

Chapter 2

Partial Least Squares Path Modeling: Updated Guidelines

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Abstract Partial least squares (PLS) path modeling is a variance-based structural equation modeling technique that is widely applied in business and social sciences. It is the method of choice if a structural equation model contains both factors and composites. This chapter aggregates new insights and offers a fresh look at PLS path modeling. It presents the newest developments, such as consistent PLS, confirmatory composite analysis, and the heterotrait-monotrait ratio of correlations (HTMT). PLS path modeling can be regarded as an instantiation of generalized canonical correlation analysis. It aims at modeling relationships between composites, i.e., linear combinations of observed variables. A recent extension, consistent PLS, makes it possible to also include factors in a PLS path model. The chapter illustrates how to specify a PLS path model consisting of construct measurement and structural relationships. It also shows how to integrate categorical variables. A particularly important consideration is model identification: Every construct measured by multiple indicators must be embedded into a nomological net, which means that there must be at least one other construct with which it is related. PLS path modeling results are useful for exploratory and confirmatory research. The chapter provides guidelines for assessing the fit of the overall model, the reliability and validity of the measurement model, and the relationships between constructs.

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Moreover, it provides a glimpse on various extensions of PLS, many of which will be described in more detail in later chapters of the book.

2.1 Introduction

Structural equation modeling (SEM) is a family of statistical techniques that have become very popular in business and social sciences. Its ability to model latent variables, to take into account various forms of measurement error, and to test entire theories makes it useful for a plethora of research questions.

Two types of SEM can be distinguished: covariance- and variance-based SEM. Covariance-based SEM estimates model parameters using the empirical variance-covariance matrix, and it is the method of choice if the hypothesized model consists of one or more common factors. In contrast, variance-based SEM first creates proxies as linear combinations of observed variables and then estimates the model parameters using these proxies. Variance-based SEM is the method of choice if the hypothesized model contains composites.

Among variance-based SEM methods, partial least squares (PLS) path modeling is regarded as the “most fully developed and general system” (McDonald 1996, p. 240) and has been called a “silver bullet” (Hair et al. 2011). PLS is widely used in information systems research (Marcoulides and Saunders 2006), strategic management (Hair et al. 2012a), marketing (Hair et al. 2012b), and beyond. Its ability to model both factors and composites is appreciated by researchers across disciplines and makes it a promising method particularly for new technology research and information systems research. Whereas factors can be used to model latent variables of behavioral research such as attitudes or personality traits, composites can be applied to model strong concepts (Höök and Löwgren 2012), i.e., the abstraction of artifacts such as management instruments, innovations, or information systems. A particularly interesting class of artifacts is success factors for businesses. Consequently, PLS path modeling is a preferred statistical tool for success factor studies (Albers 2010).

Not only has PLS and its use been subject of various reviews (c.f. Hair et al. 2012a, b), but just recently it has also undergone a series of serious examinations and has been the target of heated scientific debates. Scholars have discussed the conceptual underpinnings (Rigdon 2012, 2014; Sarstedt et al. 2014) and the strengths and weaknesses (Henseler et al. 2014; Rigdon et al. 2014) of PLS. As a fruitful outcome of these debates, substantial contributions to PLS emerged, such as bootstrap-based tests of overall model fit (Dijkstra and Henseler 2015a), consistent PLS to estimate factor models (PLSc, see Dijkstra and Henseler 2015b), and the heterotrait-monotrait ratio of correlations as a new criterion for discriminant validity (HTMT, see Henseler et al. 2015). All these changes render the extant guidelines on PLS path modeling outdated, if not even invalid. Consequently, Rigdon (2014) recommends breaking the chains and forging ahead, which implies an urgent need for updated guidelines on why, when, and how to use PLS.

The purpose of this chapter is manifold. First, it provides an updated view on what PLS actually is and which algorithmic steps it includes since the invention of consistent PLS. Second, it explains how to specify PLS path models, taking into account the nature of the measurement models (composite vs. factor), model identification, sign indeterminacy, special treatments for categorical variables, and determination of sample size. Third, it explains how to assess and report PLS results, including the novel bootstrap-based tests of model fit, the SRMR as a measure of approximate model fit, the new reliability coefficient ρ_A , and the HTMT. Fourth, it sketches several ways of how to extend PLS analyses. Finally, it contrasts the understanding of PLS as presented in this chapter with the traditional view and discusses avenues for future developments.

2.2 The Nature of PLS Path Modeling

The core of PLS is a family of alternating least squares algorithms that emulate and extend principal component analysis as well as canonical correlation analysis. The method was invented by Herman Wold (c.f. 1974, 1982) for the analysis of high-dimensional data in a low-structure environment and has undergone various extensions and modifications. In its most modern appearance (c.f. Dijkstra and Henseler 2015a, b), PLS path modeling can be understood as a full-fledged structural equation modeling method that can handle both factor models and composite models for construct measurement, estimate recursive and non-recursive structural models, and conduct tests of model fit.

