in their chosen statistical software, and is 'overwhelmed' (Russo and Stol, 2022, p. 126) by a few explanatory formulas, should best refrain from using such software. This position appears to agree with Russo and Stol (2022), who write that 'all scholars have a responsibility to study and familiarize themselves with the methods they use – this is, after all, the core business of scholars.' (p. 126).

We agree that our presentation is dense in information, but this is unavoidable when one is tasked to write a comprehensive review within the constraints of journal page limitations. For a more accessible explanation of a subset of the issues, we recommend the readers to take a look at our recent article in the European Marketing Journal (Rönkkö et al., 2022) and the accompanying video material and demonstrations.

We also appreciate Russo and Stol's (2022) suggestion to feature GSCA more prominently. Given that we were invited to initiate a debate on PLS, the suggested comparison of PLS and GSCA must, as interesting and informative as it will undoubtedly be, remain a future project. We also agree with Russo and Stol (2022) that our early critique has spurred many useful adaptations and extensions to PLS and ER21 aims to bring these advances to the attention of Information Systems researchers.

In their second point, Russo and Stol (2022) admonish us to know our audience. They suggest that our recommendations are somehow too technical and onerous for researchers to perform as 'they go well beyond the typical introductory textbooks on PLS' (p. 127). We are somewhat baffled by this. If this is in fact the case, and given our agreement on the point of researchers (and editors) needing to be well-versed in their methodology, existing textbooks must then be insufficient. However, even the introductory text by Hair et al. (2022), which lacks any technical depth on the method, provides simple how-to steps for researchers to accomplish the recommended analyses. None of our recommendations in ER21 are particularly onerous: An easy to follow method for simulations using PLS was presented in this same journal some years ago (Rönkkö & Aguirre-Urreta, 2015); the model fit statistic d_g is available, for example, in the `matrixpls` package for R (Rönkkö, 2022) and in SmartPLS and only needs to be examined and reported; using PLS for prediction is easily done in `matrixpls` and SmartPLS but, more importantly, needs to be motivated and supported in the aim of the study, using words, not math; and a comparison with unweighted composites is included in the default output of `matrixpls` and with other software requires just the calculation of simple summed (averaged) scales and a correlation of composite scores, which is possible even in spreadsheet software (Rönkkö et al., 2022).

Third, Russo and Stol (2022) present philosophical and practical differences. We agree that some constructs are best approximated as composites, and the socio-economic status is a widely used example. Though we point out that measures of SES do not cause the concept (Edwards, 2011), in line with the quoted passage of Rigdon (2016) that it is impossible to form conceptual variables out of data. However, when the indicators share the construct as a cause, as we noted above in our response to Rigdon (2022), it would be quite the coincidence if the causes of observables could be best approximated by the very specific linear combination of just those observables they are causing. But the focus on the validity of proxy scores merely distracts from the, often more important, issue of properly estimating the relationships. And while we agree that 'we should never rely on a single study that investigates important relationships' (Russo and Stol, 2022, p. 128), we strongly disagree with the 'anything goes' attitude of Russo and Stol (2022) when they write that '[t]he issue of how precise or reliable some of the parameter estimates really are loses importance because other studies may either confirm or disconfirm such findings' (p. 128). If precision and reliability do not matter, why do we bother with the scientific method at all?

On the practical side, there are two more issues that we want to address. Russo and Stol comment that CB-SEM requires the use of sum scores: 'For example, latent growth models (Bollen and Curran, 2006), which are implemented within the CB-SEM framework, require simple scores (as opposed to multiple indicator common factors), as does moderation analysis.' Both these claims are incorrect: Bollen and Curran (2006), who Russo and Stol cite to support their claim, explain the use of multiple item factors in section 8.2 of their book, and the use of latent variables in moderation models is explained in introductory textbooks (e.g., Kline, 2011, Chapter 12) so the lack of available procedures is no longer an excuse to not do latent variable moderation (Cortina et al., 2019). Russo and Stol (2022) further note that 'unweighted scores assume that all indicators (items) contribute equally, or are equally important, which may be an unreasonable assumption,' ignoring decades of evidence (as summarized in ER21 and the references therein) demonstrating that using differential item weighting rarely makes a positive difference.

