An Alternative Estimation Procedure For Partial Least Squares Path Modeling

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Since its inception, partial least squares path modeling has suffered from the absence of a single optimization criterion for estimating component weights. A new estimation procedure is proposed to address this enduring issue. The proposed procedure aims to minimize a single least squares criterion for estimating component weights under both Mode A and Mode B. An alternating least squares algorithm is developed to minimize the criterion. This procedure provides quite similar or identical solutions to those obtained from existing Lohmöller's algorithm in real and simulated data analyses. The proposed procedure can serve as an alternative to the existing one in that it is well-grounded in theory as well as performs comparably in practice.

1. Introduction

Partial least squares path modeling (PLSPM) (Wold, 1966, 1973, 1982; Lohmöller 1989) is a long-standing approach to structural equation modeling. In parameter estimation, this approach adopts a strategy of estimating a latent variable as a component or weighted composite of indicators. In this regard, PLSPM can be considered a component-based approach to structural equation modeling (Tenenhaus, 2008). It carries out two main stages sequentially to estimate parameters. The first stage estimates latent variables as components, which requires the estimation of component weights. This stage uses an iterative algorithm to estimate the component weights. The second stage estimates remaining parameters in measurement and structural models (i.e., path coefficients and/or loadings) by means of ordinary linear regression. That is, path coefficients are estimated by regressing each dependent latent variable on its explanatory latent variables, whereas loadings are estimated by regressing indicators on their corresponding latent variables. The second stage is thus non-iterative, which is based on the latent variables obtained from the first stage. Accordingly, the first stage is the most crucial estimation procedure in PLSPM (Hanafi, 2007).

Lohmöller's (1989) algorithm is best known for the first stage and implemented into most software programs for PLSPM, including LVPLS (Lohmöller, 1984), PLS Graph (Chin, 2001), SmartPLS (Ringle et al., 2005), and XLSTAT (Addinsoft, 2009). As will be explained in more detail in Section 2, this algorithm repeats two steps, called

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internal and external estimation. In the internal estimation step, a so-called inner estimate or inner component is obtained for each latent variable under different schemes such as centroid, factorial, and path weighting. In the external estimation step, component weights for each block of indicators are estimated in two different ways called Mode A and Mode B.

It is not known which criterion the Lohmöller algorithm aims to optimize by repeating the two steps (e.g., Coolen & de Leeuw, 1987; Jöreskog & Wold, 1982). A few attempts have been made to address this issue. For example, Hanafi (2007) presented association-maximization criteria for the centroid and factorial schemes under Mode B (also see Tenenhaus & Tenenhaus, 2011). To our knowledge, nevertheless, no single optimization criterion is yet available for the algorithm, which includes both Mode A and Mode B as special cases. The lack of a single optimization criterion makes it difficult to evaluate the algorithm (McDonald, 1996).

In this paper, we propose an alternative procedure for the first estimation stage of PLSPM. The proposed procedure aims to minimize a single least squares criterion for estimating component weights under both Mode A and Mode B. An alternating least squares (ALS) algorithm is used to minimize the criterion, which repeats the same two steps used in the Lohmöller algorithm. A major difference is that the ALS algorithm updates the inner estimates and component weights optimally by minimizing the least squares criterion. Consequently, the proposed procedure is well-defined in a least squares sense.

The paper is organized as follows. In Section 2, we provide a brief description of the existing Lohmöller algorithm. In Section 3, we provide a detailed account of the proposed procedure. In Section 4, we investigate the performance of the proposed and extant procedures through the analyses of real and simulated data. In the final section, we discuss implications of the proposed procedure.

2. Existing PLSPM Algorithm

We briefly describe the Lohmöller algorithm. Refer to Tenenhaus et al. (2005) for a fuller description of the algorithm.

Let η_j denote an N by 1 vector of the jth latent variable ($j = 1, \ldots, J$), where N is the number of individuals. Let X_j denote an N by P_j matrix consisting of a block of indicators associated with η_j. Let w_j denote a P_j by 1 vector of component weights assigned to X_j. In PLSPM, conventionally, both indicators and latent variables are assumed to be standardized, such that they have zero means and unit variances (e.g., $\eta_j'\eta_j = N$). However, they are to be normalized here, so that their length is equal to one (e.g., $\eta_j'\eta_j = 1$). This normalization makes the exposition of equations simpler while producing identical estimates of weights, path coefficients, and loadings. The individual scores of standardized latent variables can always be obtained by multiplying their normalized scores by $\sqrt{N}$.

The Lohmöller algorithm begins by choosing arbitrary initial values for w_j and computing $\eta_j = X_j w_j$. Then, it repeats the following two steps to estimate w_j and

η_j.

Step 1 (internal estimation): Update the inner estimate for η_j. The inner estimate, denoted here by f_j, is a weighed composite of the latent variables connected to η_j in a given structural model. Such connected latent variables contain those affecting η_j as well as those being affected by η_j. The inner estimate takes the general form as follows.

$$f_j = \sum_{q=1}^{Q_j} e_{jq}\eta_q, \tag{1}$$

where e_{jq} is a scalar value, called the inner weight, which is assigned to each of the Q_j latent variables (η_q's) that are connected to η_j. As shown in (1), updating the inner estimate amounts to updating its inner weights, given latent variables. Three different ways, so-called schemes, are available for the calculation of the inner weights: centroid (Wold, 1982), factorial (Lohmöller, 1989), and path weighting. In the centroid scheme, e_{jq}'s are the signs of the correlations between η_q's and η_j. In the factorial scheme, e_{jq}'s are the correlations between η_q's and η_j. In the path weighting scheme, e_{jq}'s are the regression coefficients of η_j on η_q's if η_j is a dependent variable, whereas they are the correlations between η_q's and η_j if η_j is an explanatory variable. The path weighting scheme is recommended over the other schemes because it takes into account both directions and magnitudes of the relationships between latent variables (Esposito Vinzi et al., 2010).