PLS path models are formally defined by two sets of linear equations: the measurement model (also called outer model) and the structural model (also called inner model). The measurement model specifies the relations between a construct and its observed indicators (also called manifest variables), whereas the structural model specifies the relationships between the constructs. Figure 2.1 depicts an example of a PLS path model.

PLS path models can contain two different forms of construct measurement: factor models or composite models (see Rigdon 2012, for a nice comparison of both types of measurement models). The factor model hypothesizes that the variance of a set of indicators can be perfectly explained by the existence of one unobserved variable (the common factor) and individual random error. It is the standard model of behavioral research. In Fig. 2.1, the exogenous construct ξ and the endogenous construct η_2 are modeled as factors. In contrast, composites are formed as linear combinations of their respective indicators. The composite model does not impose any restrictions on the covariances between indicators of the same construct, i.e., it relaxes the assumption that all the covariation between a block of indicators is explained by a common factor. The composites serve as proxies for the scientific concept under investigation (Ketterlinus et al. 1989; Maraun and Halpin 2008;

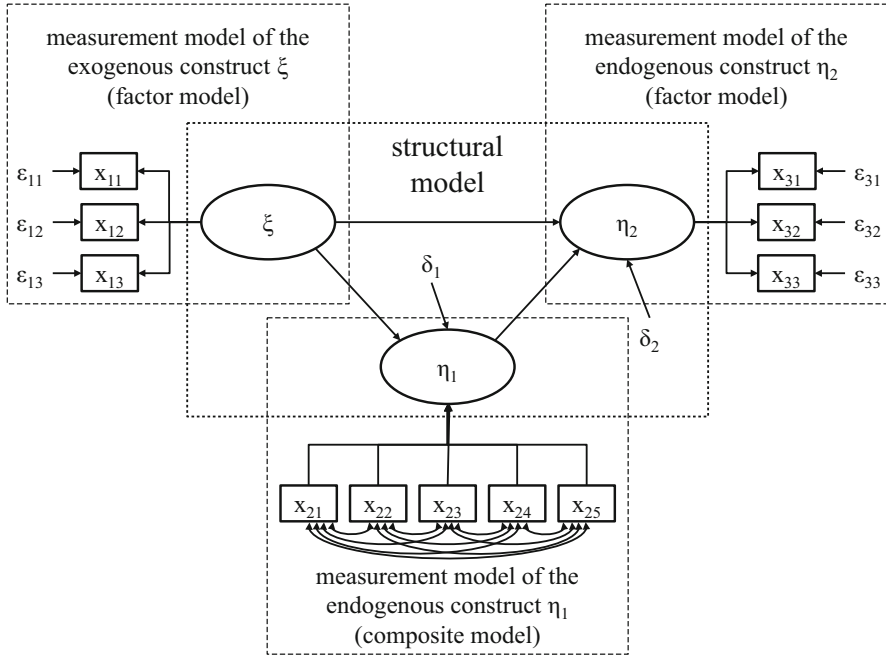


Fig. 2.1 PLS path model example

Rigdon 2012; M. Tenenhaus 2008).¹ The fact that composite models are less restrictive than factor models makes it likely that they have a higher overall model fit (Landis et al. 2000).

The structural model consists of exogenous and endogenous constructs as well as the relationships between them. The values of exogenous constructs are assumed to be given from outside the model. Thus, exogenous variables are not explained by other constructs in the model, and there must not be any arrows in the structural model that point to exogenous constructs. In contrast, endogenous constructs are at least partially explained by other constructs in the model. Each endogenous construct must have at least one arrow of the structural model pointing to it. The relationships between the constructs are usually assumed to be linear. The size and significance of path relationships are typically the focus of the scientific endeavors pursued in empirical research.

The estimation of PLS path model parameters happens in four steps: (1) an iterative algorithm that determines composite scores for each construct, (2) a correction for attenuation for those constructs that are modeled as factors (Dijkstra and Henseler 2015b), (3) parameter estimation, and (4) bootstrapping for inference testing.

¹Note that also factors are nothing else than proxies (Rigdon 2012).

Step 1 For each construct, the iterative PLS algorithm creates a proxy as a linear combination of the observed indicators. The indicator weights are determined such that each proxy shares as much variance as possible with the proxies of causally related constructs. The PLS algorithm can be viewed as an approach to extend canonical correlation analysis to more than two sets of variables; it can emulate several of Kettenring's (1971) techniques for the canonical analysis of several sets of variables (M. Tenenhaus et al. 2005). For a more detailed description of the algorithm, see Henseler (2010). The major outputs of the first step are the proxies (i.e., composite scores), the proxy correlation matrix, and the indicator weights.

Step 2 Correcting for attenuation is a necessary step if a model involves factors. As long as the indicators contain random measurement error, so will the proxies. Consequently, proxy correlations are typically underestimations of factor correlations. Consistent PLS (PLSc) corrects for this tendency (Dijkstra and Henseler 2015a, b) by dividing a proxy's correlations by the square root of its reliability (the so-called correction for attenuation). PLSc addresses the issue of what the correlation between constructs would be if there were no random measurement error. The major output of this second step is a consistent construct correlation matrix.