Fourth, in their final section on 'exceptional cases and flawed evidence', Russo and Stol (2022) suggest that we may have overstated our claims of damage to the field of IS by the early use of PLS. Specifically, they note the simplicity of some of the models that we have used. Yet, our findings generalize to the kinds of models that IS researchers estimate, as demonstrated by Rönkkö et al. (2016) who simulated data using ten models published in MIS Quarterly. Moreover, we are not aware of a single realistic simulation study where PLS provides a meaningful advantage over unit-weighted composites. Russo and Stol (2022), and others in the past, also note that some simulation studies that compare PLS with alternative methods are based on the factor model and suggest that this is invalid. We disagree: As long as applied research uses PLS to estimate factor models (cf. Section 8 below), methodology research needs to point out any strengths and weaknesses of various methods *for such factor models*. After all, methodology research is to engage with and inform applied research as it is conducted.

We have recognized in ER21 that the foundational theories have been replicated in different settings and with different methodologies, whether PLSc, summed scales, or CB-SEM. Thus, we agree with Russo and Stol (2022) that, *at this time*, there is sufficient evidence to support the findings and corroborate the theories.

6 Response to Schuberth, Zaza, and Henseler (2022)

We appreciate the thoughtful comments by Schuberth, Zaza, and Henseler (2022) (hereafter SZH22), on our paper. SZH22 note that our earlier work (Rönkkö & Evermann, 2013) led to a split in the PLS community. They position themselves in the group of researchers who 'ascribe PLS the same status as other estimators to SEM' and emphasize the 'steps of SEM'[3]. Because CAIS readers may be unfamiliar with the split, we reiterate that the split involves two groups of researchers. The first group, consisting of Hair and his coauthors, continues to advocate PLS-SEM as a set of techniques, tools, and a workflow mostly focusing on what is supported by the SmartPLS software. Importantly, this group essentially advocates the status quo of how PLS is currently used in IS. This includes, for example, the use of the AVE and CR statistics, that were shown to be problematic over a decade ago by Evermann and Tate (2010). 'It is particularly worrying that some quite influential researchers such as Hair continue to spread outdated views on PLS even against their better judgment (see, for instance, the relatively recent publications Hair, Sarstedt, & Ringle, 2019; Hair, Howard, & Nitzl, 2020)' (Henseler, 2021, p. 96). The other group, consisting of Henseler, Schuberth, the late Theo Dijkstra, and their coauthors, instead abandoned practices that are not supported by evidence, worked to develop solutions to problems of PLS (e.g. PLSc) when used as a latent variable estimation technique, and developed PLS as a fully composite-based modeling approach instead of as a second-class latent variable model estimator. The differences between the groups can also be understood within the context of Figure 1: The Hair et al. group continues to market PLS as a SEM technique (left hand side, Panel A) whereas the Henseler et al. group recognizes that the real question is whether to model with latent variables or composites and that if composites are used, PLS is just one of the available techniques for doing so.

We are grateful to SZH22 to spell out important limitations of PLS for estimating latent variable models, i.e. it cannot model restrictions on loadings or covariances, cannot express correlations between errors of manifest variables for different latent variables, and cannot estimate cross-loadings. We emphasize that all these are significant limitations, as many realistic datasets or models are likely to exhibit one or more of these characteristics (Rönkkö et al., 2022). While SZH22 point out that procedures for PLS to estimate models with latent variables that do not possess indicators exist for special cases of so-called higher order factors, these procedures are not applicable to more general cases, e.g. latent growth curve or latent cross-lagged difference models.

