Partial Least Squares Structural Equation Modeling

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Abstract

Partial least squares structural equation modeling (PLS-SEM) has become a popular method for estimating (complex) path models with latent variables and their relationships. Building on an introduction of the fundamentals of measurement and structural theory, this chapter explains how to specify and estimate path models using PLS-SEM. Complementing the introduction of the PLS-SEM method and the description of how to evaluate analysis results, the chapter also offers an overview of complementary analytical techniques. An application of the PLS-SEM method to a well-known corporate reputation model using the SmartPLS 3 software illustrates the concepts.

Keywords

Partial least squares • PLS • PLS path modeling PLS-SEM • SEM • Variance-based structural equation modeling

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Introduction

In the 1970s and 1980s the Swedish econometrician Herman O. A. Wold (1975, 1982, 1985) "vigorously pursued the creation and construction of models and methods for the social sciences, where 'soft models and soft data' were the rule rather than the exception, and where approaches strongly oriented at prediction would be of great value" (Dijkstra 2010, p. 24). One procedure that emerged from Wold's efforts was partial least squares path modeling, which later evolved to partial least squares structural equation modeling (PLS-SEM; Hair et al. 2011). PLS-SEM estimates the parameters of a set of equations in a structural equation model by combining principal components analysis with regression-based path analysis (Mateos-Aparicio 2011). Wold (1982) proposed his "soft model basic design" underlying PLS-SEM as an alternative to Jöreskog's (1973) factor-based SEM or covariance-based SEM, which has been labeled as hard modeling because of its numerous and rather restrictive assumptions for establishing a structural equation model but also in terms of data distribution and sample size. Importantly, "it is not the concepts nor the models nor the estimation techniques which are 'soft', only the distributional assumptions" (Lohmöller 1989, p. 64).

PLS-SEM enjoys widespread popularity in a broad range of disciplines including accounting (Lee et al. 2011; Nitzl 2016), group and organization management (Sosik et al. 2009), hospitality management (Ali et al. 2017), international management (Richter et al. 2016a), operations management (Peng and Lai 2012), management information systems (Hair et al. 2017a; Ringle et al. 2012), marketing (Hair et al.

2012b), strategic management (Hair et al. 2012a), supply chain management (Kaufmann and Gaeckler 2015), and tourism (do Valle and Assaker 2016). Contributions in terms of books, edited volumes, and journal articles applying PLS-SEM or proposing methodological extensions are appearing at a rapid pace (e.g., Latan and Noonan 2017; Esposito Vinzi et al. 2010; Hair et al. 2017b, 2018; Garson 2016; Ramayah et al. 2016). A main reason for PLS-SEM's attractiveness is that the method allows researchers to estimate very complex models with many constructs and indicator variables, especially when prediction is the goal of the analysis. Furthermore, PLS-SEM generally allows for much flexibility in terms of data requirements and the specification of relationships between constructs and indicator variables. Another reason is the accessibility of easy to use software with graphical user interface such as ADANCO, PLS-Graph, SmartPLS, WarpPLS, and XLSTAT. Packages for statistical computing software environments such as R complement the set of programs (e.g., semPLS).

The objective of this chapter is to explain the fundamentals of PLS-SEM. Building on Sarstedt et al. (2016b), this chapter first provides an introduction of measurement and structural theory as a basis for presenting the PLS-SEM method. Next, the chapter discusses the evaluation of results, provides an overview of complementary analytical techniques, and concludes by describing an application of the PLS-SEM method to a well-known corporate reputation model, using the SmartPLS 3 software.

Principles of Structural Equation Modeling

Path Models with Latent Variables

A path model is a diagram that displays the hypotheses and variable relationships to be estimated in an SEM analysis (Bollen 2002). Figure 1 shows an example of a path model with latent variables and their indicators.

Constructs, also referred to as latent variables, are elements in statistical models that represent conceptual variables that researchers define in their theoretical models. Constructs are visualized as circles or ovals (Y_1 to Y_3) in path models, linked via single-headed arrows that represent predictive relationships. The indicators, often also named manifest variables or items, are directly measured or observed variables that represent the raw data (e.g., respondents' answers to a questionnaire). They are represented as rectangles (x_1 to x_9) in path models and are linked to their corresponding constructs through arrows.

A path model consists of two elements. The structural model represents the structural paths between the constructs, whereas the measurement models represent the relationships between each construct and its associated indicators. In PLS-SEM, structural and measurement models are also referred to as inner and outer models. To develop path models, researchers need to draw on structural theory and measurement theory, which specify the relationships between the elements of a path model.

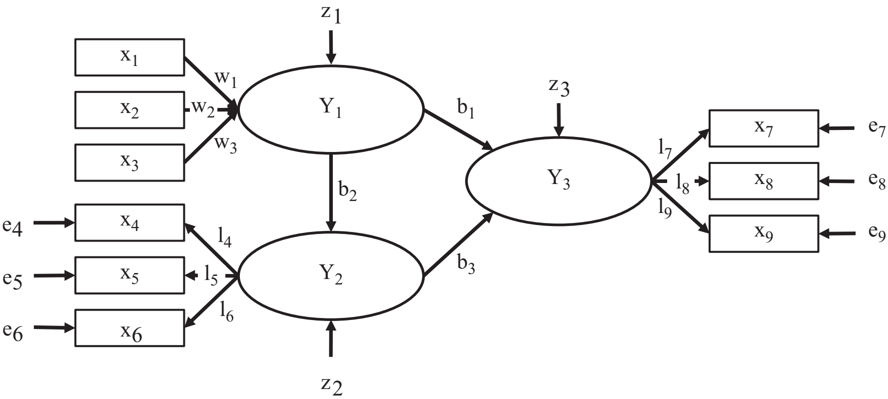

Fig. 1 Path model with latent variables

Structural Theory

Structural theory indicates the latent variables to be considered in the analysis of a certain phenomenon and their relationships. The location and sequence of the constructs are based on theory and the researcher's experience and accumulated knowledge (Falk and Miller 1992). When researchers develop path models, the sequence is typically from left to right. The latent variables on the left side of the path model are independent variables, and any latent variable on the right side is the dependent variable (Fig. 1). However, latent variables may also serve as both an independent and dependent variable in the model (Haenlein and Kaplan 2004).

When a latent variable only serves as an independent variable, it is called an exogenous latent variable (Y_1 in Fig. 1). When a latent variable only serves as a dependent variable (Y_3 in Fig. 1), or as both an independent and a dependent variable (Y_2 in Fig. 1), it is called an endogenous latent variable. Endogenous latent variables always have error terms associated with them. In Fig. 1, the endogenous latent variables Y_2 and Y_3 have one error term each (z_2 and z_3), which reflect the sources of variance not captured by the respective antecedent construct(s) in the structural model. The exogenous latent variable Y_1 also has an error term (z_1) but in PLS-SEM, this error term is constrained to zero because of the way the method treats the (formative) measurement model of this particular construct (Diamantopoulos 2011). Therefore, this error term is typically omitted in the display of a PLS path model. In case an exogenous latent variable draws on a reflective measurement model, there is no error term attached to this particular construct.

The strength of the relationships between latent variables is represented by path coefficients (i.e., b_1, b_2, and b_3), and the coefficients are the result of regressions of each endogenous latent variable on their direct predecessor constructs. For example, b_1 and b_3 result from the regression of Y_3 on Y_1 and Y_2.

Measurement Theory

The measurement theory specifies how to measure latent variables. Researchers can generally choose between two different types of measurement models (Diamantopoulos and Winklhofer 2001; Coltman et al. 2008): reflective measurement models and formative measurement models.

