PLS Pluses and Minuses
In Path Estimation Accuracy
Full Paper

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Abstract

In this paper we ask three questions. Do PLS path estimates compensate for measurement error? Do they capitalize on chance? And is PLS able to more accurately weight measurement indicators so as to make path estimations more accurate? The evidence is quite convincing that PLS path estimates do have all three of these characteristics. Our analysis suggests, however, that measurement error has by far the largest impact, followed by capitalization on chance, with better weighting of indicators having the smallest influence. MIS researchers need to consider how to respond to these findings.

Keywords

PLS, regression, path estimate accuracy, measurement error, capitalization on chance, better indicator weights

Introduction

It has been argued that Partial Least Squares (PLS) has become the statistical technique of choice in the MIS research community (Ringle et al. 2012). However, a debate concerning the efficacy of PLS versus covariance-based structural equation modeling (CB-SEM) and regression seems to be underway. In 1996, McDonald (1996, pp. 266-267), argued that both PLS and regression (but not CB-SEM) provide path estimates that are attenuated by measurement error. Goodhue et al. (2011; 2012) demonstrated exactly that in simulation studies. In addition, Goodhue et al. (2007; 2011) suggested that PLS appears to capitalize on chance correlations in the data in obtaining its path estimates. Rönkkö and Evermann (2013) and Rönkkö (2014) explained PLS's capitalization on chance mathematically, and used simulation studies to confirm it. Finally, some researchers have suggested that PLS's ability to differentially weight construct indicators by assigning higher weights to the ones that are more reliable enables PLS to achieve more accurate scales (Gefen et al 2011; Chin Marcolin and Newsted 2003, p. 190), resulting in more accurate path estimates.

These assertions can be reduced to three key questions related to path estimate accuracy. First, does PLS fail to compensate for measurement error in its estimations? Second, does PLS capitalize on chance in its estimates? Third, is PLS able to more accurately weight measurement indicators so as to get more accurate path estimations? The first two concerns might be argued to be potential "minuses" in the PLS balance sheet, the third a "plus". What has not been done previously is to quantify the relative size of these three factors when using PLS path estimation in practice.

By using Monte Carlo simulation and decomposing the "consistency-at-large" characteristic of PLS, we have been able to isolate the impact of (1) measurement error (by modifying the number of indicators of

each construct), (2) capitalization on chance (by modifying the number of cases), and (3) better weighting of indicators by varying the dispersion of these weights in the underlying model.

Our simulation studies comparing PLS and regression[1] show strong evidence for all three of these elements. The size of the biases introduced, however, suggests that measurement error has by far the largest impact, followed by capitalization on chance, with better weighting of indicators having the smallest influence.

Why is this issue important to the MIS research community? Researchers would like to avoid Type I errors, and practitioners would like to predict the actual impact of the constructs included in our theories. Both of these are compromised if our path estimates are being biased by unpredictable but systematic amounts. We conclude the paper with a discussion of what IS researchers should make of these results.

Methodology

All of our empirical work utilized Monte Carlo simulation. We began with a replication of Hue and Wold's demonstration of PLS's (and regression's) consistency-at-large. We first used Hue and Wold's underlying model (shown in Figure 1) with a path of .5, a large effect size. In additional analyses, we modified path strength, indicator loading configurations and sample size. In each of our simulations we generated 500 samples for the specified condition. Each set of 500 samples was analyzed using PLS and then regression. For each condition, we tracked the average value of the path estimates (and its standard deviation) across the 500 samples for that condition.
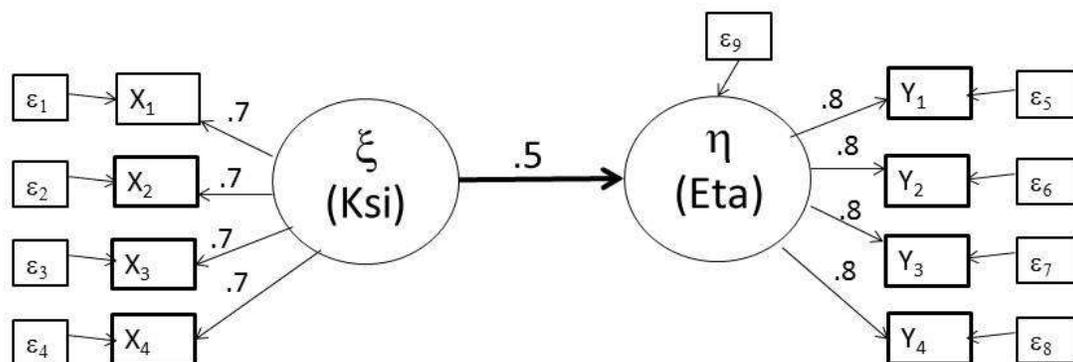
Figure 1. Replication of Hui and Wold's (1982) Simulation

(.7 loadings on Ksi and .8 loadings on Eta)

Building On Hue and Wold's Consistency-at-Large Simulation:
The Impact of Measurement Error

Joreskog and Wold (1982, p. 266, italics in the original) define consistency-at-large as follows: "Under general conditions of regularity, ML [Maximum Likelihood] estimates of the unknowns are known to be *optimal* in the large sample sense (asymptotic minimum of the confidence intervals), while the accuracy

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[1] We do not include LISREL or other CB-SEM modeling tools in this study because CB-SEM path estimates do not suffer from systematic measurement error nor do they suffer from systematic capitalization on chance correlations in the data (McDonald 1996; Goodhue et al. 2012).

of the PLS estimates is less sharp – they are asymptotically correct in the joint sense of *consistency* (large number of cases) and *consistency-at-large* (large number of indicators for each latent variable)." Or, as McDonald (1996, p. 248) stated it: "...the path coefficients estimated through PLS converge on the parameters of the latent-variable model as both the sample size and the number of indicators of each latent variable become infinite."