Figure 1 displays a prototype, structural model to illustrate the first step. This model consists of four latent variables ($J = 4$). For the prototype model, the inner estimate for each of the four latent variables is given as

$$\begin{aligned} f_1 &= e_{13}\eta_3 \\ f_2 &= e_{23}\eta_3 \\ f_3 &= e_{31}\eta_1 + e_{32}\eta_2 + e_{34}\eta_4 \\ f_4 &= e_{43}\eta_3 \end{aligned} \tag{2}$$

As explained above, the inner weights for these inner estimates are calculated based on which scheme is chosen. For example, if the path weighting scheme is adopted, e_{31} and e_{32} are the regression coefficients of η_3 on η_1 and η_2, because η_1 and η_2 are explanatory variables for η_3, whereas e_{34} are the correlation between η_3 and η_4, because η_3 is an explanatory variable for η_4. All the other inner weight estimates are simply correlations between two connected latent variables, because all latent variables are normalized and the regression coefficient of one latent variable on the other is equivalent to the correlation between them.

Step 2 (external estimation): Update w_j. There are two ways of estimating component weights on the basis of the nature of the measurement model: Mode A and Mode B. Mode A is known to be more suitable for reflective indicators, whereas Mode B is for formative indicators (e.g., Tenenhaus et al., 2005). Specifically, under Mode A, w_j is updated by regressing X_j on f_j, as follows.

$$w_j = X_j' f_j (f_j' f_j)^{-1}. \tag{3}$$

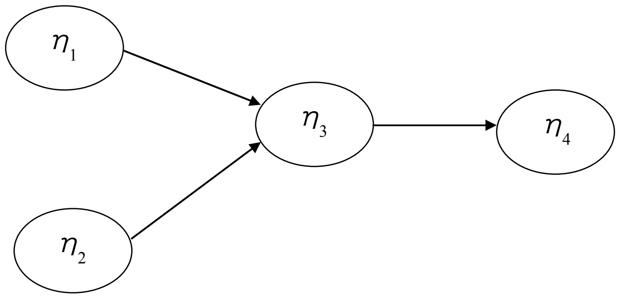

Figure 1: A prototype structural model that involves four latent variables. No residual terms are displayed.

Under Mode B, w_j is updated by regressing f_j on X_j, as follows.

$$w_j = (X_j' X_j)^{-1} X_j' f_j. \tag{4}$$

Subsequently, η_j is updated by $\eta_j = X_j w_j$, and normalized such that $\eta_j' \eta_j = w_j' X_j' X_j w_j = 1$. This normalization can be done by multiplying w_j by $(w_j' X_j' X_j w_j)^{-1/2}$, indicating that the effect of $(f_j' f_j)^{-1}$ in (3) will be cancelled out. Consequently, under Mode A, w_j can be updated simply by

$$w_j = X_j' f_j. \tag{5}$$

The above steps are repeated until no substantial differences occur between the previous and current weight estimates for all J blocks of indicators. A summary of this algorithm is provided in the Appendix.

As stated earlier, it is unknown which optimization criterion the Lohmöller algorithm seeks to maximize or minimize under Mode A and Mode B. In the next section, we propose a single least squares criterion that is to be consistently minimized for estimating component weights under both modes.

3. The Proposed Estimation Procedure for PLSPM

Let $H = [\eta_1, \ldots, \eta_J]$ denote an N by J matrix consisting of all J latent variables. Let ε_j denote a J by 1 vector consisting of Q_j inner weights for the Q_j latent variables connected to η_j, and of $J - Q_j$ zeros for the remaining unconnected latent variables. Then, let $f_j = H\varepsilon_j$ denote an N by 1 vector of the inner estimate for η_j. For example, in the prototype model depicted in Figure 1, $H = [\eta_1, \eta_2, \eta_3, \eta_4]$, $\varepsilon_1 = [0, 0, e_{13}, 0]'$, $\varepsilon_2 = [0, 0, e_{23}, 0]'$, $\varepsilon_3 = [e_{31}, e_{32}, 0, e_{34}]'$, and $\varepsilon_4 = [0, 0, e_{43}, 0]'$.

We propose a least squares criterion for estimating all weights under Mode A, as follows.

$$\text{Minimize } \varphi_A = \sum_{j=1}^{J} SS(X_j - f_j w_j'), \tag{6}$$

subject to $\eta_j' \eta_j = 1$, where $SS(M) = \text{trace}(M'M)$ for any matrix M. This criterion appears similar to a blockwise join loss function for principal component analysis

(Gifi, 1990, p. 152), where a vector of object scores is replaced by the inner estimate.

We propose a least squares criterion for estimating all weights under Mode B, as follows.

$$\text{Minimize } \varphi_B = \sum_{j=1}^{J} \mathrm{SS}(\mathbf{f}_j - \mathbf{X}_j \mathbf{w}_j), \tag{7}$$

subject to $\eta_j'\eta_j = 1$. Criterion (7) may be viewed as a blockwise meet loss version (Gifi, 1990, p. 167) of the covariance-maximization criterion for regularized generalized canonical correlation analysis (Tenenhaus & Tenenhaus, 2011).