Reflective measurement models have direct relationships from the construct to the indicators and treat the indicators as error-prone manifestations of the underlying construct (Bollen 1989). The following equation formally illustrates the relationship between a latent variable and its observed indicators:

$$x = lY + e \tag{1}$$

where x is the observed indicator variable, Y is the latent variable, the loading l is a regression coefficient quantifying the strength of the relationship between x and Y, and e represents the random measurement error. The latent variables Y_2 and Y_3 in the path model shown in Fig. 1 have reflective measurement models with three indicators each. When using reflective indicators (also called effect indicators), the items should be a representative sample of all items of the construct's conceptual domain (Nunnally and Bernstein 1994). If the items stem from the same domain, they capture the same concept and, hence, should be highly correlated (Edwards and Bagozzi 2000).

In contrast, in a formative measurement model, a linear combination of a set of indicators forms the construct (i.e., the relationship is from the indicators to the construct). Hence, "variation in the indicators precedes variation in the latent variable" (Borsboom et al. 2003, p. 2008). Indicators of formatively measured constructs do not necessarily have to correlate strongly as is the case with reflective indicators. Note that strong indicator correlations can also occur in formative measurement models and do not necessarily imply that the measurement model is reflective in nature (Nitzl and Chin 2017).

When referring to formative measurement models, researchers need to distinguish two types of indicators: causal indicators and composite indicators (Bollen 2011; Bollen and Bauldry 2011). Constructs measured with causal indicators have an error term, which implies that the construct has not been perfectly measured by its indicators (Bollen and Bauldry 2011). More precisely, causal indicators show conceptual unity in that they correspond to the researcher's definition of the concept (Bollen and Diamantopoulos 2017), but researchers will hardly ever be able to identify all indicators relevant for adequately capturing the construct's domain (e.g., Bollen and Lennox 1991). The error term captures all the other "causes" or explanations of the construct that the set of causal indicators do not capture (Diamantopoulos 2006). The existence of a construct error term in causal indicator models suggests that the construct can, in principle, be equivalent to the conceptual variable of interest, provided that the model has perfect fit (e.g., Grace and Bollen 2008). In case the indicators x_1, x_2, and x_3 represent causal indicators, Y_1's error term

z_1 would capture these other "causes" (Fig. 1). A measurement model with causal indicators can formally be described as

$$Y = \sum_{k=1}^{K} w_k \cdot x_k + z, \tag{2}$$

where w_k indicates the contribution of x_k ($k = 1, \ldots, K$) to Y, and z is an error term associated with Y.

Composite indicators constitute the second type of indicators associated with formative measurement models. When using measurement models with composite indicators, researchers assume that the indicators define the construct in full (Sarstedt et al. 2016b). Hence, the error term, which in causal indicator models represents "omitted causes," is set to zero in formative measurement models with composite indicators ($z_1 = 0$ in Fig. 1). Hence, a measurement model with composite indicators takes the following form, where Y is a linear combination of indicators x_k ($k = 1, \ldots, K$), each weighted by an indicator weight w_k (Bollen 2011; McDonald 1996):

$$Y = \sum_{k=1}^{K} w_k \cdot x_k. \tag{3}$$

According to Henseler (2017, p. 180), measurement models with composite indicators "are a prescription of how the ingredients should be arranged to form a new entity," which he refers to as artifacts. That is, composite indicators define the construct's empirical meaning. Henseler (2017) identifies Aaker's (1991) conceptualization of brand equity as a typical conceptual variable with composite indicators (i.e., an artifact) in advertising research, comprising the elements brand awareness, brand associations, brand quality, brand loyalty, and other proprietary assets. The use of artifacts is especially prevalent in the analysis of secondary and archival data, which typically lack a comprehensive substantiation on the grounds of measurement theory (Rigdon 2013a; Houston 2004). For example, a researcher may use secondary data to form an index of a company's communication activities, covering aspects such as online advertising, sponsoring, or product placement (Sarstedt and Mooi 2014). Alternatively, composite indicator models can be thought of as a means to capture the essence of a conceptual variable by means of a limited number of indicators (Dijkstra and Henseler 2011). For example, a researcher may be interested in measuring a company's corporate social responsibility using a set of five (composite) indicators that capture salient features relevant to the particular study. More recent research contends that composite indicators can be used to measure any concept including attitudes, perceptions, and behavioral intentions (Nitzl and Chin 2017). However, composite indicators are not a free ride for careless measurement. Instead, "as with any type of measurement conceptualization, however, researchers need to offer a clear construct definition and specify items that closely match this definition – that is, they must share conceptual unity" (Sarstedt et al. 2016b, p. 4002). Composite indicator models rather view construct measurement as approximation of conceptual variables, acknowledging the practical problems that come with measuring unobservable conceptual variables that populate theoretical models. Whether researchers deem an approximation as sufficient depends on their philosophy of science. From an empirical realist perspective, researchers want to see results from causal and composite indicators converging upon the conceptual variable, which they assume exists independent of observation and transcends data. An empiricist defines a certain concept in terms of data, a function of observed variables, leaving the relationship between conceptual variable and construct untapped (Rigdon et al. 2017).

Path Model Estimation with PLS-SEM

Background

Different from factor-based SEM, PLS-SEM explicitly calculates case values for the latent variables as part of the algorithm. For this purpose, the "unobservable variables are estimated as exact linear combinations of their empirical indicators" (Fornell and Bookstein 1982, p. 441) such that the resulting composites capture most of the variance of the exogenous constructs' indicators that is useful for predicting the endogenous constructs' indicators (e.g., McDonald 1996). PLS-SEM uses these composites to represent the constructs in a PLS path model, considering them as approximations of the conceptual variables under consideration (e.g., Henseler et al. 2016a; Rigdon 2012).

Since PLS-SEM-based model estimation always relies on composites, regardless of the measurement model specification, the method can process reflectively and formatively specified measurement models without identification issues (Hair et al. 2011). Identification of PLS path models only requires that each construct is linked with a significant path to the nomological net of constructs (Henseler et al. 2016a). This characteristic also applies to model settings in which endogenous constructs are specified formatively as PLS-SEM relies on a multistage estimation process, which separates measurement from structural model estimation (Rigdon et al. 2014).

Three aspects are important for understanding the interplay between data, measurement, and model estimation in PLS-SEM. First, PLS-SEM handles all indicators of formative measurement models as composite indicators. Hence, a formatively specified construct in PLS-SEM does not have an error term as is the case with causal indicators in factor-based SEM (Diamantopoulos 2011).

Second, when the data stem from a common factor model population (i.e., the indicator covariances define the data's nature), PLS-SEM's parameter estimates deviate from the prespecified values. This characteristic, also known as PLS-SEM bias, entails that the method overestimates the measurement model parameters and underestimates the structural model parameters (e.g., Chin et al. 2003). The degree of over- and underestimation decreases when both the number of indicators per construct and sample size increase (consistency at large; Hui and Wold 1982). However, some recent work on PLS-SEM urges researchers to avoid the term PLS-SEM bias since the characteristic is based on specific assumptions about the nature of the data that do not necessarily have to hold (e.g., Rigdon 2016). Specifically, when the data stem from a composite model population in which linear combinations of the indicators define the data's nature, PLS-SEM estimates are unbiased and consistent (Sarstedt et al. 2016b). Apart from that, research has shown that the bias produced by PLS-SEM when estimating data from common factor model populations is low in absolute terms (e.g., Reinartz et al. 2009), particularly when compared to the bias that common factor-based SEM produces when estimating data from composite model populations (Sarstedt et al. 2016b). "Clearly, PLS is optimal for estimating composite models while simultaneously allowing approximating common factor models with effect indicators with practically no limitations" (Sarstedt et al. 2016b, p. 4008).

Third, PLS-SEM's use of composites not only has implications for the method's philosophy of measurement but also for its area of application. In PLS-SEM, once the weights are derived, the method always produces a single specific (i.e., determinate) score for each case per composite. Using these scores as input, PLS-SEM applies a series of ordinary least squares regressions, which estimate the model parameters such that they maximize the endogenous constructs' explained variance (i.e., their R^2 values). Evermann and Tate's (2016) simulation studies show that PLS-SEM outperforms factor-based SEM in terms of prediction. In light of their results, the authors conclude that PLS-SEM allows researchers "to work with an explanatory, theory-based model, to aid in theory development, evaluation, and selection." Similarly, Becker et al.'s (2013a) simulation study provides support for PLS-SEM's superior predictive capabilities.