To test the assertion that PLS achieves consistency-at-large, Hui and Wold (1982) carried out a Monte Carlo simulation based on the model shown in Figure 1 above. Consistency-at-large would suggest that if we have an infinite number of cases and an infinite number of indicators, PLS should arrive at the correct estimate for the path. We replicated Hui and Wold's simulation using the same model and the same number of indicators (4, 8, 16, and 32). For each condition (the number of indicators), 500 datasets were generated using random number generators, and each dataset had an N of 4000 cases (an approximation of a large sample size approaching infinity).

The PLS and regression results are shown in Figure 2. The solid yellow line at path = .5 shows the true value of the path. The solid blue line shows the results for PLS; the dashed red line the results for regression. The amount of bias (estimate – true score) is shown by the green vertical arrows for each number of indicators.

As the number of indicators increases from 4 to 32, the path estimates for both PLS and regression approach the true value of .5. The graph is fairly persuasive evidence that if the number of indicators increased to 64, then 128 and on toward infinity, the PLS (and regression) lines would converge to the actual value of .5. We agree that this is confirmation of consistency-at-large for PLS (and for regression).

Note that the vertical arrows show the amount of bias from the true score, and that both PLS and regression have the same biases. The bias decreases as the number of indicators goes up. One explanation for these biases is that with more indicators, the reliability of the measures of the constructs goes up.
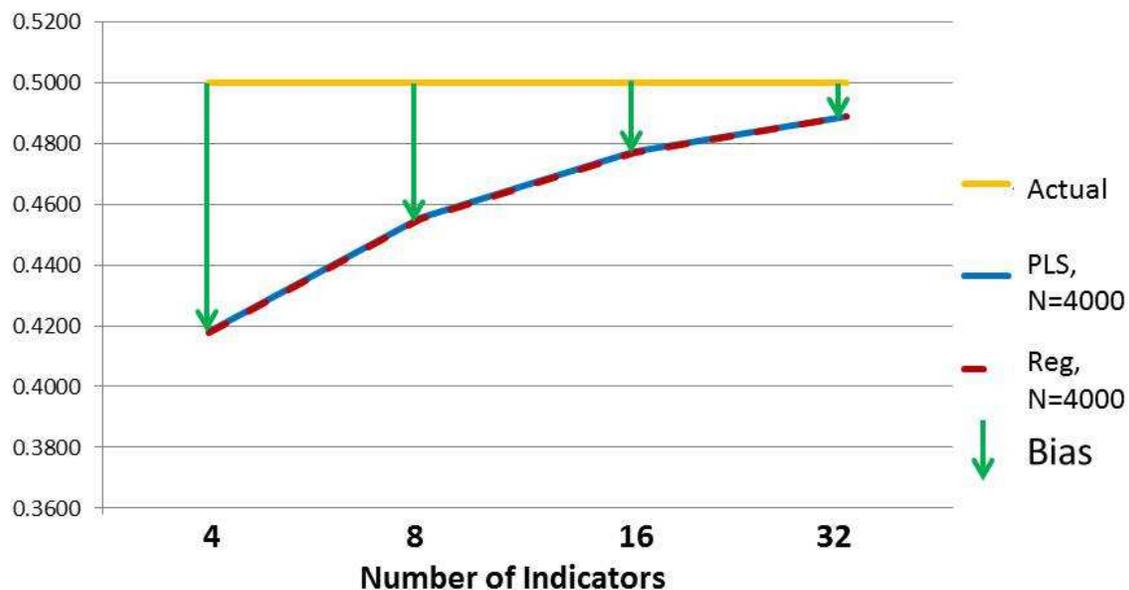
Figure 2. Replicating Hui and Wold's (1992) Simulation Results
(4, 8, 16, and 32 indicators, N=4000)

Because in a Monte Carlo simulation we know the true underlying values of the indicator loadings (as shown in Figure 1), we can calculate the reliability of our measures in this simulation. The reliability of a

collection of indicators is approximated by either Cronbach's alpha or Chin's equation for PLS Bias, as shown below, where K is the number of indicators and S is the average correlation across all indicators:

α = K * S / [1 + S (K – 1)]   (Cronbach's Alpha)

PLS Bias = S / [S + (1-S) / K]   (Chin 1998, p. 330])

Perhaps surprisingly, the two equations above are mathematically identical, that is, PLS bias equals α. With the resulting calculated reliabilities, we can calculate (and correct for!) the path bias from measurement error using Nunnally and Bernstein's equation[2] for the impact of measurement reliability on path estimates. As it turns out, ALL of the bias seen in Figure 2 is exactly the measurement bias predicted by Nunnally and Bernstein's (1994) equation, whether using Cronbach's alpha or Chin's equation. In other words, at least part of what underlies PLS's (and regression's) consistency-at-large is that with an infinite number of indicators, measurement reliability is reduced to zero. We approach that condition with 32 indicators in Figure 2. This leads us to the following hypothesis:

H1: With the underlying model as shown in Figure 1, and a sample size of n=4000, if we correct for measurement error, PLS and regression path estimates should both arrive at the true value.