Let α_j denote a binary value that indicates which mode is used for updating the component weights for the j th block of indicators. That is, $\alpha_j = 1$ if Mode A is used, and $\alpha_j = 0$ if Mode B is used. We then develop a single optimization criterion for the PLSPM algorithm by combining (6) and (7), as follows.

$$\text{Minimize } \varphi = \sum_{j=1}^{J} \alpha_j \mathrm{SS}(\mathbf{X}_j - \mathbf{f}_j \mathbf{w}_j') + \sum_{j=1}^{J} (1 - \alpha_j)\mathrm{SS}(\mathbf{f}_j - \mathbf{X}_j \mathbf{w}_j), \tag{8}$$

subject to $\eta_j'\eta_j = 1$. This criterion subsumes (6) and (7) as special cases by setting all α_j's to one or zero, respectively. Moreover, it can be used for estimating the weights for each block of indicators under either Mode A or Mode B by setting the corresponding α_j to one or zero, respectively.

We develop an ALS algorithm to minimize (8). This algorithm begins by assigning arbitrary initial values to $\mathbf{w}_j$ and obtaining $\eta_j = \mathbf{X}_j \mathbf{w}_j$. Then, it alternates the following two steps.

Step 1 (internal estimation): Update $\mathbf{f}_j$ for fixed $\mathbf{w}_j$. This step reduces to updating the inner weights in ε_j, given latent variables. It is equivalent to minimizing

$$\varphi_j = \alpha_j \mathrm{SS}(\mathbf{X}_j - \mathbf{H}\varepsilon_j \mathbf{w}_j') + (1 - \alpha_j)\mathrm{SS}(\mathbf{H}\varepsilon_j - \eta_j). \tag{9}$$

Let $\mathbf{e}_j$ denote a Q_j by 1 vector consisting of non-zero inner weights only. Let Γ_j denote an N by Q_j matrix formed by eliminating the columns of $\mathbf{H}$ corresponding to any zero elements in ε_j. Then, minimizing (9) is equivalent to minimizing

$$\varphi_j = \alpha_j \mathrm{SS}(\mathbf{X}_j - \Gamma_j \mathbf{e}_j \mathbf{w}_j') + (1 - \alpha_j)\mathrm{SS}(\Gamma_j \mathbf{e}_j - \eta_j). \tag{10}$$

By solving $\frac{1}{2}\frac{\partial \varphi_j}{\partial \mathbf{e}_j} = 0$, the least squares estimate of $\mathbf{e}_j$ is obtained as

$$\mathbf{e}_j = \left(\alpha_j \mathbf{w}_j'\mathbf{w}_j \Gamma_j'\Gamma_j + (1 - \alpha_j)\Gamma_j'\Gamma_j\right)^{-1} \Gamma_j'\eta_j. \tag{11}$$

Then, $\mathbf{f}_j$ is updated by $\mathbf{f}_j = \mathbf{H}\varepsilon_j$, where ε_j is constructed from the estimate of $\mathbf{e}_j$.

Step 2 (external estimation): Update $\mathbf{w}_j$ for fixed $\mathbf{f}_j$. This is equivalent to minimizing

$$\varphi_j = \alpha_j \mathrm{SS}(\mathbf{X}_j - \mathbf{f}_j \mathbf{w}_j') + (1 - \alpha_j)\mathrm{SS}(\mathbf{f}_j - \mathbf{X}_j \mathbf{w}_j). \tag{12}$$

Note that in (12), $\mathbf{f}_j$ does not involve $\mathbf{w}_j$ because η_j is not connected with itself.

By solving $\frac{1}{2}\frac{\partial \varphi_j}{\partial w_j} = 0$, the least squares estimate of w_j is obtained as

$$w_j = \left(\alpha_j f_j' f_j I + (1 - \alpha_j) X_j' X_j\right)^{-1} X_j' f_j, \tag{13}$$

where I is an identity matrix of size P_j. Subsequently, η_j is updated by $\eta_j = X_j w_j$, and normalized. We repeat the two steps until the difference in the values of (8) between the previous and current iterations decreases below a pre-determined threshold (e.g., .00001). A summary of the ALS algorithm is also presented in the Appendix.

A few remarks concerning the ALS algorithm are in order. First, it is easily seen that if Mode A is used or equivalently $\alpha_j = 1$, (13) reduces to (3) and (5), whereas if Mode B is used or $\alpha_j = 0$, (13) reduces to (4). This indicates that the algorithm deals with Mode A and Mode B as special cases. Second, in the first step, the estimates of the inner weights are obtained in such a way that they minimize a least squares criterion, conditionally upon the estimates of component weights. Thus, we may call the step the "least squares scheme." On the other hand, it is uncertain which criterion the existing schemes seek to optimize except for a few special cases (Hanafi, 2007; Tenenhaus & Tenenhaus, 2011). Third, the ALS algorithm defines convergence as the decrease in the value of the optimization criterion (8) beyond a certain threshold, whereas the Lohmöller algorithm defines convergence as a sort of equilibrium, i.e., the point at which no substantial difference occurs between the previous and current estimates of weights, because it does not involve an optimization criterion. Lastly, at least in theory, a third type of mode can be considered by taking any value of α_j between 0 and 1. For example, by specifying $\alpha_j = .1$, the second term of the criterion can have a greater influence on the estimation of component weights. However, in practice, it is not yet clear what such types of mode connote and whether using them is sensible substantively.

4. Empirical Comparisons

In this section, we compare the proposed procedure to the extant procedure based on the Lohmöller algorithm, using real and simulated data.

4.1 Real Data Analysis

We applied the proposed and extant procedures to fit the American customer satisfaction index (ACSI) model (Fornell et al., 1996) to a consumer-level dataset collected in 2002. This dataset consists of the responses of 774 consumers to the service units (e.g., police, garbage pick-up services, etc.) within the US sector of public administration.