The PLS-SEM Algorithm

Model estimation in PLS-SEM draws on a three-stage approach that belongs to the family of (alternating) least squares algorithms (Mateos-Aparicio 2011). Figure 2 illustrates the PLS-SEM algorithm as presented by Lohmöller (1989). Henseler et al. (2012b) offer a graphical illustration of the SEM algorithm's stages.

The algorithm starts with an initialization stage in which it establishes preliminary latent variable scores. To compute these scores, the algorithm typically uses unit weights (i.e., 1) for all indicators in the measurement models (Hair et al. 2017b).

Stage 1 of the PLS-SEM algorithm iteratively determines the inner weights and latent variable scores by means of a four-step procedure – consistent with the algorithm's original presentation (Lohmöller 1989), inner weights refer to path coefficients, while outer weights and outer loadings refer to indicator weights and loadings in the measurement models. Step #1 uses the initial latent variable scores from the initialization of the algorithm to determine the inner weights b_{ji} between the adjacent latent variables Y_j (i.e., the dependent one) and Y_i (i.e., the independent one) in the structural model. The literature suggests three approaches to determine the inner weights (Lohmöller 1989; Chin 1998; Tenenhaus et al. 2005). In the centroid scheme, the inner weights are set to $+1$ if the covariance between Y_j and Y_i is positive and -1 if this covariance is negative. In case two latent variables are unconnected, the weight is set to

Initialization

Stage 1: Iterative estimation of weights and latent variable scores

Starting at step #4, repeat steps #1 to #4 until convergence is obtained.

#1 Inner weights (here obtained by using the factor weighting scheme)

$$v_{ji} = \begin{cases} \mathrm{cov}(Y_j; Y_i) & \text{if } Y_j \text{ and } Y_i \text{ are adjacent} \\ 0 & \text{otherwise} \end{cases}$$

#2 Inside approximation

$$\tilde{Y}_j := \sum_i b_{ji} Y_i$$

#3 Outer weights; solve for

$$\tilde{Y}_{jn} = \sum_{k_j} \tilde{w}_{k_j} x_{k_j n} + d_{jn} \qquad \text{in a Mode A block}$$

$$x_{kjn} = \tilde{w}_{k_j} \tilde{Y}_{jn} + e_{k_j n} \qquad \text{in a Mode B block}$$

#4 Outside approximation

$$Y_{jn} := \sum_{k_j} \tilde{w}_{k_j} x_{k_j n}$$

Stage 2: Estimation of outer weights, outer loadings, and path coefficients

Stage 3: Estimation of location parameters

Fig. 2 The basic PLS-SEM algorithm (adapted from Lohmöller 1989, p. 29).

0. In the factor weighting scheme, the inner weight corresponds to the covariance between Y_j and Y_i and is set to zero in case the latent variables are unconnected. Finally, the path weighting scheme takes into account the direction of the inner model relationships (Lohmöller 1989). Chin (1998, p. 309) notes that the path weighting scheme "attempts to produce a component that can both ideally be predicted (as a predictand) and at the same time be a good predictor for subsequent dependent variables." As a result, the path weighting scheme leads to slightly higher R^2 values in the endogenous latent variables compared to the other schemes and should therefore be preferred. In most instances, however, the choice of the inner weighting scheme has very little bearing on the results (Noonan and Wold 1982; Lohmöller 1989).

Step #2, the inside approximation, computes proxies for all latent variables $\tilde{Y}_j$ by using the weighted sum of its adjacent latent variables scores Y_i. Then, for all the indicators in the measurement models, Step #3 computes new outer weights indicating the strength of the relationship between each latent variable $\tilde{Y}_j$ and its corresponding indicators. To do so, the PLS-SEM algorithm uses two different estimation modes. When using Mode A (i.e., correlation weights), the bivariate correlation between each indicator and the construct determine the outer weights. In contrast, Mode B (i.e., regression weights) computes indicator weights by regressing each construct on its associated indicators.

By default, estimation of reflectively specified constructs draws on Mode A, whereas PLS-SEM uses Mode B for formatively specified constructs. However, Becker et al. (2013a) show that this reflex-like use of Mode A and Mode B is not optimal under all conditions. For example, when constructs are specified formatively, Mode A estimation yields better out-of-sample prediction when the model estimation draws on more than 100 observations and when the endogenous construct's R^2 value is 0.30 or higher.

Figure 2 shows the formal representation of these two modes, where $x_{k_j n}$ represents the raw data for indicator k ($k = 1,\ldots,K$) of latent variable j ($j = 1,\ldots,J$) and observation n ($n = 1,\ldots,N$), $\tilde{Y}_{jn}$ are the latent variable scores from the inside approximation in Step #2, $\tilde{w}_{k_j}$ are the outer weights from Step #3, d_{jn} is the error term from a bivariate regression, and $e_{k_j n}$ is the error term from a multiple regression. The updated weights from Step #3 (i.e., $\tilde{w}_{k_j}$) and the indicators (i.e., $x_{k_j n}$) are linearly combined to update the latent variables scores (i.e., Y_{jn}) in Step #4 (outside approximation). Note that the PLS-SEM algorithm uses standardized data as input and always standardizes the generated latent variable scores in Step #2 and Step #4. After Step #4, a new iteration starts; the algorithm terminates when the weights obtained from Step #3 change marginally from one iteration to the next (typically 1×10^{-7}), or when the maximum number of iterations is achieved (typically 300; Henseler 2010).

Stages 2 and 3 use the final latent variable scores from Stage 1 as input for a series of ordinary least squares regressions. These regressions produce the final outer loadings, outer weights, and path coefficients as well as related elements such as indirect and total effects, R^2 values of the endogenous latent variables, and the indicator and latent variable correlations (Lohmöller 1989).

Research has proposed several variations of the original PLS-SEM algorithm. Lohmöller's (1989) extended PLS-SEM algorithm, for example, allows assigning more than one latent variable to a block of indicators and imposing orthogonality restrictions among constructs in the structural model. More recently, Becker and Ismail (2016) developed a modified version of the original PLS-SEM algorithm that uses sampling (post-stratification) weights to correct for sampling error. Their weighted PLS-SEM approach considers a weights vector defined by the researcher in order to ensure correspondence between sample and population structure (Sarstedt et al. 2017).

Moreover, Dijkstra and Henseler (2015a, b) introduced the consistent PLS (PLSc) approach, which has also been generalized to nonlinear structural equation models (Dijkstra and Schermelleh-Engel 2014). PLSc is a modified version of Lohmöller's (1989) original PLS-SEM algorithm that produces model estimates that follow a common factor model approach to measurement – see Dijkstra and Henseler (2015b) for an empirical comparison of PLSc and factor-based SEM. Note that PLSc's introduction has also been viewed critically, however, because of its focus on common factor models. As indicated by Hair et al. (2017a, p. 443): "It is unclear why researchers would use these alternative approaches to PLS-SEM when they could easily apply the much more widely recognized and validated CB-SEM [i.e., factor-based SEM] method." PLS-SEM does not produce inconsistent estimates per se but only when used to estimate common factor models, just like factor-based SEM produces inconsistent estimates when used to estimate composite models (Sarstedt et al. 2016b). In addition to the already existing but infrequently used capabilities to estimate unstandardized coefficients (with or without intercept), Dijkstra and Henseler (2015b) contend that PLS-SEM and PLSc provide a basis for the implementation of other, more versatile estimators of structural model relationships, such as two-stage least squares and seemingly unrelated regression. These extensions would facilitate analysis of path models with circular relationships between the latent variables (so called nonrecursive models).

Further methodological advances may facilitate, for example, the consideration of endogeneity in the structural model, which occurs when an endogenous latent variable's error term is correlated with the scores of one or more explanatory variables in a partial regression relationship.