Step 3 Once a consistent construct correlation matrix is available, it is possible to estimate the model parameters. If the structural model is recursive (i.e., there are no feedback loops), ordinary least squares (OLS) regression can be used to obtain consistent parameter estimates for the structural paths. In the case of non-recursive models, instrumental variable techniques such as two-stage least squares (2SLS) should be employed. In addition to the path coefficient estimates, this third step can also provide estimates for loadings, indirect effects, total effects, and several model assessment criteria.

Step 4 Finally, the bootstrap is applied in order to obtain inference statistics for all model parameters. The bootstrap is a nonparametric inferential technique which rests on the assumption that the sample distribution conveys information about the population distribution. Bootstrapping is the process of drawing a large number of resamples with replacement from the original sample and then estimating the model parameters for each bootstrap resample. The standard error of an estimate is inferred from the standard deviation of the bootstrap estimates.

The PLS path modeling algorithm has favorable convergence properties (Henseler 2010). However, as soon as PLS path models involve common factors, there is the possibility of so-called Heywood cases (Krijnen et al. 1998), meaning that one or more variances implied by the model would be negative. The occurrence of Heywood cases may be caused by an atypical or too-small sample, or the common factor structure may not hold for a particular set of indicators.

PLS path modeling is not as efficient as maximum likelihood covariance-based SEM. One possibility is to further minimize the discrepancy between the empirical and the model-implied correlation matrix, an approach followed by efficient PLS (PLSe, see Bentler and Huang 2014). Alternatively, one could embrace the notion that PLS is a limited-information estimator and is less affected by model

misspecification in some subparts of a model (Antonakis et al. 2010). Ultimately, there is no clear-cut resolution of the issues on this trade-off between efficiency and robustness with respect to model misspecification.

2.3 Model Specification

The analysts must take care that the specified statistical model complies with the conceptual model to be tested and further that the model complies with technical requirements such as identification and with the data conforming to the required format and statistical power.

Typically, the structural model is theory-based and is the prime focus of the research question and/or research hypotheses. The specification of the structural model addresses two questions: Which constructs should be included in the model? And how are they hypothesized to be interrelated? That is, what are the directions and strengths of the causal influences between and among the latent constructs? In general, analysts should keep in mind that the constructs specified in a model are only proxies and that there will always be a validity gap between these proxies and the theoretical concepts that are the intended modeling target (Rigdon 2012). The paths, specified as arrows in a PLS model, represent directional linear relationships between proxies. The structural model, and the indicated relationships among the latent constructs, is regarded as separate from the measurement model.

The specification of the measurement model entails decisions for composite or factor models and the assignment of indicators to constructs. Factor models are the predominant measurement model for behavioral constructs such as attitudes or personality traits. Factor models are strongly linked to true score theory (McDonald 1999), the most important measurement paradigm in behavioral sciences. If a construct has this background and random measurement error is likely to be an issue, analysts should choose the factor model. Composites help model emergent constructs, for which elements are combined to form a new entity. Composites can be applied to model strong concepts (Höök and Löwgren 2012), i.e., the abstraction of artifacts (man-made objects). Typical artifacts in new technology research would include innovations, technologies, systems, processes, strategies, management instruments, or portfolios. Whenever a model contains this type of construct, it is preferable to use a composite model.

Measurement models of PLS path models may appear less detailed than those of covariance-based structural equation modeling, but in fact some specifications are implicit and are not visualized. For instance, neither the unique indicator errors (nor their correlations) of factor models nor the correlations between indicators of composite models are drawn. Because PLS currently does not allow to either constrain these parameters or to free the error correlations of factor models, by convention these model elements are not drawn. No matter which type of measurement is chosen to measure a construct, PLS requires that there is at least

one indicator available. Constructs without indicators, so-called phantom variables (Rindskopf 1984), cannot be included in PLS path models.

In some PLS path modeling software (e.g., SmartPLS and PLS-Graph), the direction of arrows depicted in the measurement model does not indicate whether a factor or composite model is estimated but whether correlation weights (Mode A, represented by arrows pointing from a construct to its indicators) or regression weights (Mode B, represented by arrows pointing from indicators to their construct) shall be used to create the proxy. In both cases PLS will estimate a composite model. Indicator weights estimated by Mode B are consistent (Dijkstra 2010), whereas indicator weights estimated by Mode A are not, but the latter excel in out-of-sample prediction (Rigdon 2012).

Some model specifications are made automatically and cannot be manually changed: Measurement errors are assumed to be uncorrelated with all other variables and errors in the model; structural disturbance terms are assumed to be orthogonal to their predictor variables as well as to each other²; correlations between exogenous variables are free. Because these specifications hold across models, it has become customary not to draw them in PLS path models.