The ACSI model specifies the relationships among antecedent and consequent latent variables of customer satisfaction. As depicted in Figure 2, the ACSI model includes fourteen indicators: x_1 = customer expectations about overall quality, x_2 = customer expectations about reliability, x_3 = customer expectations about customization, x_4

= overall quality, x_5 = reliability, x_6 = customization, x_7 = price given quality, x_8 = quality given price, x_9 = overall customer satisfaction, x_{10} = confirmation of expectations, x_{11} = distance to ideal product or service, x_{12} = formal or informal complaint behavior, x_{13} = repurchase intention, and x_{14} = price tolerance. The measures and scales of these indicators are available in Fornell et al. (1996). The ACSI model also involves six latent variables that underlie the fourteen indicators, as follows: CE = customer expectations, PQ = perceived quality, PV = perceived value, CS = customer satisfaction, CC = customer complaints, and CL = customer loyalty.

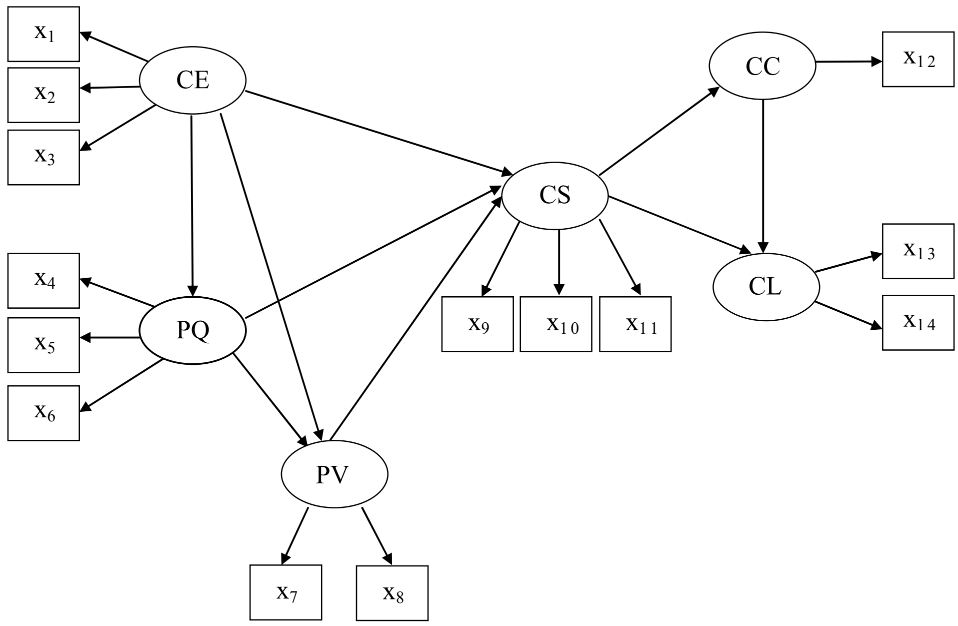

Figure 2: The American customer satisfaction index model. No residual terms are displayed.

We used SmartPLS (Ringle et al., 2005) to implement the extant procedure in combination with the path weighting scheme. As displayed in Figure 2, the ACSI model assumes that all indicators are reflective. This suggests that Mode A should be more appropriate for estimating weights.

Tables 1 and 2 present the estimates of weights, loadings, and path coefficients obtained from the proposed and extant procedures under Mode A. As shown in the tables, both procedures resulted in quite similar parameter estimates, leading to the same interpretations.

4.2 Simulated Data Analysis

We further compared the performance of the proposed and extant procedures based on simulated data. In particular, we focused on how similarly the proposed and extant procedures would perform under two different models.

Table 1: The estimates of weights and loadings of the ACSI model obtained from the proposed and extant proceduresfor PLSPM.

Latent	Indicator	Weight estimates		Loading estimates	
		Proposed	Extant	Proposed	Extant
CE	x_1	.4447	.4523	.8651	.8679
	x_2	.4375	.4310	.8772	.8750
	x_3	.3219	.3207	.7189	.7179
PQ	x_4	.4042	.4048	.9336	.9328
	x_5	.4114	.4034	.9325	.9303
	x_6	.2986	.3072	.8004	.8045
PV	x_7	.4251	.4229	.8024	.8012
	x_8	.7060	.7080	.9332	.9339
CS	x_9	.3851	.3855	.9388	.9387
	x_{10}	.3480	.3414	.9232	.9216
	x_{11}	.3487	.3550	.9097	.9113
CC	x_{12}	1.000	1.000	1.000	1.000
CL	x_{13}	.5827	.5827	.9507	.9507
	x_{14}	.4812	.4813	.9268	.9268

Table 2: The estimates of path coefficients of the ACSI model obtained from the proposed and extant procedures for PLSPM.

	Proposed	Extant
CE $\rightarrow$ PQ	.5822	.5819
CE $\rightarrow$ PV	.1220	.1230
CE $\rightarrow$ CS	.0330	.0353
PQ $\rightarrow$ PV	.6469	.6466
PQ $\rightarrow$ CS	.6707	.6668
PV $\rightarrow$ CS	.2656	.2676
CS $\rightarrow$ CC	−.4000	−.4002
CS $\rightarrow$ CL	.5824	.5831
CC $\rightarrow$ CL	−.0976	−.0972

4.2.1 Simulation 1

Figure 3 displays the structural equation model considered in the first simulation study, along with its unstandardized and standardized parameter values. In this model, three latent variables were specified, each of which underlay three indicators. Individual-level multivariate normal data were drawn from $N(0, \Sigma)$, where Σ is the implied population covariance matrix derived based on the unstandardized parameter values in the framework of covariance structure analysis (e.g., Jöreskog, 1970). This indicates that the latent variables in the model were assumed to be equivalent to common factors.