Moving outside the discussion of PLS, SZH22 briefly introduce the 'Henseler-Ogasawara' specification that allows modelling of composites in covariance models, outside of special cases where identification is achieved in the form of MIMIC ("multiple indicator multiple causes") models. This specification further limits the use of PLS in the estimation of structural equation models, as it addresses the motivation of many PLS-based studies that covariance estimation cannot model composites.

In their Section 3, SZH22 engage in detail with many of our recommendations to 'suggest updates and improvements where necessary'. To limit the length of this rejoinder, we provide only brief responses in order.

We thank SZH22 for providing additional details on the re-sampling and information theoretic model selection (our recommendations 6 and 7) and the HTMT2 metric that relaxes some assumptions of the HTMT (our recommendation 9). On SZH22's recommendation to use established terminology (cf. our recommendation 10), we only note that the debate between Aguirre-Urreta and Marakas (2014) and Rigdon et al. (2014) in the Journal of the AIS took place despite such established terminology. Critically, the way that a graphical specification is translated into equations differs between methods and applied researchers must be aware what their chosen software tool is actually doing. Whether that necessarily requires drawing the editor's ire by including such equations may remain unanswered here. We further note that our recommendation to compare PLS composites against unit weighted composites (Recommendation 14) stands even if a composite model is assumed to be the ideal modeling approach. Whether differential

[3] As an aside, we note that the 'steps of SEM' are a tacit social agreement among researchers that has emerged over many years, is continuously debated, and subject to change. In fact, what SZH22 call the typical steps of SEM, 'namely model specification, model identification, model estimation, and model assessment' is so broad as to apply to any statistical model. In particular, it encompasses the way that the 'PLS-SEM' stream around Hair and colleagues uses PLS.

weights make a difference is partially an empirical matter and it is important to increase our understanding when differential weights are warranted and when simpler unit weights will suffice.

SZH22 attempt to provide an answer to the question of when a population model might be composite. We agree up to the point that there exist what they call ‘forged concepts’. While researchers are of course free to postulate any number of ontologically non-real concepts, it would be rare indeed if forged concepts, such as SZH22’s ‘IT capability’ did not represent ontologically real entities: Most IS researchers would ascribe IT capability ontologically real causal force in that it allows firms to take certain observable, manifest actions; else, why study it? But SZH22’s example requires further examination: Following SZH22’s citation of Chae et al. (2014) we note that Bharadwaj (2000) writes ‘A firm’s IT infrastructure, its human IT skills, and its ability to leverage IT for intangible benefits serve as firm-specific resources, which in combination create a firm-wide IT capability’ (p. 176). The reader may be misled by the use of the term ‘in combination’ but Bharadwaj (2000) elaborates that ‘firms that achieve competitive advantage through IT have also learned to combine effectively their IT resources to create an overall IT capability’ (p. 176). Importantly, the ‘combining’ happens in the very complex real world, not in the simple linear statistical model and a numerical composite (‘forged concept’) would appear to be a poor approximation of a complex and possibly non-linear real-world causal process. Of course, as regression equations in a statistical model may express causality, composition, or any number of other notions, the statistical model is unable to differentiate between these notions (Evermann & Tate, 2012). In summary, unless explicitly defined by theory as a composite of observations, such as the socioeconomic status (SES), we continue to have significant doubts that many concepts are composite by nature.

7 Response to Sharma, Liengaard, Saarstedt, Hair and Ringle (2022)

We thank Sharma, Liengaard, Sarstedt, Hair, and Ringle (2022) (SLSHR22 in the following) for their reply. The title of their contribution suggests that we have made “extraordinary” claims, but we have done no such thing and no “extraordinary” evidence is required. SLSHR22 discuss five claims they believe we have made in ER21 and we respond to each of their points in turn.