The above correction is an attempt to achieve the same goal sought by Dijkstra and Henseler (2015) – to correct for measurement error. Dijkstra and Henseler do this through a technique they call "Consistent PLS", although the actual method they use is somewhat different from ours.

In Figure 3 we test Hypothesis H1. The figure may be a little hard to read because the lines for (1) the actual path values, (2) the PLS 4000-Corrected values, and (3) the Reg 4000-Corrected values are all on top of one another. They stretch horizontally at the .5 level across all numbers of indicators. In this scenario, when corrected for measurement error, PLS and regression estimates return the true values. This is strong support for Hypothesis 1.
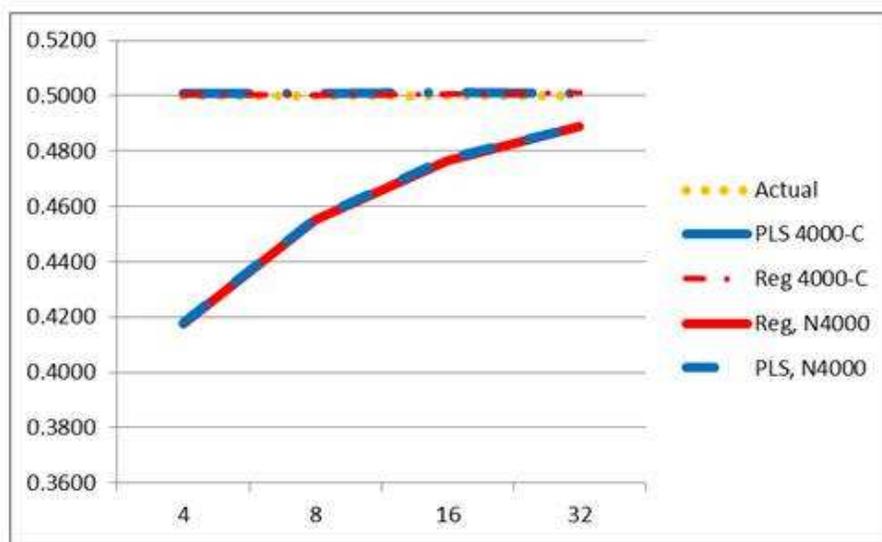

Figure 3. Hui and Wold's (1992) Simulation Results Corrected For Measurement Error

(Using Nunnally and Bernstein's with Chin's or Cronbach's Equations)

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[2] Nunnally and Bernstein's equation is for the bias in the estimation of the correlation between two constructs, based on their reliabilities. Nunnally and Bernstein (1994, pp. 241, 257): Apparent Correlation$_{XY}$ = Actual Correlation$_{XY}$ * (Reliability$_X$ * Reliability$_Y$)$^{(1/2)}$. For regression when the independent variables are uncorrelated, the same equation can be used for the bias of the regression paths.