We considered three different levels of sample size ($N = 25, 100, 400$). Five hundred samples were generated at each sample size. We used the same initial values per sample for the proposed and extant procedures. In the model, all indicators were reflective, so that we used Mode A for both procedures. The path weighting scheme was employed for the extant procedure.

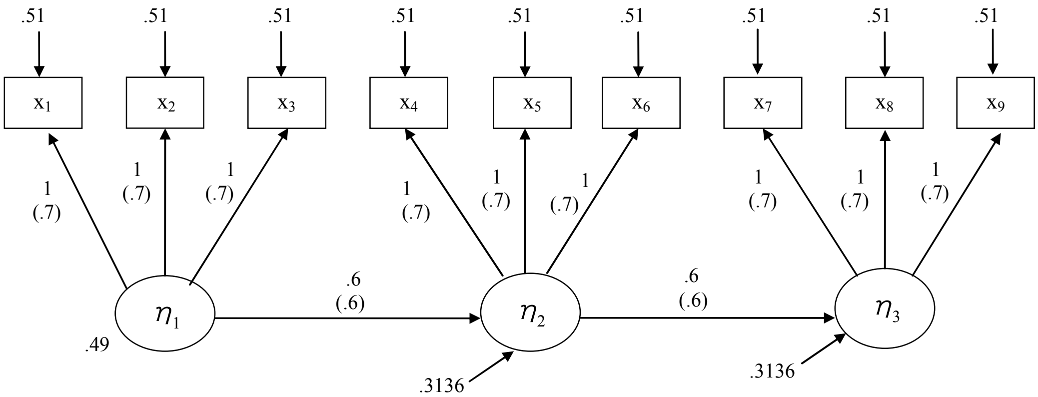

Figure 3: The structural equation model specified for the first simulation study. Standardized parameters are given in parentheses.

PLSPM provides standardized parameter estimates. Table 3 presents the bias, standard deviation, and mean square error of each standardized parameter estimate obtained from the two procedures. As shown in the table, the parameter estimates of both procedures shared the same properties. In general, their loading estimates were positively biased, whereas their path coefficients were negatively biased. As stated above, in this study, the simulated data were generated under the assumption that a latent variable was equivalent to a common factor. Under this assumption, PLSPM is known to yield biased estimates (e.g., Dijkstra, 2010) because it regards latent variables as components rather than common factors. The standard deviations of the loading and path coefficient estimates decreased with sample size. The mean square errors of these estimates became closer to zero with sample size. Notably, all the parameter estimates obtained from both procedures exhibited quite similar biases, standard deviations, and mean square errors across all sample sizes. This indicates that the proposed procedure resulted in virtually identical parameter estimates as those from the extant one.

As discussed in Section 3, technically, the proposed procedure allows a compromise between Mode A and Mode B by taking the value of α_j between 0 and 1. As a reviewer suggested, we have investigated the effect of adopting such a third type of mode on parameter estimation. Specifically, we applied the proposed procedure under $\alpha_j = .5$, so that Mode A and Mode B contributed simultaneously to obtaining estimates. As shown in Table 3, this case tended to produce less biased estimates particularly in small samples, whereas it tended to yield larger standard deviations of the estimates. Consequently, its estimates tended to show larger mean square errors than those obtained under Mode A. Thus, at least in this study, adopting $\alpha_j = .5$ was of little benefit over using Mode A in estimating parameters. Although permitting a compromise between the two conventional modes is a technically novel feature, as stated earlier, it is unclear what such a compromise indicates substantively, when it can be useful, and how the value of α_j can be chosen.

Table 3: The bias, standard deviation (SD), and mean square error (MSE) of each parameter estimate obtained from the proposed and extant procedures for PLSPM in the first simulation study. PP^1: Proposed procedure under $\alpha_j = 1$; PP^2: Proposed procedure under $\alpha_j = .5$; EP: Extant procedure.