Identification has always been an important issue for SEM, although it has been neglected in the realm of PLS path modeling in the past. It refers to the necessity to specify a model such that only one set of estimates exists that yields the same model-implied correlation matrix. It is possible that a complete model is unidentified, but also only parts of a model can be unidentified. In general, it is not possible to derive useful conclusions from unidentified (parts of) models. In order to achieve identification, PLS fixes the variance of factors and composites to one. An important requirement of composite models is a so-called nomological net. It means that composites cannot be estimated in isolation but need at least one other variable (either observed or latent) to have a relation with. Since PLS also estimates factor models via composites, this requirement extends to all factor models estimated using PLS. If a factor model has exactly two indicators, it does not matter which form of SEM is used—a nomological net is then required to achieve identification. If a construct is only measured by one indicator, one speaks of single-indicator measurement (Diamantopoulos et al. 2012). The construct scores are then identical to the standardized indicator values. In this case it is not possible to determine the amount of random measurement error in this indicator. If an indicator is error-prone, the only possibility to account for the error is to utilize external knowledge about the reliability of this indicator to manually define the indicator's reliability.

A typical characteristic of SEM and factor-analytical tools in general is sign indeterminacy, in which the weight or loading estimates for a factor or a composite can only be determined jointly for their value but not for their sign. For example, if a factor is extracted from the strongly negatively correlated customer satisfaction indicators “How satisfied are you with provider X?” and “How much does provider X differ from an ideal provider?” the method cannot “know” whether the extracted

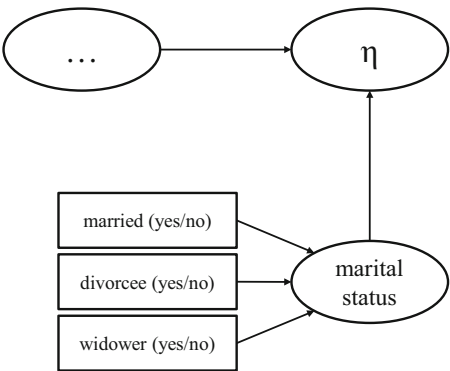
²This assumption should be relaxed in case of non-recursive models (Dijkstra and Henseler 2015a).

factor should correlate positively with the first or with the second indicator. Depending on the sign of the loadings, the meaning of the factor would either be “customer satisfaction” or “customer non-satisfaction.” To avoid this ambiguity, it has become practice in SEM to determine one particular indicator per construct with which the construct scores are forced to correlate positively. Since this indicator dictates the orientation of the construct, it is called the “dominant indicator.” While in covariance-based structural equation modeling this dominant indicator also dictates the construct’s variance, in PLS path modeling, the construct variance is simply set to one.

Like multiple regression, PLS path modeling requires metric data for the dependent variables. Dependent variables are the indicators of the factor model(s) as well as the endogenous constructs. Quasi-metric data stemming from multipoint scales such as Likert scales or semantic differential scales are also acceptable as long as the scale points can be assumed to be equidistant and the number of scale points is sufficiently high (Rhemtulla et al. 2012). If these assumptions are not fulfilled, but the data are ordinal, researchers should rely on dedicated PLS-based approaches such as OrdPLSc (Schuberth et al. 2016; see also Chap. 6 of this book). To some extent it is also possible to include categorical variables in a model. Categorical variables (which are not necessarily ordinal) are particularly relevant for analyzing experiments (c.f. Streukens et al. 2010) or for control variables such as industry (Braojos-Gomez et al. 2015) or ownership structure (Chen et al. 2015). Figure 2.2 illustrates how a categorical variable “marital status” would be included in a PLS path model. If a categorical variable has only two levels (i.e., it is dichotomous), it can serve immediately as a construct indicator. If a categorical variable has more than two levels, it should be transformed into as many dummy variables as there are levels. A composite model is formed out of all but one dummy variable. The remaining dummy variable characterizes the reference level. Preferably, categorical variables should only play the role of exogenous variables in a structural model.

Sample size plays a dual role, namely, technically and in terms of inference statistics. Technically, the number of observations must be high enough that the regressions that form part of the PLS algorithm do not evoke singularities. It can

Fig. 2.2 Including a categorical control variable in a PLS path model (here marital status with the four categories “unmarried,” “married,” “divorcee,” “widower”; the reference category is “unmarried”)



thus be that the number of parameters or the number of variables in a model exceeds the number of observations. Inference statistics become relevant if an analyst wants to generalize from a sample to a population. The larger the sample size, the smaller the confidence intervals of the model's parameter estimates, and the smaller the chance that a parameter estimate's deviation from zero are due to sampling variation. Moreover, a larger sample size increases the likelihood to detect model misspecification (see Sect. 2.4 for PLS' tests of model fit). Hence, a larger sample size increases the rigor to falsify the model in the Popperian sense, but at the same time, the likelihood increases that a model gets rejected due to minor and hardly relevant aspects. The statistical power of PLS should not be expected to supersede that of covariance-based SEM.³ Consequently, there is no reason to prefer PLS over other forms of SEM with regard to inference statistics. In research practice, there are typically many issues that have an impact on the final sample size. One important consideration should be the statistical power, i.e., the likelihood to find an effect in the sample if it indeed exists in the population. Optimally, researchers make use of Monte Carlo simulations to quantify the statistical power achieved at a certain sample size (for a tutorial, see Aguirre-Urreta and Rönkkö 2015).