The Effect of Sample Size

We have seen how reducing the number of indicators increases measurement error in both PLS and regression. Let us now investigate how reducing sample size affects both techniques, a condition not tested by Hui and Wold. Figure 4 shows the result of reducing the sample size to something closer to what we typically see in MIS research, n = 100. The figure actually shows the results for n = 100 superimposed on the diagram from Figure 2. Here the regression results for n = 100 are shown with a dotted red line, and the PLS results for N = 100 are shown with a dotted blue line.
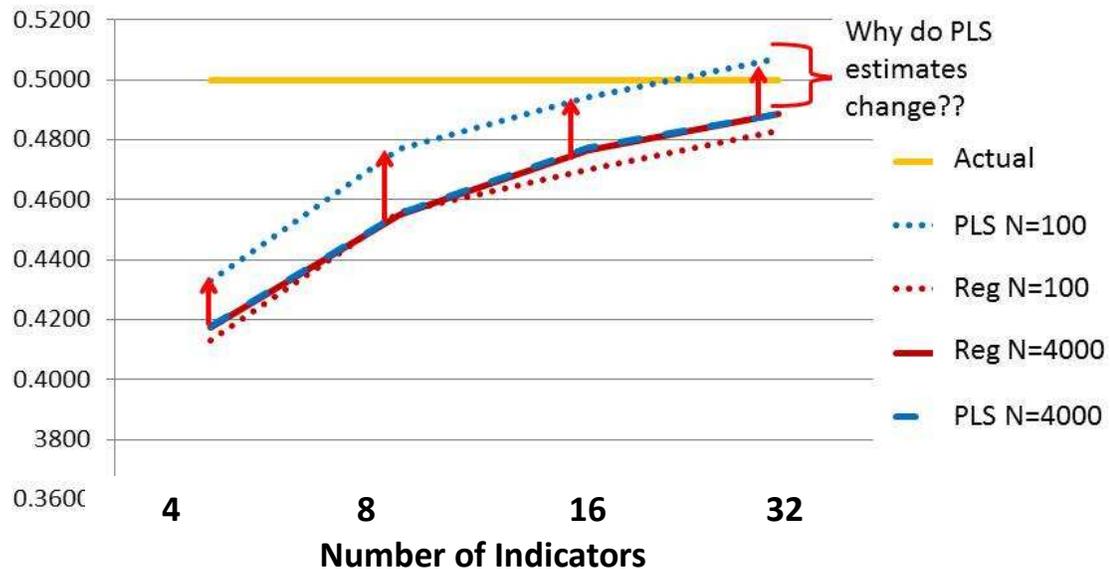
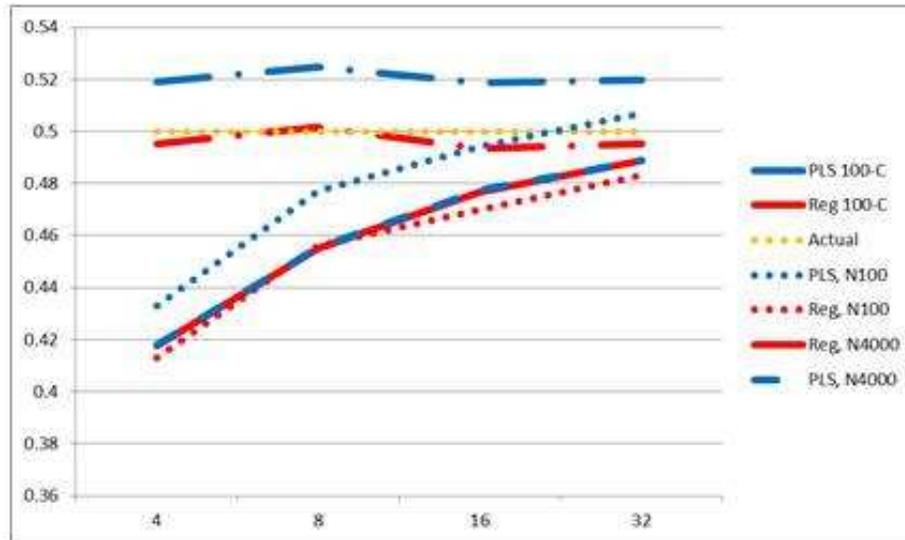**Figure 4. Path Estimates Moving From N = 4000 to N = 100.**

In Figure 4 we see that as the sample size decreases from 4000 to 100, the regression estimates do not change appreciably. But PLS has a considerably larger change -- an increase of about the same amount regardless of the number of indicators. Furthermore, if we extended the N = 100 PLS dotted blue line to more than 32 indicators (64? 128?), PLS would likely overestimate the true value.

In Figures 2 and 3 we showed that we can correct for measurement error using Nunnally and Bernstein's equation along with either Cronbach's or Chin's equation for reliability. Since measurement error is not a function of sample size -- note that sample size does not appear in either Cronbach's or Chin's equations for measurement bias – we could similarly correct for measurement error in Figure 4 by again using the same correction.

Figure 5 adds that correction to Figure 4. The corrected regression estimates (the red dashes and dots line) track fairly closely to the true value of .5 (shown with the dotted yellow line). The corrected PLS line (shown with the blue dashes and dots line) overestimates the true value by about 4%.

We know that with a sufficiently large sample size and a sufficiently large number of indicators, PLS will achieve the correct path value. Therefore it is hard to argue that by decreasing the sample size from 4000 to 100 we have "improved" PLS's estimate. It would appear that something else is biasing PLS estimates upward.

Both Goodhue et al. (2007) and Rönkkö (2014) argued that the more random variance affecting the indicator correlation matrix, the more variety PLS would have to choose from, and the more extensive the opportunity for capitalization on chance would likely be. Our general hypothesis is that random error in the cross-construct indicator correlations causes PLS to capitalize on chance and potentially overestimated path values. In this case, it is actually fairly straightforward to predict when PLS will have more capitalization on chance. We have only to look at those situations that would cause the indicator correlation matrix to have the most variance. Any characteristic of an underlying model that increases the amount of variance in the indicator correlation matrix, will increase PLS's tendency to capitalize on chance.


Figure 5. Path Estimates Moving From N = 4000 to N = 100
Plus N = 100 Corrected for Measurement Error

For example with a very large number of cases, random variance in indicator scores and in correlations across indicators would tend to cancel out, resulting in an indicator correlation matrix where random noise was less apparent. Under this circumstance, PLS would have little opportunity to capitalize on chance as it determined the weights for each construct's indicators. More specifically, with smaller sample size, there is more random variance in the estimates of the indicator correlations, and more opportunity for PLS to capitalize on chance. This leads to the following hypothesis.

H2: PLS will experience more capitalization on chance as sample size decreases.

Figure 6 shows a test of H2. Note that for Figures 6 through 8 we use only 4 indicators, and we have modified the underlying model to have a path of .35, a medium effect size. These are more realistic values for most MIS research. A yellow solid line indicates the true value of the path, and a solid orange line indicates the predicted value for regression (.294) using Nunnally and Bernstein's equation for bias in regression due to underlying measurement error. The uncorrected regression results are shown with the dashed red line, and the uncorrected PLS results with the dashed blue line.