Parameters	N	Bias			SD			MSE		
		PP^1	PP^2	EP	PP^1	PP^2	EP	PP^1	PP^2	EP
Loading 1 (.7)	25	.0842	.0052	.0842	.1590	.2900	.1633	.0324	.0841	.0338
	100	.1067	.0957	.1067	.0537	.0970	.0536	.0143	.0186	.0143
	400	.1120	.1092	.1120	.0250	.0448	.0250	.0132	.0139	.0132
Loading2 (.7)	25	.0977	−.0110	.0973	.1242	.2959	.1241	.0250	.0877	.0249
	100	.1064	.0930	.1064	.0519	.0994	.0518	.0140	.0185	.0140
	400	.1103	.1078	.1103	.0256	.0467	.0256	.0128	.0138	.0128
Loading3 (.7)	25	.0766	−.0021	.0775	.1573	.3137	.1543	.0306	.0984	.0298
	100	.1106	.0869	.1106	.0490	.1073	.0489	.0146	.0191	.0146
	400	.1121	.1068	.1121	.0236	.0468	.0236	.0131	.0136	.0131
Loading4 (.7)	25	.1016	.0672	.1023	.1164	.1813	.1139	.0239	.0374	.0234
	100	.1079	.1013	.1079	.0442	.0762	.0440	.0136	.0161	.0136
	400	.1110	.1098	.1110	.0210	.0326	.0209	.0128	.0131	.0128
Loading5 (.7)	25	.1042	.0675	.1039	.1136	.1774	.1139	.0237	.0360	.0238
	100	.1092	.1112	.1092	.0461	.0702	.0460	.0141	.0173	.0140
	400	.1121	.1113	.1121	.0215	.0315	.0214	.0130	.0134	.0130
Loading6 (.7)	25	.0992	.0617	.1006	.1098	.1993	.1039	.0219	.0435	.0209
	100	.1077	.1001	.1077	.0464	.0757	.0465	.0138	.0158	.0138
	400	.1120	.1114	.1120	.0215	.0308	.0215	.0130	.0134	.0131
Loading7 (.7)	25	.0938	.0013	.0951	.1569	.2969	.1449	.0334	.0882	.0300
	100	.1097	.0930	.1097	.0489	.1044	.0489	.0144	.0195	.0144
	400	.1097	.1117	.1097	.0229	.0453	.0229	.0126	.0145	.0126
Loading8 (.7)	25	.0757	−.0127	.0764	.1837	.2888	.1835	.0395	.0835	.0395
	100	.1055	.0844	.1055	.0540	.0983	.0539	.0140	.0168	.0140
	400	.1114	.1048	.1114	.0242	.0453	.0242	.0130	.0130	.0130
Loading9 (.7)	25	.0605	−.0015	.0615	.2162	.2788	.2182	.0504	.0777	.0514
	100	.1084	.0966	.1084	.0488	.1066	.0488	.0141	.0207	.0141
	400	.1125	.1068	.1125	.0224	.0464	.0224	.0132	.0135	.0132
Path 1 (.6)	25	−.1024	−.0664	−.1021	.1655	.1854	.1635	.0379	.0388	.0372
	100	−.1555	−.1382	−.1554	.0801	.0808	.0799	.0306	.0256	.0305
	400	−.1531	−.1451	−.1531	.0405	.0396	.0405	.0251	.0226	.0251
Path 2 (.6)	25	−.1091	−.0703	−.1091	.1576	.1769	.1573	.0368	.0362	.0366
	100	−.1461	−.1300	−.1461	.0812	.0762	.0810	.0279	.0227	.0279
	400	−.1500	−.1493	−.1500	.0396	.0401	.0396	.0241	.0239	.0241

4.2.2 Simulation 2

The first simulation study was useful to evaluate how similarly the proposed and extant procedures performed. Nonetheless, this study may be somewhat too simple in that it involved only three blocks of reflective indicators and assumed the same correlations among each block of indicators. Thus, we conducted another simulation study, which considered both formative and reflective indictors as well as different correlations among each block of indicators. Specifically, we used the model specified in Ringle et al. (2009) for the second simulation study. Figure 4 displays the model given in Ringle et al. (2009), along with its parameter values. Ringle et al. (2009) did not provide population residual variances. Instead, they provided the population correlation matrix of indicators, derived based on the specified model (see Table 5 in Ringle et al., 2009). We generated multivariate normal data, using the correlation matrix.

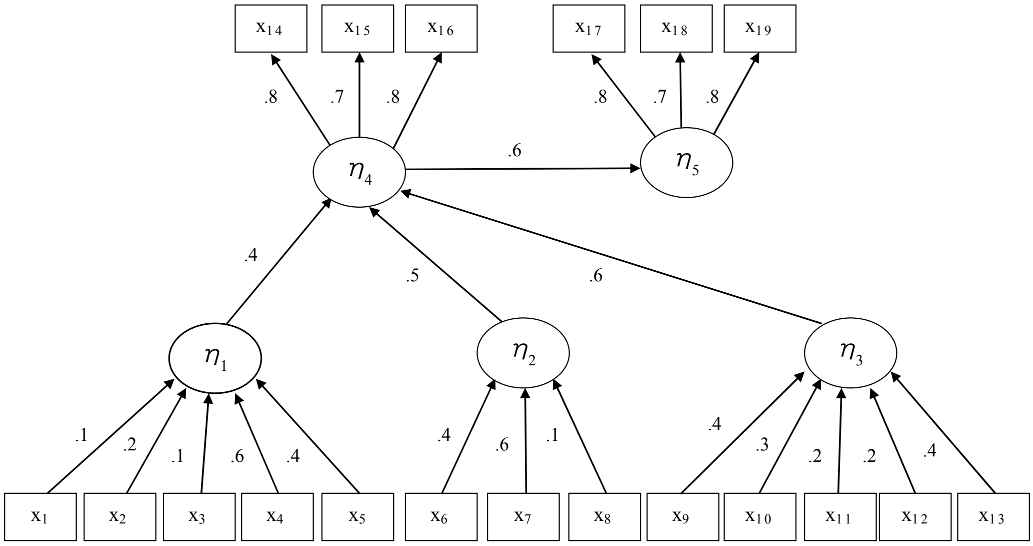

Figure 4: Ringle et al. (2009)'s structural equation model used for the second simulation study.

As in the first simulation study, we considered three different levels of sample size ($N = 25, 100, 400$). Five hundred samples were generated at each sample size. We used the same initial values per sample for the proposed and extant procedures. Mode A was applied for estimating the weights for reflective indicators, whereas Mode B was used for estimating those for formative indicators. The path weighting scheme was employed for the extant procedure.

Table 4 provides the bias, standard deviation, and mean square error of each standardized parameter estimate obtained from the two procedures. The parameter estimates of both procedures showed the same behaviors, although it was somewhat difficult to characterize them clearly. For example, some weight estimates for formative indicators were negatively biased, other estimates were positively biased, and the others were biased in different directions over sample size. Conversely, all loading estimates were positively biased regardless of sample size. Two estimates of path coefficients were negatively biased, whereas one estimate was positively biased, across sample sizes. It was difficult to explain where these biases came from because Ringle et al. (2009) did not discuss explicitly whether their population correlation matrix was generated based on the assumption that the latent variables were equivalent to common factors as in the first study. The standard deviations and mean square errors of all parameter estimates decreased with sample size. Importantly, all the parameter estimates obtained from both procedures involved quite similar biases, standard

Table 4: The bias, standard deviation (SD), and mean square error (MSE) of each parameter estimate obtained from the proposed and extant procedures for PLSPM in the second simulation study.