2.4 Assessing and Reporting PLS Analyses

PLS path modeling can be used both for explanatory and predictive research. Depending on the analyst's aim—either explanation or prediction—the model assessment will be different. If the analyst's aim is to predict, the assessment should focus on blindfolding (M. Tenenhaus et al. 2005) and the model's performance with regard to holdout samples (Cepeda Carrión et al. 2016; Lancelot-Miltgen et al. 2016). However, since prediction-orientation still tends to be scarce in business research (Shmueli and Koppius 2011), in the remainder we will focus on model assessment if the analyst's aim is explanation.

PLS path modeling results can be assessed globally (i.e., for the overall model) and locally (for the measurement models and the structural model). For a long time, it was said that PLS path modeling did not optimize any global scalar and therefore did not allow for global model assessment. However, because PLS in the form as described above provides consistent estimates for factor and composite models, it is possible to meaningfully compare the model-implied correlation matrix with the empirical correlation matrix, which opens up the possibility for the assessment of global model fit.

³An allegedly higher statistical power of PLS (Reinartz et al. 2009) can be traced back to model misspecification, namely, making use of a composite model although the factor model would have been true (Goodhue et al. 2011).

The overall goodness of fit of the model should be the starting point of model assessment. If the model does not fit the data, the data contains more information than the model conveys. The obtained estimates may be meaningless, and the conclusions drawn from them become questionable. The global model fit can be assessed in two non-exclusive ways: by means of inference statistics, i.e., so-called tests of model fit, or through the use of fit indices, i.e., an assessment of approximate model fit. In order to have some frame of reference, it has become customary to determine the model fit both for the estimated model and for the saturated model. Saturation refers to the structural model, which means that in the saturated model all constructs correlate freely.

PLS path modeling's tests of model fit rely on the bootstrap to determine the likelihood of obtaining a discrepancy between the empirical and the model-implied correlation matrix that is as high as the one obtained for the sample at hand if the hypothesized model was indeed correct (Dijkstra and Henseler 2015a). Bootstrap samples are drawn from modified sample data. This modification entails an orthogonalization of all variables and a subsequent imposition of the model-implied correlation matrix. In covariance-based SEM, this approach is known as Bollen-Stine bootstrap (Bollen and Stine 1992). If more than 5% (or a different percentage if an alpha-level different from 0.05 is chosen) of the bootstrap samples yield discrepancy values above the ones of the actual model, it is not that unlikely that the sample data stems from a population that functions according to the hypothesized model. The model thus cannot be rejected. There is more than one way to quantify the discrepancy between two matrices, for instance, the maximum likelihood discrepancy, the geodesic discrepancy d_G , or the unweighted least squares discrepancy d_{ULS} (Dijkstra and Henseler 2015a), and so there are several tests of model fit. Monte Carlo simulations confirm that the tests of model fit can indeed discriminate between well-fitting and ill-fitting models (Henseler et al. 2014). More precisely, both measurement model misspecification and structural model misspecification can be detected through the tests of model fit (Dijkstra and Henseler 2014). Because it is possible that different tests have different results, a transparent reporting practice would always include several tests.

In addition to conducting the tests of model fit, it is also possible to determine the approximate model fit. Approximate model fit criteria help answer the question how substantial the discrepancy between the model-implied and the empirical correlation matrix is. This question is particularly relevant if this discrepancy is significant. Currently, the only approximate model fit criterion implemented for PLS path modeling is the standardized root mean square residual (SRMR, Hu and Bentler 1998, 1999). As can be derived from its name, the SRMR is the square root of the sum of the squared differences between the model-implied and the empirical correlation matrix, i.e., the Euclidean distance between the two matrices. A value of 0 for SRMR would indicate a perfect fit, and generally, an SRMR value less than 0.05 indicates an acceptable fit (Byrne 2013). A recent simulation study shows that even entirely correctly specified model can yield SRMR values of 0.06 and higher (Henseler et al. 2014). Therefore, a cutoff value of 0.08 as proposed by Hu and Bentler (1999) appears to be more adequate for PLS path models. Another useful