Additional Considerations When Using PLS-SEM

Research has witnessed a considerable debate about situations that favor or hinder the use of PLS-SEM (e.g., Goodhue et al. 2012; Marcoulides et al. 2012; Marcoulides and Saunders 2006; Rigdon 2014a; Henseler et al. 2014). Complementing our above discussion of the method's treatment of latent variables and the consequences for measurement model specification and estimation, in the following sections we introduce further aspects that are relevant when considering using PLS-SEM, and which have been discussed in the literature (e.g., Hair et al. 2013). Where necessary, we refer to differences to factor-based SEM even though such comparisons should not be made indiscriminately (e.g., Marcoulides and Chin 2013; Rigdon 2016; Rigdon et al. 2017; Hair et al. 2017c).

Distributional Assumptions

Many researchers indicate that they prefer the nonparametric PLS-SEM approach because their data's distribution does not meet the requirements of the parametric factor-based SEM approach (e.g., Hair et al. 2012b; Nitzl 2016; do Valle and Assaker 2016). Methods researchers have long noted, however, that this sole justification for PLS-SEM use is inappropriate since maximum likelihood estimation in factor-based SEM is robust against violations of normality (e.g., Chou et al. 1991; Olsson et al. 2000). Furthermore, factor-based SEM literature offers robust procedures for parameter estimation, which work well at smaller sample sizes (Lei and Wu 2012).

Consequently, justifying the use of PLS-SEM solely on the grounds of data distribution is not sufficient (Rigdon 2016). Researchers should rather choose the PLS-SEM method for more profound reasons (see Richter et al. 2016b) such as the goal of their analysis.

Statistical Power

When using PLS-SEM, researchers benefit from the method's greater statistical power compared to factor-based SEM, even when estimating data generated from a common factor model population. Because of its greater statistical power, the PLS-SEM method is more likely to identify an effect as significant when it is indeed significant. However, while several studies have offered evidence for PLS-SEM's increased statistical power (e.g., Reinartz et al. 2009; Goodhue et al. 2012), also vis-á-vis other composite-based approaches to SEM (Hair et al. 2017c), prior research has not examined the origins of this feature.

The characteristic of higher statistical power makes PLS-SEM particularly suitable for exploratory research settings where theory is less developed and the goal is to reveal substantial (i.e., strong) effects (Chin 2010). As Wold (1980, p. 70) notes, "the arrow scheme is usually tentative since the model construction is an evolutionary process. The empirical content of the model is extracted from the data, and the model is improved by interactions through the estimation procedure between the model and the data and the reactions of the researcher."

Model Complexity and Sample Size

PLS-SEM works efficiently with small sample sizes when models are complex (e.g., Fornell and Bookstein 1982; Willaby et al. 2015). Prior reviews of SEM use show that the average number of constructs per model is clearly higher in PLS-SEM (approximately eight constructs; e.g., Kaufmann and Gaeckler 2015; Ringle et al. 2012) compared to factor-based SEM (approximately five constructs; e.g., Shah and Goldstein 2006; Baumgartner and Homburg 1996). Similarly, the number of indicators per construct is typically higher in PLS-SEM compared to factor-based SEM, which is not surprising considering the negative effect of more indicators on χ^2-based fit measures in factor-based SEM. Different from factor-based SEM, the PLS-SEM algorithm does not simultaneously compute all the model relationships (see previous section), but instead uses separate ordinary least squares regressions to estimate the model's partial regression relationships – as implied by its name. As a result, the overall number of model parameters can be extremely high in relation to the sample size as long as each partial regression relationship draws on a sufficient number of observations. Reinartz et al. (2009), Henseler et al. (2014), and Sarstedt et al. (2016b) show that PLS-SEM provides solutions when other methods do not converge, or develop inadmissible solutions, regardless of whether using common factor or composite model data. However, as Hair et al. (2013, p. 2) note, "some researchers abuse this advantage by relying on extremely small samples relative to the underlying population" and that "PLS-SEM has an erroneous reputation for offering special sampling capabilities that no other multivariate analysis tool has" (also see Marcoulides et al. 2009).

PLS-SEM can be applied with smaller samples in many instances when other methods fail, but the legitimacy of such analyses depends on the size and the nature of the population (e.g., in terms of its heterogeneity). No statistical method – including PLS-SEM – can offset a badly designed sample (Sarstedt et al. 2017). To determine the necessary sample size, researchers should run power analyses that take into account the model structure expected effect sizes and the significance level (e.g. Marcoulides and Chin 2013) and provide power tables for a range of path model constellations. Kock and Hadaya (2017) suggest two new methods for determining the minimum sample size in PLS-SEM applications.

While much focus has been devoted to PLS-SEM's small sample size capabilities (e.g., Goodhue et al. 2012), discussions often ignore that the method is also suitable for the analysis of large data quantities such as those produced in Internet research, social media, and social network applications (e.g., Akter et al. 2017). Analyses of social media data typically focus on prediction, rely on complex models with little theoretical substantiation (Stieglitz et al. 2014), and often lack a comprehensive substantiation on the grounds of measurement theory (Rigdon 2013b). PLS-SEM's nonparametric nature, its ability to handle complex models with many (e.g., say eight or considerably more) constructs and indicators along with its high statistical power, makes the method a valuable method for social media analytics and the analysis of other types of large-scale data.

Goodness-of-Fit

PLS-SEM does not have an established goodness-of-fit measure. As a consequence, some researchers conclude that PLS-SEM's use for theory testing and confirmation is limited (e.g., Westland 2015). Recent research has, however, started reexamining goodness-of-fit measures proposed in the early days of PLS-SEM (Lohmöller 1989) or suggesting new ones, thereby broadening the method's applicability (Henseler et al. 2014; Dijkstra and Henseler 2015a). Examples of goodness-of-fit measures suggested in a PLS-SEM context include standardized root mean square residual (SRMR), the root mean square residual covariance (RMS_{theta}), the normed fit index (NFI; also referred to as Bentler-Bonett index), the non-normed fit index (NNFI; also referred to as Tucker-Lewis index), and the exact model fit test (Dijkstra and Henseler 2015a; Lohmöller 1989; Henseler et al. 2014). Note that the goodness-of-fit criterion proposed by Tenenhaus et al. (2005) does not represent a valid measure of model fit (Henseler and Sarstedt 2013). Also, the use of the NFI usually is not recommended as it systematically improves for more complex models (Hu and Bentler 1998).

Several notes of caution are important regarding the use of goodness-of-fit measures in PLS-SEM: First and foremost, literature casts doubt on whether measured fit – as understood in a factor-based SEM context – is a relevant concept for PLS-SEM (Hair et al. 2017b; Rigdon 2012; Lohmöller 1989). Factor-based SEM follows an explanatory modeling perspective in that the algorithm estimates all the model parameters such that the divergence between the empirical covariance matrix and the model-implied covariance matrix is minimized. In contrast, the PLS-SEM algorithm follows a prediction modeling perspective in that the method aims to maximize the amount of explained variance of the endogenous latent variables. Explanation and prediction are two distinct concepts of statistical modeling and estimation. "In explanatory modeling the focus is on minimizing bias to obtain the most accurate representation of the underlying theory. In contrast, predictive modeling seeks to minimize the combination of bias and estimation variance, occasionally sacrificing theoretical accuracy for improved empirical precision" (Shmueli 2010, p. 293). Correspondingly, a grossly misspecified model can yield superior predictions whereas a correctly specified model can perform extremely poor in terms of prediction – see the Appendix in Shmueli (2010) for an illustration. Researchers using PLS-SEM overcome this seeming dichotomy between explanatory and predictive modeling since they expect their model to have high predictive accuracy, while also being grounded in well-developed causal explanations. Gregor (2006, p. 626) refers