SLSHR22 claim that we "create unnecessary doubt among researchers applying the method” when we explicitly state that PLS is a method with a known bias when applied to factor models. SLSHR22 start their paper by explaining the history of the development and purpose of the PLS method. They begin with Wold (1982) and Jöreskog & Wold (1982), emphasizing the fact that PLS was designed for prediction, and hence makes a trade-off between predictive ability and parameter estimate bias. We do not disagree with their characterization of the origins of PLS, but note that the very simulation studies cited by SLSHR22 show, for the common factor model that is at the heart of the foundational IS studies that SLSHR22 are concerned with, large differences in the parameter estimates between CB-SEM and PLS. For example, Reinartz, Haenlein, & Henseler (2009) report PLS estimates of 0.4 for structural parameters with a true value (and CB-SEM estimate) of 0.5, a 20% difference. Sarstedt, Hair, Ringle, Thiele, and Gudergan (2016) report a mean absolute error for CB-SEM estimates that is 30% less than that of PLS (0.05 versus 0.07) noting that ‘our results confirm the well-known PLS bias when using the method to estimate the path model with common factor model-based data’ (p. 4005). Differences of the order of 20 to 30 percent should give any researcher grounds to pause and reflect.

However, our main response to the first point raised by SLSHR22 is that the foundational IS studies they are so concerned about did not focus on prediction; they used PLS to test hypotheses in a common factor model. For that application, PLS was a known-to-be-biased estimator.

In their second point, on the goals of explanation and prediction, SLSHR22 see disagreement where there is none. We are aware of the recent call for and research into explainable AI in a variety of fields. We agree with SLSHR22 that a trade-off between explainability and predictive ability is useful in some contexts. In fact, the sentence from ER21 that is quoted by SLSHR22 says precisely that! However, there may well be situations where explainability at the expense of predictive performance is not desirable: In a hypothetical case of successfully treating a patient using a predictive model and of letting the patient die using an explainable model, we believe that most decision makers would forego the explainability. In those situations, predictability is a 'must have' hard requirement, explainability is the 'nice to have' icing on the cake[4].

The third point raised by SLSHR22 concerns the development and nature of additions to PLS. In response to their tour through the topics of string theory, the standard model of physics, the periodic table of elements, and carbon dating, we note that many PLS improvements are more akin to the epi-cycles in Kopernican astronomy or phlogiston in chemistry, in that they cling to a fundamentally ill-suited foundation. It is true that retrofitting can be useful. Yet, it makes no sense to take a motorcycle and make it more car-like by installing two additional wheels, replacing the steering bar with a steering wheel, and building a cabin around the seat if you already have a car available. Similarly, building additions and corrections to PLS to make it produce results that are closer to CB-SEM results makes little sense when CB-SEM already provides an elegant answer to the problem.

SLSHR22 further make the argument that PLS is simply different from CB-SEM, and hence, should have the freedom to develop in ways that make it useful for its, still somewhat unclear, purpose. SLSHR22 claim that 'complex socio-technical processes that give rise to noisy multivariate data do not care about what makes statisticians happy, or whether they believe in common factors or composites.' (p. 4) However, researchers ought to take care to utilize their tools responsibly, as noted by SLSHR22, i.e. in a way that reflects their assumptions about the nature and the purpose of their research. As we note in Section 8 below, this is unfortunately not the case.

In presenting their fourth point, on the extent to which published models are particularly susceptible to problems for inference and testing, SLSHR22 commit a logical fallacy. Given the preponderance of PLS-based analyses in the Information Systems discipline and the demonstrated bias of PLS parameter estimates away from zero, it is little surprise that Blut et al. (2021) find hardly any zero effects. Unfortunately, their study does not disaggregate findings by analysis method. More importantly, do SLSHR22 really wish to suggest that researchers should assume a non-zero effect a priori and select a tool that fails in the zero effect condition? Why then do we bother testing for the significance of the effect?