At each value for the sample size, the regression estimates are almost exactly what is predicted by Nunnally and Bernstein's equation for regression bias due to measurement error. The PLS estimates at N = 4000 are virtually identical to the regression estimates. As sample size decreases from N = 4000, the PLS estimate gets larger, eventually exceeding the true path value of .35 when N = 50. More specifically, at N = 50, the average PLS estimate exceeds the true value by .0102, significantly different from zero at the p<.02 level.
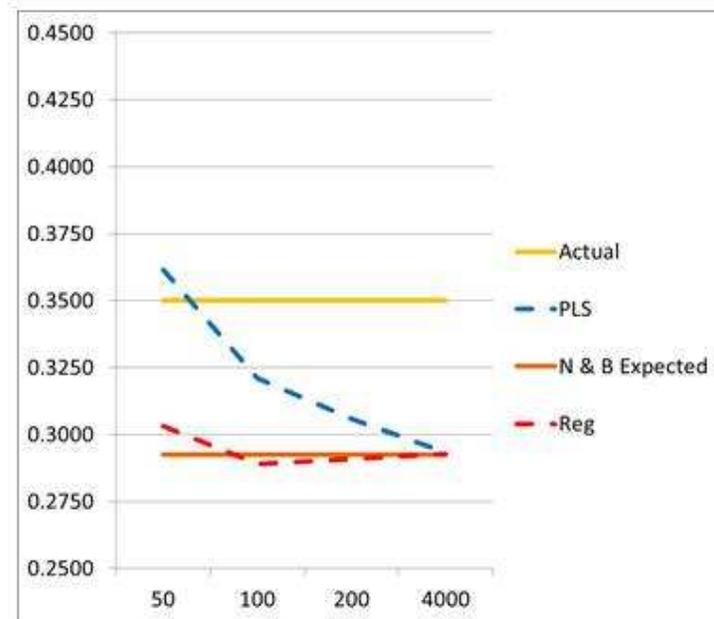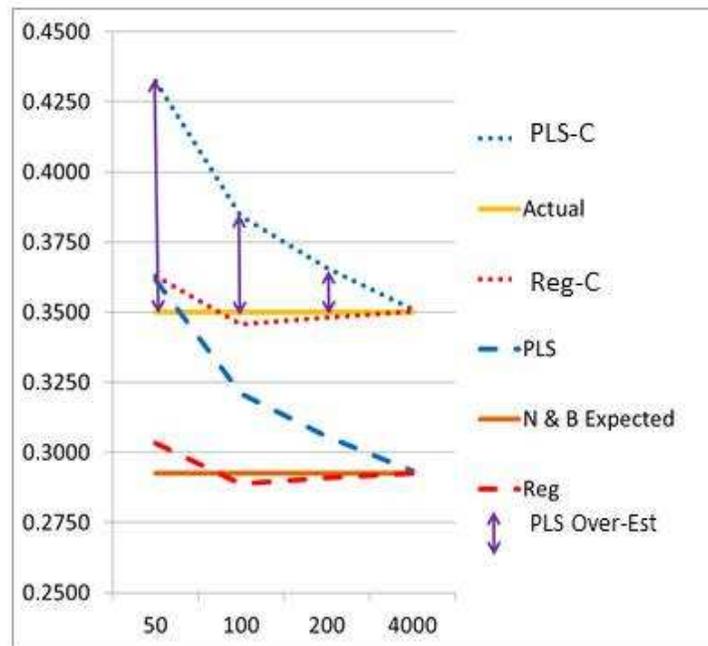
Figure 6. Test of Hypothesis #2 (Part 1--Uncorrected)
(True Path = .35, Loadings on Ksi = .7, .7, .7, .7; on Eta = .8, .8, .8, .8)

Figure 7 repeats the Figure 6 data but adds the correction for known measurement error to the regression and PLS estimates. Corrected regression estimates are shown with the dotted red line, with corrected PLS estimates shown with the dotted blue line. The corrected regression results track the true value quite closely. But from the graph it is clear that something else is affecting the corrected PLS path estimates beyond the true underlying value and measurement error. That something else is absent at N = 4000 (the dotted blue line is almost exactly .35), but increases with decreasing N. The result is that the dotted blue line for corrected PLS gradually overestimates the true value by more and more as sample size is reduced, with the overestimation shown by the two-headed purple arrows. We conclude that Hypothesis #2 is supported.

Interestingly, for PLS under these conditions and with an N about 60, the amount of capitalization on chance (increasing the path estimate) just about matches the amount of measurement error (decreasing the path estimate). The dashed blue line for uncorrected PLS crosses the true value of .35 near the left side of the graph. One might be inclined to conclude that PLS is actually quite accurate at this number of cases. However, our analysis makes clear that the truth is that under these conditions the error introduced by PLS's capitalization on chance *just happens* to counterbalance the error introduced by PLS's failure to take into account measurement error. This may explain why some researchers thought that PLS was more accurate than regression at small sample size.

Looking at N = 100 (a typical sample size that might be used in MIS research), the uncorrected PLS estimate is about .32; the PLS estimate corrected for measurement error is about .38. A PLS researcher interested in the true value (.35) might be forced to choose between the uncorrected estimate (low by about 8%) or the estimate corrected for measurement error (high by about 8%).