approximate model fit criterion could be the Bentler-Bonett index or normed fit index (NFI, Bentler and Bonett 1980). The suggestion to use the NFI in connection with PLS path modeling can be attributed to Lohmöller (1989). For factor models, NFI values above 0.90 are considered as acceptable (Byrne 2013). For composite models, thresholds for the NFI are still to be determined. Because the NFI does not penalize for adding parameters, it should be used with caution for model comparisons. In general, the usage of the NFI is still rare.⁴ Another promising approximate model fit criterion is the root mean square error correlation (RMS_{θ} , see Lohmöller 1989). A recent simulation study (Henseler et al. 2014) provides evidence that the RMS_{θ} can indeed distinguish well-specified from ill-specified models. However, thresholds for the RMS_{θ} are yet to be determined, and PLS software still needs to implement this approximate model fit criterion. Note that early suggestions for PLS-based goodness-of-fit measures such as the “goodness-of-fit” (GoF, see M. Tenenhaus et al. 2004) or the “relative goodness-of-fit” [GoF_{rel} , proposed by Esposito Vinzi et al. (2010)] are—contrary to what their name might suggest—not informative about the goodness of model fit (Henseler et al. 2014; Henseler and Sarstedt 2013). Consequently, there is no reason to evaluate and report them if the analyst’s aim is to test or to compare models.

If the specified measurement (or outer) model does not possess minimum required properties of acceptable reliability and validity, then the structural (inner) model estimates become meaningless. That is, a necessary condition to even proceed to assess the “goodness” of the inner structural model is that the outer measurement model has already demonstrated acceptable levels of reliability and validity. There must be a sound measurement model before one can begin to assess the “goodness” of the inner structural model or to rely on the magnitude, direction, and/or statistical strength of the structural model’s estimated parameters. Factor and composite models are assessed in a different way.

Factor models can be assessed in various ways. The bootstrap-based tests of overall model fit can indicate whether the data is coherent with a factor model, i.e., it represents a confirmatory factor analysis. In essence, the test of model fit provides an answer to the question “Does empirical evidence speak against the existence of the factor?” This quest for truth illustrates that testing factor models is rooted in the positivist research paradigm. If the test of overall model fit has not provided evidence against the existence of a factor,⁵ several questions with regard to the factor structure emerge: Does the data support a factor structure at all? Is it clear that a factor can be extracted? How well has this factor been measured? Note that tests of overall model fit cannot answer these questions; in particular, entirely uncorrelated empirical variables do not necessarily lead to the rejection of the factor model. To

⁴For an application of the NFI, see Ziggers and Henseler (2016).

⁵Interestingly, the methodological literature on factor models is quite silent about what to do if the test speaks against a factor model. Some researchers suggest considering the alternative of a composite model, because it is less restrictive (Henseler et al. 2014) and not subject to factor indeterminacy (Rigdon 2012).

answer these questions, one should rather rely on several local assessment criteria with regard to the reliability and validity of measurement.

The amount of random error in construct scores should be acceptable, or in other words, the reliability of construct scores should be sufficiently high. Nunnally and Bernstein (1994) recommend a minimum reliability of 0.7. The most important reliability measure for PLS is ρ_A (Dijkstra and Henseler 2015b); it currently is the only consistent reliability measure for PLS construct scores. Most PLS software also provides a measure of composite reliability (also called Dillon-Goldstein's ρ , factor reliability, Jöreskog's ρ , omega, or ρ_c) as well as Cronbach's alpha. Both refer to sum scores, not construct scores. In particular, Cronbach's alpha typically underestimates the true reliability and should therefore only be regarded as a lower boundary to the reliability (Sijtsma 2009).

The measurement of factors should also be free from systematic measurement error. This quest for validity can be fulfilled in several non-exclusive ways. First, a factor should be unidimensional, a characteristic examined through convergent validity. The dominant measure of convergent validity is the average variance extracted (AVE, Fornell and Larcker 1981).⁶ If the first factor extracted from a set of indicators explains more than one half of their variance, there cannot be any second, equally important factor. An AVE of 0.5 or higher is therefore regarded as acceptable. A somewhat more liberal criterion was proposed by Sahmer et al. (2006): They find evidence for unidimensionality as long as a factor explains significantly more variance than the second factor extracted from the same indicators. Second, each pair of factors that stand in for theoretically different concepts should also statistically be different, which raises the question of discriminant validity. Two criteria have been shown to be informative about discriminant validity (Voorhees et al. 2016): the Fornell-Larcker criterion (proposed by Fornell and Larcker 1981) and the heterotrait-monotrait ratio of correlations (HTMT, developed by Henseler et al. 2015). The Fornell-Larcker criterion says that a factor's AVE should be higher than its squared correlations with all other factors in the model. The HTMT is an estimate for the factor correlation (more precisely, an upper boundary). In order to clearly discriminate between two factors, the HTMT should be significantly smaller than one. Third, the cross-loadings should be assessed to make sure that no indicator is incorrectly assigned to a wrong factor.