SLSHR22 also present a simulation, which they argue shows that PLS has no problems with weak paths. Yet, their presentation of the results is highly misleading. First, the fact that PLSc produces inadmissible estimates is a sign that the PLS weights are not identified (Rönkkö, McIntosh, & Aguirre-Urreta, 2016). Second, by just presenting the average of the estimates over all replications, SLSHR22 essentially mask the problem caused by the PLS weights. To demonstrate, we replicated their third simulation for the effect = 0.1 condition[5] and plotted the distribution of the six path estimates in Figure 2. The plots show a clear bimodal (two-peaked) shape for the effects of PE, EE, and SI on BI (top row in Figure 2) which all had just a single path in the estimated model. The effect of FC on USE and BI are bimodal to but to a lesser extent because this FC had two outgoing paths of which one was non-zero in the population. The path from BI to USE is least affected because this composite had two incoming paths that were both from composites that had at least two paths themselves. Still, the effect of PLS weights is visible in the clearly non-normal distribution of the estimates. As these plots show, the simulation by SLSHR22 does not demonstrate the robustness of PLS against weak paths but the opposite.

[4] As an aside, we note that SLSHR22 begin their discussion by claiming that "ER claim that PLS finds itself between a 'rock and a hard place' ... This is incorrect" (p. 125) only to close by stating that "PLS was deliberately designed to occupy the demanding space 'between a rock and a hard place'" (p. 126). We do wonder about the arrangements of rocks, hard places, and PLS.

[5] SLSHR22 did not provide sufficient information to fully reproduce their study so we had to make educated guesses of some of the model parameter values. We provide our simulation code in the appendix.