Parameters	N	Bias		SD		MSE	
		Proposed	Extant	Proposed	Extant	Proposed	Extant
Weight 1 (.1)	25	−.1443	−.1442	.2812	.2811	.0999	.0998
	100	−.1461	−.1461	.1206	.1206	.0359	.0359
	400	−.1577	−.1579	.0575	.0575	.0282	.0282
Weight 2 (.2)	25	−.0773	−.0771	.2355	.2356	.0614	.0615
	100	−.0772	−.0770	.1149	.1149	.0192	.0191
	400	−.0655	−.0654	.0545	.0545	.0073	.0072
Weight 3 (.1)	25	−.1354	−.1356	.2630	.2631	.0875	.0876
	100	−.1391	−.1393	.1148	.1148	.0325	.0326
	400	−.1338	−.1340	.0519	.0519	.0206	.0207
Weight 4 (.6)	25	.0298	.0297	.2252	.2252	.0516	.0516
	100	.0614	.0615	.0763	.0763	.0096	.0096
	400	.0687	.0688	.0366	.0366	.0061	.0061
Weight 5 (.4)	25	.2674	.2675	.2026	.2026	.1125	.1126
	100	.3090	.3089	.0724	.0724	.1007	.1007
	400	.3103	.3102	.0366	.0367	.0976	.0976
Weight6 (.4)	25	.0294	.0299	.4651	.4649	.2172	.2171
	100	.1421	.1426	.3178	.3176	.1212	.1212
	400	.2276	.2280	.1591	.1589	.0771	.0772
Weight7 (.6)	25	−.1872	−.1867	.4839	.4835	.2691	.2686
	100	.0410	.0410	.3089	.3087	.0971	.0970
	400	.1298	.1295	.1492	.1491	.0391	.0390
Weight 8 (.1)	25	.0705	.0701	.5018	.5017	.2568	.2566
	100	−.0989	−.0991	.3496	.3494	.1320	.1319
	400	−.1255	−.1259	.2161	.2159	.0625	.0625
Weight9 (.4)	25	−.2287	−.2288	.5146	.5149	.3171	.3175
	100	−.1280	−.1281	.5045	.5046	.2709	.2710
	400	.1415	.1411	.4416	.4416	.2150	.2149
Weight 10 (.3)	25	−.1332	−.1333	.6262	.6261	.4099	.4098
	100	−.1598	−.1597	.5498	.5498	.3278	.3278
	400	.0085	.0090	.4136	.4137	.1711	.1712
Weight 11 (.2)	25	−.1197	−.1194	.6373	.6371	.4204	.4202
	100	−.1571	−.1567	.6042	.6039	.3897	.3893
	400	−.3426	−.3424	.4836	.4834	.3513	.3510
Weight 12 (.2)	25	−.1170	−.1169	.5816	.5814	.3520	.3517
	100	−.1023	−.1022	.5153	.5152	.2760	.2759
	400	−.0963	−.0963	.4253	.4253	.1902	.1901
Weight 13 (.4)	25	−.3089	−.3088	.5303	.5302	.3767	.3765
	100	−.3531	−.3531	.4463	.4462	.3238	.3238
	400	−.4782	−.4784	.3686	.3687	.3645	.3648
Loading 1 (.8)	25	.1596	.1599	.0177	.0174	.0258	.0259
	100	.1623	.1623	.0074	.0074	.0264	.0264
	400	.1624	.1625	.0036	.0036	.0264	.0264
Loading 2 (.7)	25	.2347	.2346	.0265	.0268	.0558	.0558
	100	.2364	.2367	.0137	.0136	.0561	.0562
	400	.2370	.2373	.0062	.0062	.0562	.0563

Parameters	N	Bias		SD		MSE	
		Proposed	Extant	Proposed	Extant	Proposed	Extant
Loading 3 (.8)	25	.1517	.1515	.0202	.0205	.0234	.0234
	100	.1533	.1529	.0096	.0098	.0236	.0235
	400	.1540	.1536	.0045	.0046	.0237	.0236
Loading 4 (.8)	25	.1476	.1476	.0266	.0266	.0225	.0225
	100	.1494	.1494	.0102	.0102	.0224	.0224
	400	.1499	.1499	.0052	.0052	.0225	.0225
Loading 5 (.7)	25	.2337	.2337	.0353	.0353	.0559	.0559
	100	.2385	.2385	.0135	.0135	.0571	.0571
	400	.2390	.2390	.0065	.0065	.0572	.0572
Loading 6 (.8)	25	.1618	.1618	.0161	.0161	.0264	.0264
	100	.1632	.1632	.0070	.0070	.0267	.0267
	400	.1630	.1630	.0034	.0034	.0266	.0266
Path 1 (.4)	25	.3332	.3329	.1918	.1917	.1478	.1476
	100	.3827	.3825	.0408	.0409	.1481	.1480
	400	.3981	.3980	.0194	.0194	.1589	.1588
Path 2 (.5)	25	−.3533	−.3528	.1422	.1423	.1450	.1447
	100	−.3047	−.3044	.0620	.0620	.0967	.0965
	400	−.2934	−.2932	.0293	.0292	.0869	.0868
Path 3 (.6)	25	−.5769	−.5765	.1868	.1865	.3677	.3671
	100	−.5737	−.5736	.0937	.0937	.3379	.3378
	400	−.5618	−.5618	.0510	.0509	.3182	.3182
Path 4 (.6)	25	.0066	.0075	.1375	.1371	.0189	.0189
	100	.0224	.0227	.0612	.0611	.0042	.0042
	400	.0167	.0168	.0299	.0299	.0012	.0012

deviations, and mean square errors of all parameter estimates across all sample sizes, indicating that the two procedures yielded almost identical parameter estimates.