The assessment of composite models is somewhat less developed. Again, the major point of departure should be the tests of model fit. The tests of model fit for the saturated model provide evidence for the external validity of the composites. Henseler et al. (2014) call this step a "confirmatory composite analysis." For composite models, the major research question is "Does it make sense to create this composite?" This different question shows that testing composite models

⁶The AVE must be calculated based on consistent loadings; otherwise, the assessment of convergent and discriminant validity based on the AVE is meaningless.

follows a different research paradigm, namely, pragmatism (Henseler 2015). Once confirmatory composite analysis has provided support for the composite, it can be analyzed further. One follow-up suggests itself: How is the composite made? Do all the ingredients contribute significantly and substantially? To answer these questions, an analyst should assess the sign and the magnitude of the indicator weights as well as their significance. Particularly if indicators weights have unexpected signs or are insignificant, this can be due to multicollinearity. It is therefore recommendable to assess the variance inflation factor (VIF) of the indicators. VIF values much higher than one indicate that multicollinearity might play a role.

Once the measurement model is deemed to be of sufficient quality, the analyst can proceed and assess the structural model. If OLS is used for the structural model, the endogenous constructs' R^2 values would be the point of departure. They indicate the % of variability accounted for by the precursor constructs in the model. The adjusted R^2 values take into account model complexity and sample size and are thus helpful to compare different models or the explanatory power of a model across different datasets.

If the analyst's aim is to generalize from a sample to a population, the path coefficients should be evaluated for significance. Inference statistics include the empirical bootstrap confidence intervals as well as one-sided or two-sided p -values. We recommend to use 4999 bootstrap samples. This number is sufficiently close to infinity for usual situations, is tractable with regard to computation time, and allows for an unambiguous determination of empirical bootstrap confidence intervals (for instance, the 2.5% [97.5%] quantile would be the 125th [4875th] element of the sorted list of bootstrap values). A path coefficient is regarded as significant (i.e., unlikely to purely result from sampling error) if its confidence interval does not include the value of zero or if the p -value is below the predefined alpha-level. Despite strong pleas for the use of confidence intervals (Cohen 1994), reporting p -values still seems to be more common in business research.

For the significant effects, it makes sense to quantify how substantial they are, which can be accomplished by assessing their effect size f^2 . Values for f^2 above 0.35, 0.15, and 0.02 can be regarded as strong, moderate, and weak, respectively (Cohen 1988). The path coefficients are essentially standardized regression coefficients, which can be assessed with regard to their sign and their absolute size. They should be interpreted as the change in the dependent variable if the independent variable is increased by one and all other independent variables remain constant. Indirect effects and their inference statistics are important for mediation analysis (Zhao et al. 2010), and total effects are useful for success factor analysis (Albers 2010). Table 2.1 sums up the discussed criteria for model assessment.

Table 2.1 Assessment of PLS path modeling results in explanatory research settings

Assessment	Criterion
<i>Overall model</i>	
Test of model fit (estimated model)	SRMR < 95% bootstrap quantile (HI95 of SRMR) $d_{\text{ULS}} < 95\%$ bootstrap quantile (HI95 of d_{ULS}) $d_{\text{G}} < 95\%$ bootstrap quantile (HI95 of d_{G})
Approximate model fit (estimated model)	SRMR < 0.08
<i>Measurement model</i>	
Confirmatory composite and/or factor analysis (saturated model)	SRMR < 95% bootstrap quantile (HI95 of SRMR) $d_{\text{ULS}} < 95\%$ bootstrap quantile (HI95 of d_{ULS}) $d_{\text{G}} < 95\%$ bootstrap quantile (HI95 of d_{G})
Approximate model fit (saturated model)	SRMR < 0.08
Internal consistency reliability	Dijkstra-Henseler's $\rho_{\text{A}} > 0.7$ Dillon-Goldstein's $\rho_{\text{c}} > 0.7$ Cronbach's $\alpha > 0.7$
Convergent validity	AVE > 0.5
Discriminant validity	HTMT significantly smaller than 1 Fornell-Larcker criterion Loadings exceed cross-loadings
<i>Structural model</i>	
Endogenous variables	R^2 , adjusted R^2
Direct effects	Path coefficient (absolute size, sign) Significance (p -value, confidence interval) Effect size
Indirect effects	Coefficient (absolute size, sign) Significance (p -value, confidence interval)
Total effects	Coefficient (absolute size, sign) Significance (p -value, confidence interval)

2.5 Extensions

PLS path modeling as described so far analyzes linear relationships between factors or composites of observed indicator variables. There are many ways how this rather basic model can be extended.

A first extension is to depart from the assumption of linearity. Researchers have developed approaches to include nonlinear relationships into the structural model. In particular, interaction effects and quadratic effects can be easily analyzed by means of some rudimentary extensions to the standard PLS path modeling setup (Dijkstra and Henseler 2011; Dijkstra and Schermelleh-Engel 2014; Henseler and Chin 2010; Henseler and Fassott 2010; Henseler et al. 2012). Interaction effects pay tribute to the fact that not all individuals function according to the same mechanism but that the strength of relationships depends on contingencies.