Table 1 Reasons for using PLS-SEM

Reasons for using PLS-SEM
The goal is to predict and explain a key target construct and/or to identify its relevant antecedent constructs
The path model is relatively complex as evidenced in many constructs per model (six or more) and indicators per construct (more than four indicators)
The path model includes formatively measured constructs; note that factor-based SEM can also include formative measures but doing so requires conducting certain model adjustments to meet identification requirements; alternatively, formative constructs may be included as simple composites (based on equal weighting of the composite's indicators; Grace and Bollen 2008)
The sample size is limited (e.g., in business-to-business research)
The research is based on secondary or archival data, which lack a comprehensive substantiation on the grounds of measurement theory
The objective is to use latent variable scores in subsequent analyses
The goal is to mimic factor-based SEM results of common factor models by using PLSc (e.g., when the model and/or data do not meet the requirements of factor-based SEM)

to this interplay as explanation and prediction theory, noting that this approach "implies both understanding of underlying causes and prediction, as well as description of theoretical constructs and the relationships among them." This perspective corresponds to Jöreskog and Wold's (1982, p. 270) understanding of PLS-SEM who labeled the method as a "causal-predictive" technique, meaning that when structural theory is strong, path relationships can be interpreted as causal. Hence, validation using goodness-of-fit measures is also relevant in a PLS-SEM context but less so compared to factor-based SEM. Instead, researchers should primarily rely on criteria that assess the model's predictive performance (e.g., Rigdon 2012, 2014b). For example, Shmueli et al. (2016) introduced a new approach to assess PLS-SEM's out-of-sample prediction on the item level, which extends Stone-Geisser's cross-validation for measuring the predictive relevance of PLS path models (Wold 1982).

Table 1 summarizes the rules of thumb researchers should consider when determining whether PLS-SEM is the appropriate statistical tool for their research.

Evaluation of PLS-SEM Results

Procedure

Evaluating PLS-SEM results involves completing two stages, as illustrated in Fig. 3. Stage 1 addresses the examination of reflective measurement models (Stage 1.1), formative measurement models (Stage 1.2), or both. If the evaluation provides support for the measurement quality, the researcher continues with the structural model evaluation in Stage 2 (Hair et al. 2017b). In brief, Stage 1 examines the measurement theory, while Stage 2 covers the structural theory that involves testing the proposed hypotheses and that addresses the relationships among the latent variables.

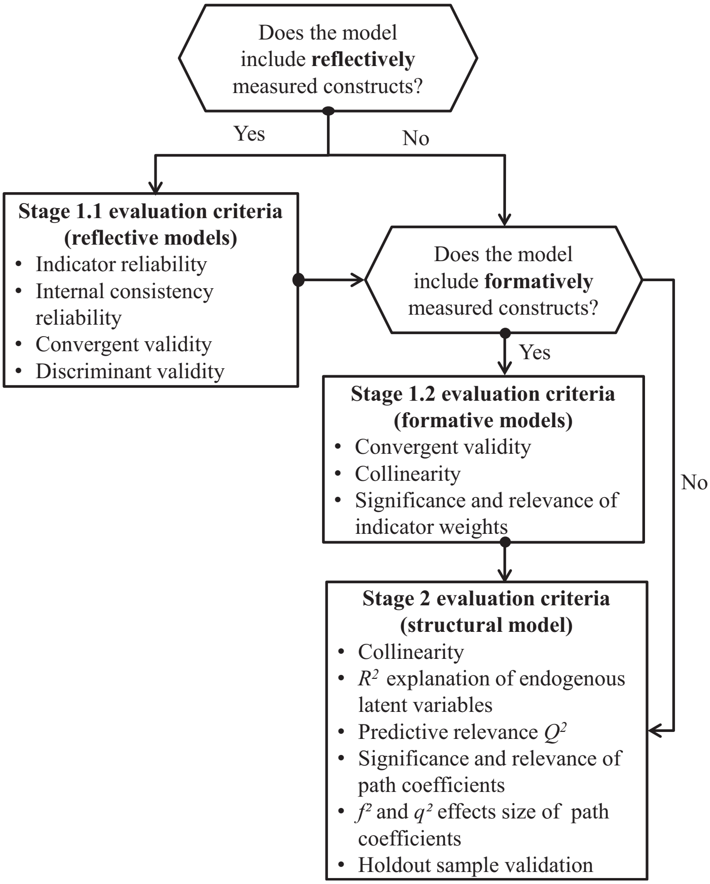

Fig. 3 PLS-SEM model evaluation (Adapted From Sarstedt et al. 2014)

Researchers have developed numerous guidelines for assessing PLS-SEM results (Chin 1998, 2010; Götz et al. 2010; Henseler et al. 2009; Tenenhaus et al. 2005; Roldán and Sánchez-Franco 2012; Hair et al. 2017b). Starting with the measurement model assessment and continuing with the structural model assessment, these guidelines offer rules of thumb for interpreting the adequacy of the results. Note that a rule of thumb is a broadly applicable and easily applied guideline for decision-making that should not be strictly interpreted for every situation. Therefore, the threshold for a rule of thumb may vary.

Stage 1.1: Reflective Measurement Model Assessment

In the case of reflectively specified constructs, a researcher begins Stage 1 by examining the indicator loadings. Loadings above 0.70 indicate that the construct explains more than 50% of the indicator's variance, demonstrating that the indicator exhibits a satisfactory degree of reliability.

The next step involves the assessment of the constructs' internal consistency reliability. When using PLS-SEM, internal consistency reliability is generally evaluated using Jöreskog's (1971) composite reliability ρ_c, which is defined as follows (for standardized data):

$$\rho_c = \frac{\left(\sum_{k=1}^{K} l_k\right)^2}{\left(\sum_{k=1}^{K} l_k\right)^2 + \sum_{k=1}^{K} \mathrm{var}(e_k)}, \tag{4}$$

where l_k symbolizes the standardized outer loading of the indicator variable k of a specific construct measured with K indicators, e_k is the measurement error of indicator variable k, and $var(e_k)$ denotes the variance of the measurement error, which is defined as $1 - l_k^2$.

For the composite reliability criterion, higher values indicate higher levels of reliability. For instance, researchers can consider values between 0.60 and 0.70 as "acceptable in exploratory research," whereas results between 0.70 and 0.95 represent "satisfactory to good" reliability levels (Hair et al. 2017b, p. 112). However, values that are too high (e.g., higher than 0.95) are problematic, as they suggest that the items are almost identical and redundant. The reason may be (almost) the same item questions in a survey or undesirable response patterns such as straight lining (Diamantopoulos et al. 2012).

Cronbach's alpha is another measure of internal consistency reliability that assumes the same thresholds but yields lower values than the composite reliability (ρ_c). This statistic is defined in its standardized form as follows, where K represents the construct's number of indicators and $-r$ the average nonredundant indicator correlation coefficient (i.e., the mean of the lower or upper triangular correlation matrix):

$$\text{Cronbach's } \alpha = \frac{K \cdot \overline{r}}{[1 + (K-1) \cdot \overline{r}]}. \tag{5}$$

Generally, in PLS-SEM Cronbach's alpha is the lower bound, while ρ_c is the upper bound of internal consistency reliability when estimating reflective measurement models with PLS-SEM. Researchers should therefore consider both measures in their internal consistency reliability assessment. Alternatively, they may also consider assessing the reliability coefficient ρ_A (Dijkstra and Henseler 2015b), which usually returns a value between Cronbach's alpha and the composite reliability ρ_c.

The next step in assessing reflective measurement models addresses convergent validity, which is the extent to which a construct converges in its indicators by explaining the items' variance. Convergent validity is assessed by the average variance extracted (AVE) across all items associated with a particular construct and is also referred to as communality. The AVE is calculated as the mean of the squared loadings of each indicator associated with a construct (for standardized data):

$$\mathrm{AVE} = \frac{\left(\sum_{k=1}^{K} l_k^2\right)}{K}, \tag{6}$$

where l_k and K are defined as explained above. An acceptable threshold for the AVE is 0.50 or higher. This level or higher indicates that, on average, the construct explains (more than) 50% of the variance of its items.