These error amounts are both different from zero by a statistically significant amount (p<.001). On the other hand, a researcher using regression and correcting for measurement errors would arrive at a much better estimate, in this case low by .005 or 1.4%, not significantly different from zero.

Figure 7. Test of Hypothesis #2 (Part 2 – Corrections for Measurement Error)
(True Path = .35, Loadings on Ksi = .7, .7, .7, .7; on Eta = .8, .8, .8, .8))

Effect of Unequal Indicator Loadings

PLS is reputed to have an advantage over regression because it is able to recognize when some indicators are actually better (have stronger loadings on the underlying construct than others). "Rather than assume equal weights for all indicators of a scale, the PLS algorithm allows each indicator to vary in how much it contributes to the composite score of the latent variable. Thus, indicators with weaker relationships to related indicators and the latent construct are given lower weightings…" (Chin et al., 2003, pg. 197). If indicator loadings for individual constructs are truly different, and if PLS can more accurately detect the true loadings and vary the indicator weights accordingly, then PLS uncorrected path estimates should be more reliable than regression uncorrected path estimates.

Rönkkö and Ylitalo (2010, p 5.) suggested that PLS assumes that all cross-construct indicator correlation is "useful" correlation. According to the understanding of capitalization on chance developed in this paper, in PLS when all capitalization on chance is removed (by very large sample size), then all remaining correlation actually *is* "useful" and does reflect the true (even if unequal) contributions of the different indicators. Thus with very large sample size, PLS should be able to weight indicators more appropriately, and achieve a higher reliability. Its uncorrected path estimates should produce more accurate path estimates than regression's uncorrected estimates with its equally weighted indicators. Thus:

H3: When measurement error and capitalization on chance are removed, if the underlying model has constructs with unequal indicator loadings, the PLS algorithm can achieve higher scale reliability.

In Figure 8 we repeated the analysis of Figure 7, but changed the indicators loadings to .7, .7, .9, and .9 for both the Ksi and the Eta constructs. In Figure 7, with equal underlying indicator loadings, with n = 4000 PLS and regression had exactly the same uncorrected path estimates and exactly the same measurement

bias. Therefore with n = 4000 and different indicator loadings, any differences in the uncorrected estimates of PLS and regression will be due solely to PLS's ability to better weight the indicators.

Figure 8 shows a noticeable difference between the PLS and regression path estimates for n = 4000, shown by the double-headed green arrow. This is persuasive evidence supporting Hypothesis #3 – PLS can have a reliability advantage by differentially weighting indicators. Note, however, that the advantage is not large.
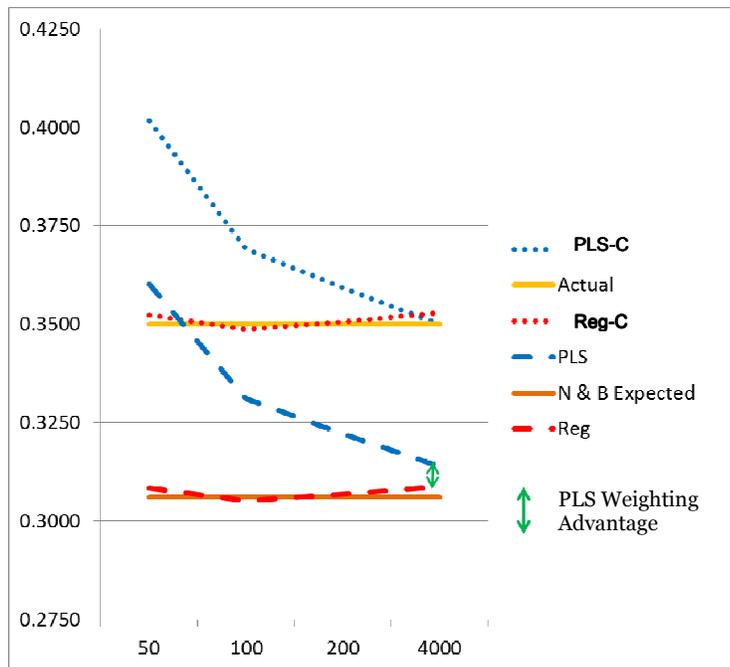
Figure 8. Test of Hypothesis #3: Does PLS's Differential Indicator Weighting Improve Reliability Over Regression's Equal Indicator Weighting?
(True Path = .35, Loading On Each Construct = .7, .7, .9, .9)

What is the relative size of the "better weighting" advantage versus the disadvantage of capitalization on chance?

We have shown evidence that three factors (neglecting to take measurement error into account, capitalization on chance, and differential weighting of indicators) have an impact on PLS path estimates. We've also shown that not taking measurement error into account has an impact on regression. In fact, corrections for measurement error could potentially be used for both PLS and regression (along the lines of Nunnally and Bernstein's equation or Djikstra and Henseler's "Consistent PLS") to remove that source of bias. It is harder to know the impact of, or to correct for, the other two factors that affect PLS. One of these (better weights) is conceptually quite attractive. The other (capitalization-on-chance) is unattractive. It would seem quite important to understand the relative size of these two impacts on PLS.