5. Conclusion

We proposed an alternative estimation procedure for estimating component weights in PLSPM. From technical perspectives, this procedure has several advantages over the extant one. First, it adopts a single optimization criterion to estimate the weights under both Mode A and Mode B. Thus, this addresses the enduring issue of lack of a single optimization criterion in PLSPM. Second, the proposed procedure applies an ALS algorithm to minimize the single criterion. This algorithm has been proven to converge (de Leeuw et al., 1976). In contrast, convergence of the extant algorithm has not been fully proven except for the cases of dealing with only one or two latent variables (Hanafi, 2007; Henseler, 2010). Third, the proposed procedure estimates the inner weights optimally in a least squares sense. On the other hand, in the extant procedure, it is unclear how the existing schemes were derived and in what sense their estimates of the inner weights are optimal. Lastly, the least squares criterion (8) can serve as a vehicle for furthering technical extensions of PLSPM. For example, multicollinearity among a block of indicators can have a negative influence on the estimation of component weights under Mode B (Esposito Vinzi et al., 2010; Tenenhaus

& Tenenhaus, 2011). To address this issue, we may integrate a ridge penalty into (8), as follows.

$$\varphi = \sum_{j=1}^{J} \alpha_j \, SS(X_j - f_j w_j') + \sum_{J=1}^{J} (1 - \alpha_j)\,(SS(f_j - X_j w_j) + \lambda_j \, SS(w_j)), \tag{14}$$

where λ_j is a block wise ridge parameter. Moreover, (8) can be minimized in combination with optimal scaling (e.g., Gifi, 1990; Young, 1981). This nonlinear extension can be of use in dealing with discrete indicators.

Besides these technical implications, the proposed procedure was found to provide quite comparable parameter estimates to those obtained from the extant one in a real

Appendix: A summary of the Lohmöller and ALS algorithms.

The Lohmöller algorithm	The ALS algorithm
Step 0 (Initialization) For $j = 1, \ldots, J$ choose the jth arbitrary weight vector (w_j^0) $\eta_j^0 = \frac{X_j w_j^0}{\\|X_j w_j^0\\|}$ End For $s = 0, 1, 2, \ldots$ (until convergence) Step 1 (Internal Estimation) For $j = 1, \ldots, J$ $f_j^s = \sum_{q=1}^{Q_j} e_{jq} \eta_q^s$, where e_{jq} is calculated as follows: For the centroid scheme, $e_{jq} = \mathrm{sign}(\mathrm{corr}(\eta_j^s, \eta_q^s))$ For the factorial scheme, $e_{jq} = \mathrm{corr}(\eta_j^s, \eta_q^s)$ For the path weighting scheme, $e_{jq} = \begin{cases} \mathrm{corr}(\eta_j^s, \eta_q^s), & \text{if } \eta_j \text{ affects } \eta_q \\ \omega_{jq}, & \text{otherwise} \end{cases}$ where ω_{jq} is the qth element of the regression coefficients of η_j on η_q's. End Step 2 (External Estimation) For $j = 1 \ldots J$ $w_j^{s+1} = X_j' f_j^s (f_j^{s\prime} f_j^s)^{-1}$, if Mode A $w_j^{s+1} = (X_j' X_j)^{-1} X_j' f_j^s$, if Mode B $\eta_j^{s+1} = \frac{X_j w_j^{s+1}}{\\|X_j w_j^{s+1}\\|}$ End Check if $\sum_{j=1}^{J} \sum_{p=1}^{P_j} (w_{jp}^s - w_{jp}^{s+1}) < .00001$. If not, go back to Step 1. End	Step 0 (Initialization) For $j = 1, \ldots, J$ choose the jth arbitrary weight vector (w_j^0) $\eta_j^0 = \frac{X_j w_j^0}{\\|X_j w_j^0\\|}$ End For $s = 0, 1, 2, \ldots$ (until convergence) Step 1 (Internal Estimation) For $j = 1, \ldots, J$ $\alpha_j = 1$, if Mode A $\alpha_j = 0$, if Mode B $f_j^s = \sum_{q=1}^{Q_j} e_{jq} \eta_q^s$, where e_{jq} is the qth element of $e_j^s = (\alpha_j w_j^{s\prime} w_j^s \Gamma_j^{s\prime} \Gamma_j^s + (1 - \alpha_j) \Gamma_j^{s\prime} \Gamma_j^s)^{-1} \Gamma_j^{s\prime} \eta_j^s$ End Step 2 (External Estimation) For $j = 1 \ldots J$ $\alpha_j = 1$, if Mode A $\alpha_j = 0$, if Mode B $w_j^{s+1} = (\alpha_j f_j^{s\prime} f_j^s I + (1 - \alpha_j) X_j' X_j)^{-1} X_j' f_j^s$, $\eta_j^{s+1} = \frac{X_j w_j^{s+1}}{\\|X_j w_j^{s+1}\\|}$ End Check if $\varphi^s - \varphi^{s+1} < .00001$. If not, go back to Step 1. End

data analysis. In addition, it resulted in virtually identical parameter estimates to those from the extant one in two simulation studies. Although the simulation studies were not exhaustive, they were of help in evaluating how similarly the proposed and extant procedures performed under different models at different sample sizes.

In sum, empirically the proposed procedure performs equally to the extant one, while technically it is well-founded in a least squares sense. Thus, the proposed procedure can serve as a substitute for the extant estimation procedure for PLSPM.

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