Once the reliability and the convergent validity of reflectively measured constructs have been successfully established, the final step is to assess their discriminant validity. This analysis reveals to which extent a construct is empirically distinct from other constructs both in terms of how much it correlates with other constructs and how distinctly the indicators represent only this single construct. Discriminant validity assessment in PLS-SEM involves analyzing Henseler et al.'s (2015) heterotrait-monotrait ratio (HTMT) of correlations. The HTMT criterion is defined as the mean value of the indicator correlations across constructs (i.e., the heterotrait-heteromethod correlations) relative to the (geometric) mean of the average correlations of indicators measuring the same construct. The HTMT of the constructs Y_i and Y_j with, respectively, K_i and K_j indicators is defined as follows:

$$\begin{aligned}
&\mathrm{HTMT}_{ij} \\
&= \underbrace{\frac{1}{K_i K_j} \sum_{g=1}^{K_i} \sum_{h=1}^{K_j} r_{ig,jh}}_{\substack{\text{average} \\ \text{heterotrait}- \\ \text{heteromethod} \\ \text{correlation}}} \\
&\div \underbrace{\left(\frac{2}{K_i(K_i-1)} \cdot \sum_{g=1}^{K_i-1} \sum_{h=g+1}^{K_i} r_{ig,ih} \cdot \frac{2}{K_j(K_j-1)} \cdot \sum_{g=1}^{K_j-1} \sum_{h=g+1}^{K_j} r_{jg,jh} \right)^{\frac{1}{2}}}_{\substack{\text{geometric mean of the average monotrait}-\text{heteromethod} \\ \text{correlation of construct } Y_i \text{ and the average} \\ \text{monotrait}-\text{heteromethod correlation of construct } Y_j}},
\end{aligned} \tag{7}$$

where $r_{ig,jh}$ represents the correlations of the indicators (i.e., within and across the measurement models of latent variables Y_i and Y_j). Figure 4 shows the correlation matrix of the six indicators used in the reflective measurement models of constructs Y_2 and Y_3 from Fig. 1.

Therefore, high HTMT values indicate discriminant validity problems. Based on prior research and their simulation study results, Henseler et al. (2015) suggest a threshold value of 0.90 if the path model includes constructs that are conceptually very similar (e.g., affective satisfaction, cognitive satisfaction, and loyalty); that is, in this situation, an HTMT value exceeding 0.90 suggests a lack of discriminant validity. However, when the constructs in the path model are conceptually more distinct, researchers should consider 0.85 as threshold for HTMT (Henseler et al. 2015). Furthermore, using the bootstrapping procedure, researchers can formally test whether the HTMT value is significantly lower than one (also referred to as $\mathrm{HTMT}_{\mathrm{inference}}$).

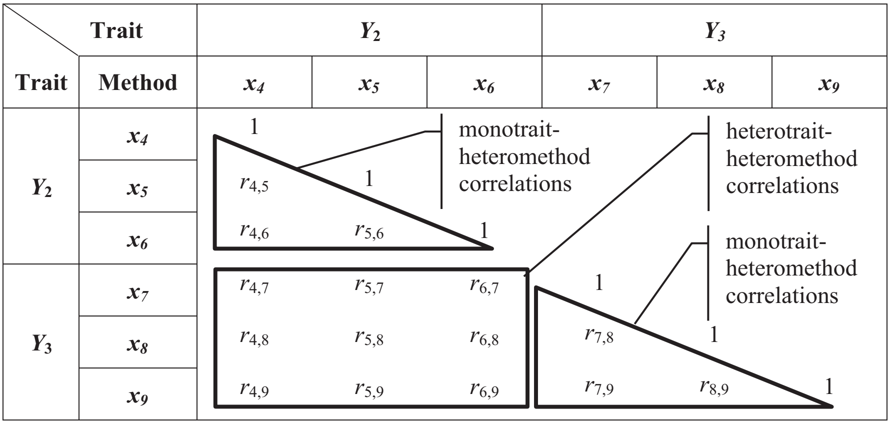

Fig. 4 Correlation matrix example

Stage 1.2: Formative Measurement Model Assessment

Formatively specified constructs are evaluated differently from reflectively measured constructs. Their evaluation involves examination of (1) the convergent validity, (2) indicator collinearity, and (3) statistical significance and relevance of the indicator weights – see Fig. 3.

The convergent validity of formatively measured constructs is determined on the basis of the extent to which the construct correlates with a reflectively measured (or single-item) construct capturing the same concept (also referred to as redundancy analysis; Chin 1998). Accordingly, researchers must plan for the assessment of convergent validity in the research design stage by including a reflectively measured construct, or single-item measure, of the formatively measured construct in the final questionnaire. Note that one should generally try to avoid using single items for construct measurement. Single items exhibit significantly lower levels of predictive validity compared to multi-item scales (Sarstedt et al. 2016a), which can be particularly problematic when using a variance-based analysis technique such as PLS-SEM.

Collinearity assessment involves computing each item's variance inflation factor (VIF) by running a multiple regression of each indicator in the measurement model of the formatively measured construct on all the other items of the same construct. The R^2 values of the k-th regression facilitate the computation of the VIF for the k-th indicator, using the following formula:

$$VIF_k = \frac{1}{1 - R_k^2} \tag{8}$$

Higher R^2 values in the k-th regression imply that the variance of the k-th item can be explained by the other items in the same measurement model, which indicates collinearity issues. Likewise, the higher the VIF, the greater the level of collinearity. As a rule of thumb, VIF values above 5 are indicative of collinearity among the indicators.

The third step in assessing formatively measured constructs is examining the statistical significance and relevance (i.e., the size) of the indicator weights. In contrast to regression analysis, PLS-SEM does not make any distributional assumptions regarding the error terms that would facilitate the immediate testing of the weights' significance based on, for example, the normal distribution. Instead, the researcher must run bootstrapping, a procedure that draws a large number of subsamples (typically 5,000) from the original data with replacement. The model is then estimated for each of the subsamples, yielding a high number of estimates for each model parameter.

Using the subsamples from bootstrapping, the researcher can construct a distribution of the parameter under consideration and compute bootstrap standard errors, which allow for determining the statistical significance of the original indicator weights. More precisely, bootstrap standard errors allow for computing t values (and corresponding p values). When interpreting the results, reviewers and editors should be aware that bootstrapping is a random process, which yields different results every time it is initiated. While the results from one bootstrapping run to the next generally do not differ fundamentally when using a large number of bootstrap samples such as 5,000, bootstrapping-based p values slightly lower than a predefined cutoff level should give rise to concern. In such a case, researchers may have repeatedly applied bootstrapping until a certain parameter has become significant, a practice referred to as p-hacking.

As an alternative, researchers can use the bootstrapping results to construct different types of confidence intervals. Recent research by Aguirre-Urreta and Rönkkö (2017) in the context of PLSc shows that bias-corrected and accelerated (BCa) bootstrap confidence intervals (Efron and Tibshirani 1993) perform very well in terms of coverage (i.e., the proportion of times the population value of the parameter is included in the 1-α% confidence interval in repeated samples) and balance (i.e., how α% of cases fall to the right or to the left of the interval). If a weight's confidence interval includes zero, this provides evidence that the weight is not statistically significant, making the indicator a candidate for removal from the measurement model. However, instead of mechanically deleting the indicator, researchers should first consider its loading, which represents the indicator's absolute contribution to the construct. While an indicator might not have a strong relative contribution (e.g., because of the great number of indicators in the formative measurement model), its absolute contribution can still be substantial (Cenfetelli and Bassellier 2009). Based on these considerations, the following rules of thumb apply (Hair et al. 2017b):

- If the weight is statistically significant, the indicator is retained.
- If the weight is nonsignificant, but the indicator's loading is 0.50 or higher, the indicator is still retained if theory and expert judgment support its inclusion.
- If the weight is nonsignificant and the loading is low (i.e., below 0.50), the indicator should be deleted from the measurement model.