Table 1 shows the relevant values from our simulation using data generated with different loadings (e.g. .7, .7, .9, .9) and true path values as shown in the left hand margin. Row 1 shows the results for the same condition as shown in Figure 8. Rows 2 and 3 show different combinations of loadings and true paths.

For each row, column A shows the true path value. Columns B and C show the uncorrected results with n=4000 for PLS and regression. PLS's advantage due to its ability to differentially weight the indicators (column D) is the difference between column B and column C. PLS's advantage from better weighting will be most obvious at very large sample size (because capitalization on chance is eliminated), but the same

advantage would presumably carry over to any sample size -- remember that measurement reliability is not a function of sample size.

PLS's capitalization on chance (column F) is calculated by subtracting PLS's uncorrected n=4000 value (column B) from the PLS's uncorrected n=100 value (column E). This is because a high sample size removes the possibility of capitalizing on chance, while n=100 makes capitalization on chance possible. Finally, the ratio of capitalization on chance to better weighting is show in column F.

|	(A) True Path	(B) PLS4000 Estimate (With Weight Adv.) [SIM]	(C) Reg4000 (No Weight Adv.) [SIM]	(D) PLS Weight Adv. at n=4000 (& at any n) [B-C]	(E) PLS100 Estimate, [SIM]	(F) PLS100 C-On-C [E-B]	(G) PLS n=100 C-On-C / Weight Adv. [F / D]
P=.35; L=.7,.9 α=.88	0.35	0.314	.308	.006	0.331	0.017	2.8
P=.50; L=.7,.9 α=.88	0.50	0.447	.440	.007	0.462	0.015	2.1
P=.35; L=.6,.8 α=.80	0.35	0.286	.280	.006	0.323	0.037	6.2

Table 1. Relative Impact From Capitalization On Chance Vs. Differential Weighting

In row 1 of Table 1, with loadings leading to an underlying Cronbach's alpha of .88 (quite strong) for both Ksi and Eta, and a medium effect size path (β=.35) between the two constructs, PLS's capitalization on chance is almost three times as large as its improvement due to more correctly weighting the indictors.

In the second row, again with indicator loadings of .7, .7, .9. .9 (Cronbach's alpha of 88) and now a strong effect size path (β=.5), there is about twice as large a negative impact (capitalization on chance) as a positive impact (better weighting). The third row of Table 1 shows the situation if the path value is .35 but the underlying indicator loadings are lower (.6, .6, .8, .8, for an underlying Cronbach's alpha of .80).

This third row is probably closer to what we would think about as typical in MIS research. For that line of Table 1 the different sources of bias are displayed graphically in Figure 9. Here the ratio of capitalization on chance to weighting advantage is about 6 to one. Clearly the advantage from PLS's ability to differentially weight indicators is relatively small compared to the other bias factors at play.

From Figures 8 and 9 and Table 1 we conclude that Hypothesis #3 is supported. But we also see that PLS's advantage from being able to more accurately determine indicator loadings, though real, is small. In general, this small advantage is overshadowed by PLS's capitalization on chance. These findings are likely not comforting to researchers interested in accurate path estimates.
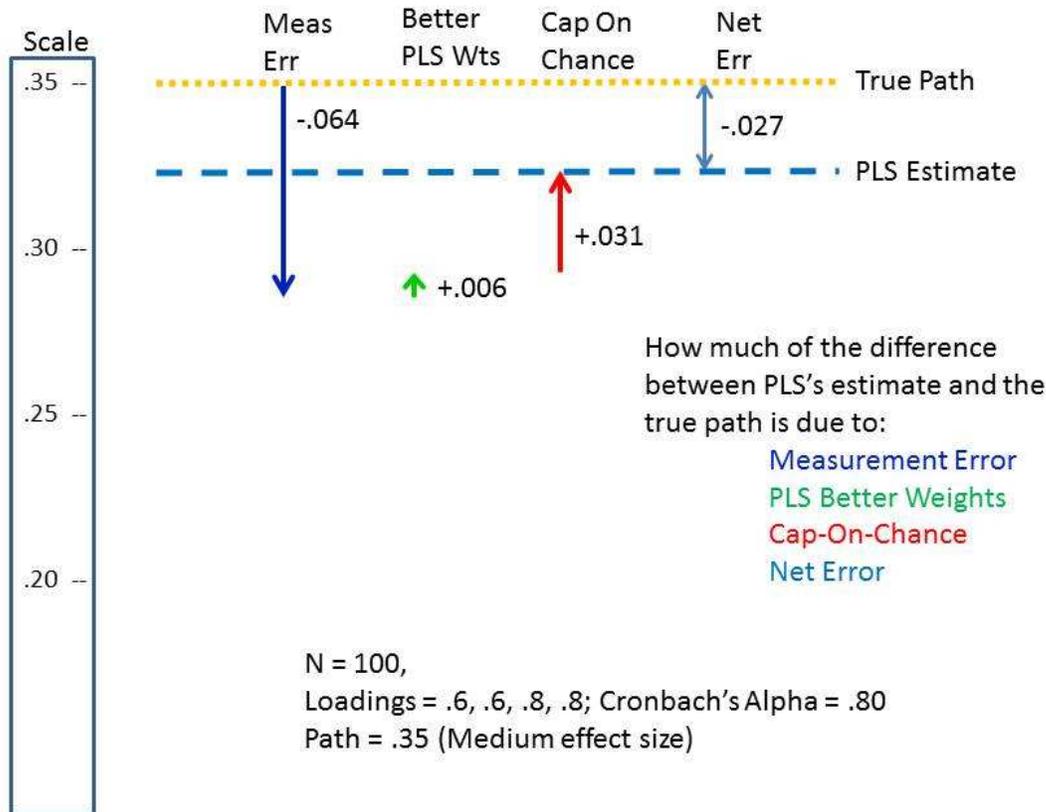
**Figure 9. The Relative Size of PLS's Ability to Differentially Weight Indicators
(From the bottom row of Table 1)**