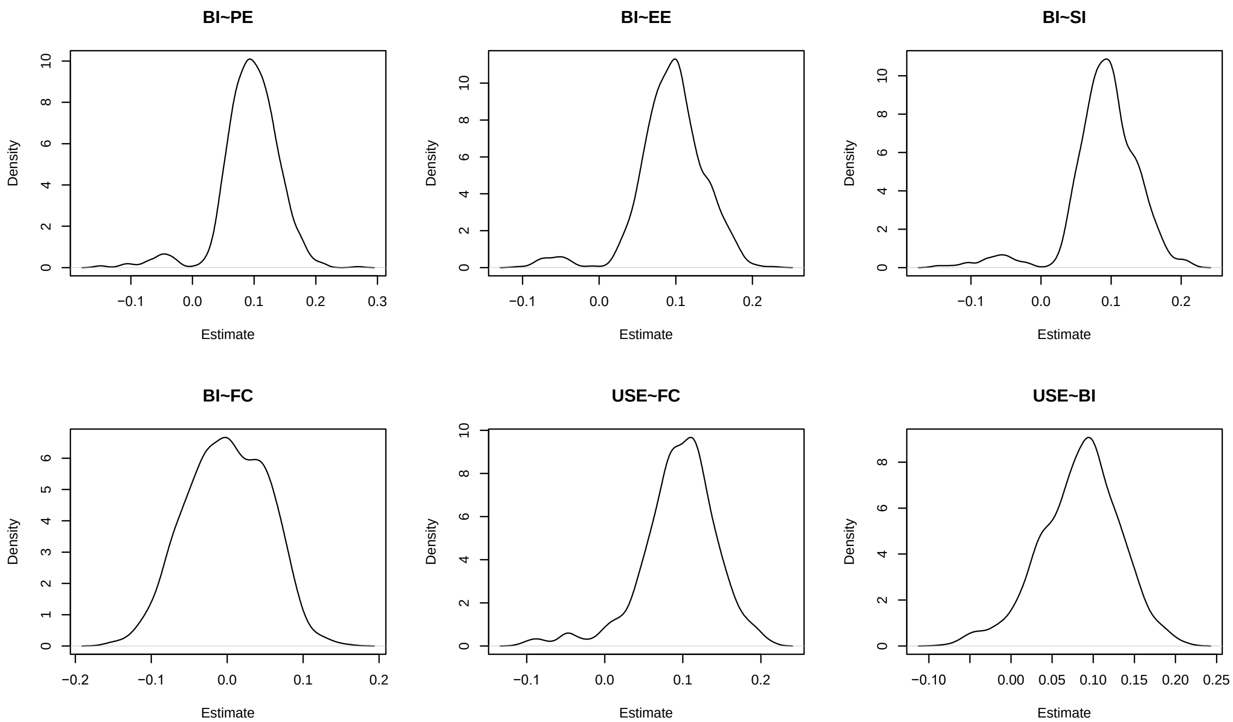

Figure 2 Distribution of parameter estimates over 1000 replications for the SLSHR22 model when effect is 0.1

We issue only a brief reply to their fifth point that we "cast doubt on foundational IS research by renowned scholars". First, we do not subscribe to their *argumentum ad verecundiam* and we do not believe that scholarly renown should make a study immune to criticism. We understand that the seminal studies that we cite in our original paper have been replicated using different methods and in many different settings, as indicated by Blut et al. (2021). We acknowledged this when we wrote that 'these theories have been expanded, extended, adopted, or replicated, sometimes with other statistical methods, and that may lend more credibility to them,' (ER21, p. 6) a statement that SLSHR22 overlook. Our argument focused on the historical first evaluation and publication of the model and we stand by this: When faced with less-than-ideal conditions with respect to appropriateness of model, effect sizes, sample size, cross-loadings, correlated errors, and a number of other conditions, a researcher would do well to look for methods other than PLS. Given the many replications of, for example UTAUT, we are now much more certain about effect sizes, we understand cross-loadings and error correlations, and, using recommendations such as those we provide in ER21, PLS may well produce acceptable results.

8 Literature Review – State of PLS Application in CAIS

Over the years, even staunch PLS proponents such as SLSHR22, have come to acknowledge that PLS may not be a 'silver bullet' but should be limited to specific situations, e.g. for prediction or for composite models. However, while PLS defenders like to point back to 10 years or more of shifting emphasis in the discussion of PLS, applied research has not appeared to come along on this journey. This section illustrates the disconnect between the arguments made in this debate and the actual use of PLS in applied research.

We searched the *Communication of the AIS* journal in the AIS electronic library for articles with the keyword 'PLS' (37 hits) or 'partial least squares' (47 hits) (in any search field) for the years from 2016 to 2021 (inclusive). Of the total of 56 identified articles, 29 presented studies that applied PLS[6]. Of those 29 studies,

[6] With no discernable trend: 5 in 2016, 5 in 2017, 4 in 2018, 9 in 2019, 4 in 2020 and 2 in 2021.

24 studies employed a factor model, 4 employed a mixed formative and factor model (we emphasize that a formative model is not the same as a composite model), and one was unclear in its presentation.

All of the 29 studies report testing a theoretically motivated model containing their hypotheses. All studies except Liu, Song, Wang, Tang (2021) and Klesel, Kampling, Bretschneider and Niehaves (2018) report CR, AVE and Cronbach alpha statistics, and only those, to assess their measurement model, apparently oblivious to the problems with this procedure. All 29 studies report parameter significance tests and R2 results, but only two studies report any predictive metrics: Ostermann, Holten, and Franzmann (2020) and Prasad and Green (2016) report the Q2 metric. While some of the studies appealed to prediction, all but these two studies assume this is covered by reporting the R2 metric, and none of the studies provide any justification in their study purpose for the prediction of case values.

Most of the 29 PLS studies report very little detail about their estimation procedure. None of the studies reported which PLS composites (Mode A or B) were used, and only one study reported the use of PLSc (Klesel, Kampling, Bretschneider and Niehaves, 2018). One may assume the remainder used whatever default their particular software package, also mostly unreported, provided at the time, possibly without any corrections for attenuation bias in the factor model.