Researchers must be cautious when deleting formative indicators based on statistical outcomes for at least the following two reasons. First, the indicator weight is a function of the number of indicators used to measure a construct: The higher the number of indicators, the lower their average weight. In other words, formative measurement models have an inherent limit to the number of indicators that can retain a statistically significant weight (e.g., Cenfetelli and Bassellier 2009). Second, as formative indicators define the construct's empirical meaning, indicator deletion should be considered with caution and should generally be the exception. Content validity considerations are imperative before deleting formative indicators (e.g., Diamantopoulos and Winklhofer 2001).

Having assessed the formative indicator weights' statistical significance, the final step is to examine each indicator's relevance for shaping the construct (i.e., the relevance). In terms of relevance, indicator weights are standardized to values that are usually between -1 and $+1$, with weights closer to $+1$ (or -1) representing strong positive (or negative) relationships, and weights closer to 0 indicating weak relationships. Note that values below -1 and above $+1$ may technically occur, for instance, when collinearity is at critical levels.

Stage 2: Structural Model Assessment

Provided the measurement model assessment indicates satisfactory quality, the researcher moves to the assessment of the structural model in Stage 2 of the PLS-SEM evaluation process (Fig. 3). After checking for potential collinearity issues among the constructs, this stage primarily focuses on learning about the predictive capabilities of the model, as indicated by the following criteria: coefficient of determination (R^2), cross-validated redundancy (Q^2), and the path coefficients.

Computation of the path coefficients linking the constructs is based on a series of regression analyses. Therefore, the researcher must ascertain that collinearity issues do not bias the regression results. This step is analogous to the formative measurement model assessment, with the difference that the scores of the exogenous latent variables serve as input for the *VIF* assessments. *VIF* values above 5 are indicative of collinearity among the predictor constructs.

The next step involves reviewing the R^2, which indicates the variance explained in each of the endogenous constructs. The R^2 ranges from 0 to 1, with higher levels indicting more predictive accuracy. As a rough rule of thumb, the R^2 values of 0.75, 0.50, and 0.25 can be considered substantial, moderate, and weak (Henseler et al. 2009; Hair et al. 2011). It is important to note, however, that, in some research contexts, R^2 values of 0.10 are considered satisfactory, for example, in the context of predicting stock returns (e.g., Raithel et al. 2012). Against this background, the researcher should always interpret the R^2 in the context of the study at hand by considering R^2 values from related studies.

In addition to evaluating the R^2 values of all endogenous constructs, the change in the R^2 value when a specific predictor construct is omitted from the model can be used to evaluate whether the omitted construct has a substantive impact on the endogenous constructs. This measure is referred to as the f^2 effect size and can be calculated as

$$f^2 = \frac{R^2_{\text{included}} - R^2_{\text{excluded}}}{1 - R^2_{\text{included}}} \tag{9}$$

where R^2_{included} and R^2_{excluded} are the R^2 values of the endogenous latent variable when a specific predictor construct is included in or excluded from the model. Technically, the change in the R^2 values is calculated by estimating a specific partial regression in the structural model twice (i.e., with the same latent variable scores). First, it is estimated with all exogenous latent variables included (yielding R^2_{included}) and, second, with a selected exogenous latent variable excluded (yielding R^2_{excluded}). As a guideline, f^2 values of 0.02, 0.15, and 0.35, respectively, represent small, medium, and large effects (Cohen 1988) of an exogenous latent variable. Effect size values of less than 0.02 indicate that there is no effect.

Another means to assess the model's predictive accuracy is the Q^2 value (Geisser 1974; Stone 1974). The Q^2 value builds on the blindfolding procedure, which omits single points in the data matrix, imputes the omitted elements, and estimates the model parameters. Using these estimates as input, the blindfolding procedure predicts the omitted data points. This process is repeated until every data point has been omitted and the model reestimated. The smaller the difference between the predicted and the original values, the greater the Q^2 criterion and, thus, the model's predictive accuracy and relevance. As a rule of thumb, Q^2 values larger than zero for a particular endogenous construct indicate that the path model's predictive accuracy is acceptable for this particular construct.

To initiate the blindfolding procedure, researchers need to determine the sequence of data points to be omitted in each run. An omission distance of 7, for example, implies that every seventh data point of the endogenous construct's indicators is eliminated in a single blindfolding run. Hair et al. (2017a) suggest using an omission distance between 5 and 10. Furthermore, there are two approaches to calculating the Q^2 value: cross-validated redundancy and cross-validated communality, the former of which is generally recommended to explore the predictive relevance of the PLS path model (Wold 1982). Analogous to the f^2 effect size, researchers can also analyze the q^2 effect size, which indicates the change in the Q^2 value when a specified exogenous construct is omitted from the model. As a relative measure of predictive relevance, q^2 values of 0.02, 0.15, and 0.35 indicate that an exogenous construct has a small, medium, or large predictive relevance, respectively, for a certain endogenous construct.

A downside of these metrics is that they tend to overfit a particular sample if predictive validity is evaluated in the same sample used for estimation (Shmueli 2010). This critique holds particularly for the R^2, which is considered a measure of the model's predictive accuracy in terms of in-sample prediction (Rigdon 2012). Predictive validity assessment, however, requires assessing prediction on the grounds of holdout samples. But the overfitting problem also applies to the Q^2 values, whose computation does not draw on holdout samples, but on single data points (as opposed to entire observations) being omitted and imputed. Hence, the Q^2 values can only be partly considered a measure of out-of-sample prediction, because the sample structure remains largely intact in its computation. As Shmueli et al.

(2016) point out, “fundamental to a proper predictive procedure is the ability to predict measurable information on new cases.” As a remedy, Shmueli et al. (2016) developed the PLSpredict procedure for generating holdout sample-based point predictions in PLS path models on an item or construct level.

Subsequently, the strength and significance of the path coefficients is evaluated regarding the relationships (structural paths) hypothesized between the constructs. Similar to the assessment of formative indicator weights, the significance assessment builds on bootstrapping standard errors as a basis for calculating t and p values of path coefficients, or – as recommended in recent literature – their (bias-corrected and accelerated) confidence intervals (Aguirre-Urreta and Rönkkö 2017). A path coefficient is significant at the 5% probability of error level if zero does not fall into the 95% (bias-corrected and accelerated) confidence interval. For example, a path coefficient of 0.15 with 0.1 and 0.2 as lower and upper bounds of the 95% (bias-corrected and accelerated) confidence interval would be considered significant since zero does not fall into this confidence interval. On the contrary, with a lower bound of −0.05 and an upper bound of 0.35, we would consider this coefficient as not significant.

In terms of relevance, path coefficients are usually between −1 to +1, with coefficients closer to +1 representing strong positive relationships, and those closer to −1 indicating strong negative relationships (note that values below −1 and above +1 may technically occur, for instance, when collinearity is at critical levels). A path coefficient of say 0.5 implies that if the independent construct increases by one standard deviation unit, the dependent construct will increase by 0.5 standard deviation units when keeping all other independent constructs constant. Determining whether the size of the coefficient is meaningful should be decided within the research context. When examining the structural model results, researchers should also interpret total effects. These correspond to the sum of the direct effect and all indirect effects between two constructs in the path model. With regard to the path model shown in Fig. 1, Y_1 has a direct effect (b_1) and an indirect effect ($b_2 \cdot b_3$) via Y_2 on the endogenous construct Y_3. Hence, the total effect of Y_1 on Y_3 is $b_1 + b_2 \cdot b_3$. The examination of total effects between constructs, including all their indirect effects, provides a more comprehensive picture of the structural model relationships (Nitzl et al. 2016).

Research Application

Corporate Reputation Model

The empirical application builds on the corporate reputation model and data that Hair et al. (2017b) use in their book *Primer on Partial Least Squares Structural Equation Modeling (PLS-SEM)*, and that Hair et al. (2018) also employ in their *Advanced Issues in Partial Least Squares Structural Equation Modeling*. The PLS path model creation and estimation draws on the software SmartPLS 3. The software, model files, and datasets used in this market research application can be downloaded at http://www.smartpls.com.