Other Effects That Could Increase Or Decrease Capitalization On Chance

Other factors might also influence the amount of capitalization on chance. We surmised that both weaker measurement reliability and weaker paths would both increase it. Though not shown here (because of space limitations), we explicitly tested these two possibilities, and found support for both.

Further, the model (Figure 1) we used in this study for testing hypotheses involves only two constructs and a single path. We presume that having more paths into or out of a given construct might reduce the opportunity for capitalization on chance. We also tested this possibility, and found that having two paths into or out of each construct cuts the size of the capitalization on chance roughly in half.

The above is certainly an important caveat to our findings. Admittedly, our Figure 1 is less complicated than models typically found in IS research. However, a scan of models tested in MISQ revealed many that included at least one construct with a single path into or out of it. These single paths would be quite susceptible to capitalization on chance. Those with only two paths (into or out of any given construct) would also be susceptible to the problem. Table 1 suggests that even if capitalization on chance were cut in half, it is still possibly several times larger than PLS's improvement due to more correctly weighting the indicators, even when there are relatively large differences between the underlying indicator loadings. When there are no important differences between underlying indicator weights, the net effect of PLS's special technique for weighting indicators is a clear net disadvantage due to overestimation because of capitalization on chance.

Discussion and Conclusion

The evidence presented in this paper is quite convincing that PLS does capitalize on chance, exaggerating path estimates. The evidence also shows that PLS can more accurately weight indicator loadings when the underlying loadings are quite different, which would improve path estimates. It is useful to place this in the context of the underlying similarities between PLS and regression.

Following Rönkkö and Ylitalo (2010), we can think of the PLS and regression estimation processes as proceeding in three distinct steps, as shown in Figure 10. First, the weights and loadings of the indicators are determined, and construct scores are derived from those. Secondly, those constructs scores are used in a traditional ordinary least squares regression to determine path values between constructs. Thirdly, the standard deviations of the path values and the t statistics are determined. For those unfamiliar with the PLS algorithm, rest assured that Figure 10 is an accurate depiction of its workings.

Figure 10. Similarities and Differences in PLS versus Regression Path Estimation
(Used with permission)

In the first step PLS and regression are decidedly different, as we know. In the second step, PLS and regression are exactly the same – OLS regression is used with the construct scores from step one to determine path values. Since the third step has no impact on the path estimates, the only difference between regression and PLS in how path estimates are determined is the way the weights are determined in step one. If PLS path estimates are at all different from regression in a substantive way, it is only because PLS comes up with different weights and loadings for use in determining construct values.

We have seen that there are two reasons that PLS might arrive at different weights for its indicators. The first is that PLS might recognize that some indicators were better measures of the construct and give those higher weights. The second is that, depending upon sample size, the amount of error present in the underlying model, and the number of paths into or out of individual constructs, PLS will capitalize on chance and overestimate path values. In fact it is impossible to have the first (an advantage) of these without also getting the second (a disadvantage). We have shown that under conditions frequently found in MIS research, capitalization on chance will be at least as strong a detriment as any advantage achieved from better weighting, possibly many times as large.

Both regression and PLS suffer from not taking measurement error into account. As shown in Figure 9, this is probably the biggest source of bias for both techniques. In this paper we showed one way to correct for this blind spot (by using Cronbach's alpha to overcome the measurement bias). Dijkstra and Henseler (forthcoming) with their "consistent PLS" have developed a different means for doing the same thing. But neither using Nunnally and Bernstein's equations or Dijkstra and Henseler's "consistent PLS" addresses the problem of PLS's capitalization on chance. Unfortunately, when measurement error is compensated for by either of the above approaches, all capitalization on chance becomes overestimation.

If MIS researchers could avoid models that had constructs with only a single path entering or leaving, a portion of the capitalization on chance could be removed. Even then the disadvantage of capitalization on change might still dominate the advantage of better indicator weighting. By avoiding models with fewer than three paths for each construct, sample sizes as small as n=100, reliabilities lower than .88, and paths that are weaker than a medium effect size, we could probably do away with most capitalization on chance. But do we really want to limit MIS research in this way?

Clearly more work needs to be done to more definitively identify the conditions where PLS will not be unduly affected by capitalization on chance. In the meantime, awareness of this particular characteristic of PLS is becoming more widespread across other behavioral disciplines, as indicated by Rönkkö's recent (2014) paper in *Organizational Research Methods*. In light of the findings reported there and here, MIS researchers need to consider whether and how the case for PLS can be justified to the larger scientific community.

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