In only 10 cases do the authors report that they used bootstrapping for confidence intervals; the other studies may have used whatever default the particular software system at the time provided, which may or may not have been t-tests based on normality assumptions (Aguirre-Urreta & Rönkkö, 2018).

Only four studies were concerned about model fit but those four studies report the GoF and use it to argue for a well-fitting model, unaware that the GoF does not measure model fit as commonly understood in this context (Henseler & Sarstedt, 2013).

9 Conclusion

We have received six insightful replies to our recommendations in ER21. Despite many disagreements on a range of issues, none of the replying authors have rejected or dismissed our recommendations. In fact, some have called for more or stronger recommendations, and in reply to Russo & Stol (2022) who are concerned about the accessibility to applied researchers, we have noted that modern PLS tools offer easy ways to conduct all the recommended analyses and report all recommended numbers.

In closing, we wish to reiterate what we consider important recommendations. PLS composites should always be compared against unit weighted composites. If there are no meaningful differences, the simpler approach should be chosen. If the composites differ in a meaningful way, the weights should be interpreted, and the differentially weighted composites can be used if there is a theoretically justifiable reason for the weights to differ. Similarly, if a statistic is used to assess model quality, the statistic should be calculated also for models that should not fit the data. It there is no difference between the statistics for the assumed correct and assumed incorrect model, then it should not be trusted. We provide several examples of such easy to apply checks and series of screencast demonstrating their use in our recent article (Rönkkö et al., 2022).

In summary, it appears to us that most of the PLS methodology community has largely given up on the use of ‘basic’ PLS for explanatory theory testing work on factor models that has been its traditional use case in IS research. We applaud this movement and wish that practitioners took note of these shifts in the PLS community. Unfortunately, our brief literature review shows a significant disconnect between recommended best practice and actual application. This underscores the importance of our guidelines in ER21 for the CAIS and wider social sciences researcher community. And while a debate such as this is useful for the methodological understanding and development, we hope that it does not make applied researchers hesitant to engage with the topic, or to become dismissive of this important research as esoteric. To be absolutely clear, methodological debates such as the present one are decidedly *not* akin to answering the question of how many angels can dance on the head of a pin. The CAIS and social science research community, authors, reviewers, and editors, should take note of this debate to improve the validity of our research. We close by again calling for all stakeholders in IS research to stay abreast of methodological developments, and to fully understand the methods and tools they use. Our recommendations aid in this, and we continue to stand by them as we see nothing in the responses to ER21 that would invalidate them.

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Appendix A: Simulation Study R Code

This appendix provides the R code for the simulation study presented in Section 7. It uses the matrixpls package (Rönkkö, 2022).

```
library(matrixpls)

# Set seed for reproducibility
set.seed(1)

#Define Simulation Parameters

SAMPLE <- 500
REPS <- 1000
EFFECT <- .1

POPULATION <- "
PE =~ pe1 + pe2 + pe3 + pe4
EE =~ ee1 + ee2 + ee3 + ee4
SI =~ si1 + si2 + si3 + si4
FC =~ fc1 + fc2 + fc3
BI =~ bi1 + bi2 + bi3
USE =~ use1 + use2 + use3 + use4

BI ~ [E]*PE + [E]*EE + [E]*SI + 0*FC
USE ~ [E]*FC + [E]*BI

BI ~~ [V1]*BI
USE ~~ [V2]*USE
"

# Set the values based on the design

population <- gsub("[E]", EFFECT, POPULATION, fixed = TRUE)
population <- gsub("[V1]", 1-3*EFFECT^2, population, fixed = TRUE)
population <- gsub("[V2]", 1-2*EFFECT^2, population, fixed = TRUE)

results <- matrixpls.sim(nRep = REPS, model = population, n= SAMPLE,
                          multicore = TRUE, boot.R = FALSE)

par(mfrow = c(2,3))

for(i in 1:6){
  plot(density(results@coef[,i]),
       main = colnames(results@coef[i]),
       xlab = "Estimate")
}
```

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