In addition to interaction effects, there are more comprehensive tools to take into account the heterogeneity between individuals. Heterogeneity can be observed, i.e., it can be traced back to an identified variable, or unobserved, i.e., there is no a priori explanation for why an individual's mechanism would differ from others. Because incorrectly assuming that all individuals function according to the same mechanism represents a validity threat (Becker et al. 2013b), several PLS-based approaches to discover unobserved heterogeneity have been proposed. Prominent examples include finite mixture PLS (Ringle et al. 2010a, c), PLS prediction-oriented segmentation (PLS-POS, Becker et al. 2013b), and PLS genetic algorithm segmentation (PLS-GAS, Ringle et al. 2010b, 2014). In order to assess observed heterogeneity, analysts should make use of multigroup analysis (Sarstedt et al. 2011). No matter whether heterogeneity is observed or unobserved, another concern for the analysts must be not to confound heterogeneity in the structural model with variation in measurement. Particularly in cross-cultural research, it has therefore become a common practice to assess the measurement model invariance before drawing conclusions about structural model heterogeneity. There is a plethora of papers discussing how to assess the measurement invariance of factor models (see, e.g., French and Finch 2006); there is only one approach for assessing the measurement invariance of composite models (Henseler et al. 2016).

2.6 Discussion

The plethora of discussions and developments around PLS path modeling called for a fresh look at this technique as well as new guidelines. As important aspect of this endeavor, we provide an answer to the question “What has changed?” This answer is given in Table 2.2, which contrasts traditional and modern perspectives on PLS. It is particularly helpful for researchers who have been educated in PLS path modeling in the past and who would like to update their understanding of the method.

The fact that PLS today strongly differs from how it used to be has also implications for the users of PLS software. They should verify that they use a software that has implemented the newest developments in the PLS field. One possibility would be ADANCO (Henseler and Dijkstra 2015), a new software for variance-based SEM, which also includes PLS path modeling.

The modularity of PLS path modeling as introduced in the second section opens up the possibility of replacing one or more steps by other approaches. For instance, the least squares estimators of the third step could be replaced by neural networks (Buckler and Hennig-Thurau 2008; Turkyilmaz et al. 2013). One could even replace the PLS algorithm in Step 1 by alternative indicator weight generators, such as principal component analysis (M. Tenenhaus 2008), generalized structured component analysis (Henseler 2012; Hwang and Takane 2004), regularized generalized canonical correlation analysis (A. Tenenhaus and Tenenhaus 2011), or even plain sum scores. Because in these instances the iterative PLS algorithm would not serve as eponym, one could not speak of PLS path modeling anymore. However, it still would be variance-based structural equation modeling.

Table 2.2 Contrasting traditional and modern perspectives on PLS

Traditional view on PLS	Modern view on PLS
PLS has some but not all abilities of structural equation modeling	PLS is a full-fledged structural equation modeling approach
PLS can estimate formative (using Mode B) and reflective measurement models (using Mode A)	PLS can consistently estimate composite models (using Mode B), formative models (MIMIC specification), and factor models (using consistent PLS for the latter)
Identification is not an issue for PLS	To ensure identification, analysts must provide a nomological net for each multi-item construct
PLS path models must be recursive	PLS path models can contain feedback loops or take into account endogeneity if an adequate estimator is used for the structural model. A sufficient number of exogenous variables must be available
PLS needs fewer observations than other SEM techniques	PLS does not need fewer observations than other techniques when it comes to inference statistics. Analysts should ensure sufficient statistical power and representativeness of data
In contrast to other SEM techniques, PLS does not rely on the assumption of normality	With regard to assumptions made for the estimation of parameters, PLS does not differ from other SEM techniques. For inference statistics, PLS applies a nonparametric technique, namely, bootstrapping, which can equally be applied by other SEM techniques
PLS only permits local model assessment by means of certain criteria	PLS path models can and should be assessed globally by means of tests of model fit and approximate measures of model fit. Models should be locally assessed, too
The reliability of PLS construct scores is indicated by Cronbach's alpha and/or composite reliability	The reliability coefficient ρ_A is a consistent estimate of the reliability of PLS construct scores; composite reliability (based on consistent loadings) is a consistent estimate of the reliability of sum scores
Discriminant validity should be assessed by comparing each construct's average variance extracted with its squared construct correlations	Discriminant validity should be assessed by means of the heterotrait-monotrait ratio of correlations (HTMT) and by comparing each construct's average variance extracted (based on consistent loadings) with its squared consistent construct correlations
Bootstrapping should be conducted in combination with sign change correction in order to avoid inflated standard errors	For each construct, a dominant indicator should be defined in order to avoid sign indeterminacy

Finally, recent research confirms that PLS serves as a promising technique for prediction purposes (Becker et al. 2013a). Both measurement models and structural models can be assessed with regard to their predictive validity. Blindfolding is the standard approach used to examine if the model or a single effect of it can predict values of reflective indicators. It is already widely applied (Hair et al. 2012b; Ringle et al. 2012). Criteria for the predictive capability of structural models have

been proposed (c.f. Chin 2010) but still need to disseminate. We anticipate that once business and social science researchers' interest in prediction becomes more pronounced, PLS will face an additional substantial increase in popularity.

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