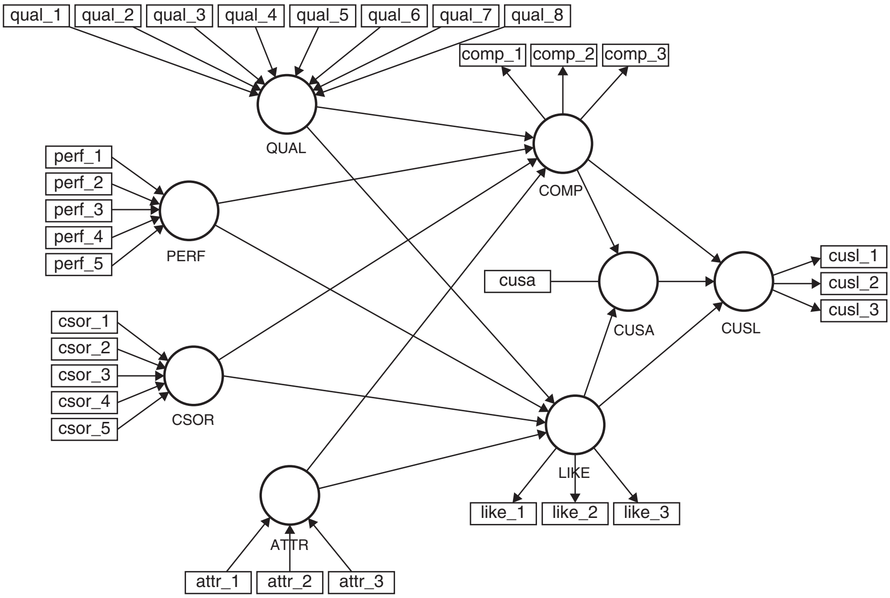

Fig. 5 Corporate reputation model in SmartPLS 3

Figure 5 shows the corporate reputation model as displayed in SmartPLS 3. Originally presented by Eberl (2010), the goal of this model is to explain the effects of corporate reputation on customer satisfaction (*CUSA*) and, ultimately, customer loyalty (*CUSL*). Corporate reputation represents a company's overall evaluation by its stakeholder (Helm et al. 2010), which comprises two dimensions (Schwaiger 2004). The first dimension captures cognitive evaluations of the company, and the construct is the company's competence (*COMP*). The second dimension captures affective judgments, which determine the company's likeability (*LIKE*). This two-dimensional reputation measurement has been validated in different countries and applied in various research studies (e.g., Eberl and Schwaiger 2005; Raithel and Schwaiger 2015; Schloderer et al. 2014). Research has shown that the approach performs favorably (in terms of convergent validity and predictive validity) compared with alternative reputation measures (e.g., Sarstedt et al. 2013). Schwaiger (2004) also identified four exogenous constructs that represent the key sources of the two corporate reputation dimensions: (1) the quality of a company's products and services, as well as the quality of its customer orientation (*QUAL*); (2) the company's economic and managerial performance (*PERF*); (3) the company's corporate social responsibility (*CSOR*); and (4) the company's attractiveness (*ATTR*).

In terms of construct measurement, *COMP*, *LIKE*, and *CUSL* have reflectively specified measurement models with three items. *CUSA* draws – for illustrative purposes – on a single-item measure. The four exogenous latent variables *QUAL*, *PERF*, *CSOR*, and *ATTR* have formative measurement models. Table 2 provides an overview of all items' wordings.

Table 2 Item wordings (Hair et al. 2017b)

Attractiveness (ATTR) – formative	
attr_1	[The company] is successful in attracting high-quality employees
attr_2	I could see myself working at [the company]
attr_3	I like the physical appearance of [the company] (company, buildings, shops, etc.)
Competence (COMP) – reflective	
comp_1	[The company] is a top competitor in its market
comp_2	As far as I know, [the company] is recognized worldwide
comp_3	I believe that [the company] performs at a premium level
Corporate Social Responsibility (CSOR) – formative	
csor_1	[The company] behaves in a socially conscious way
csor_2	[The company] is forthright in giving information to the public
csor_3	[The company] has a fair attitude toward competitors
csor_4	[The company] is concerned about the preservation of the environment
csor_5	[The company] is not only concerned about profits
Customer loyalty (CUSL) – reflective	
cusl_1	I would recommend [company] to friends and relatives.
cusl_2	If I had to choose again, I would choose [company] as my mobile phone services provider
cusl_3	I will remain a customer of [company] in the future
Customer satisfaction (CUSA) – single item	
cusa	If you consider your experiences with [company], how satisfied are you with [company]?
Likeability (LIKE) – reflective	
like_1	[The company] is a company that I can better identify with than other companies
like_2	[The company] is a company that I would regret more not having if it no longer existed than I would other companies
like_3	I regard [the company] as a likeable company
Quality (QUAL) – formative	
qual_1	The products/services offered by [the company] are of high quality
qual_2	[The company] is an innovator, rather than an imitator with respect to [industry]
qual_3	[The company]'s products/services offer good value for money
qual_4	The services [the company] offers are good
qual_5	Customer concerns are held in high regard at [the company]
qual_6	[The company] is a reliable partner for customers
qual_7	[The company] is a trustworthy company
qual_8	I have a lot of respect for [the company]
Performance (PERF) – formative	
perf_1	[The company] is a very well-managed company
perf_2	[The company] is an economically stable company
perf_3	The business risk for [the company] is modest compared to its competitors
perf_4	[The company] has growth potential
perf_5	[The company] has a clear vision about the future of the company

Data

The model estimation draws on data from four German mobile communications network providers. A total of 344 respondents rated the questions related to the items on a 7-point Likert scale, whereby a value of 7 always represents the best possible judgment and a value of 1 the opposite. The most complex partial regression in the PLS path model has eight independent variables (i.e., the formative measurement model of *QUAL*). Hence, based on power statistics as suggested by, this sample size is technically large enough to estimate the PLS path model. Specifically, to detect R^2 values of around 0.25 and assuming a power level of 80% and a significance level of 5%, one would need merely 54 observations. The dataset has only 11 missing values, which are coded with the value −99. The maximum number of missing data points per item is 4 of 334 (1.16%) in *cusl_2*. Since the relative number of missing values is very small, we continue the analysis by using the mean value replacement of missing data option. Box plots diagnostic by means of IBM SPSS Statistics (see chapter 5 in Sarstedt and Mooi 2014) reveals influential observations, but no outliers. Finally, the skewness and excess kurtosis values, as provided by the SmartPLS 3 data view, show that all the indicators are within the −1 and +1 acceptable range. The only slight exception is the *cusl_2* indicator (i.e., skewness of −1.30). However, this degree of non-normality of data in a single indicator is not a critical issue.

Model Estimation

The model estimation uses the basic PLS-SEM algorithm by Lohmöller (1989), the path weighting scheme, a maximum of 300 iterations, a stop criterion of 0.0000001 (or 1×10^{-7}), and equal indicator weights for the initialization (default settings in the SmartPLS 3 software). After running the algorithm, it is important to ascertain that the algorithm converged (i.e., the stop criterion has been reached) and did not reach the maximum number of iterations. However, the PLS-SEM algorithm practically always converges, even in very complex market research applications (Henseler 2010).

Figure 6 shows the PLS-SEM results. The numbers on the path relationships represent the standardized regression coefficients, while the numbers displayed in the circles of the endogenous latent variables represent the R^2 values. An initial assessment shows that *CUSA* has the strongest effect (0.505) on *CUSL*, followed by *LIKE* (0.344) and *COMP* (0.006). These three constructs explain 56.2% (i.e., the R^2 value) of the variance of the endogenous construct *CUSL*. Similarly, we can interpret the relationships between the exogenous latent variables *ATTR*, *CSOR*, *PERF*, and *QUAL*, as well as the two corporate reputation dimensions *COMP* and *LIKE*. But before we address the interpretation of these results, we must assess the constructs' reflective and formative measurement models.

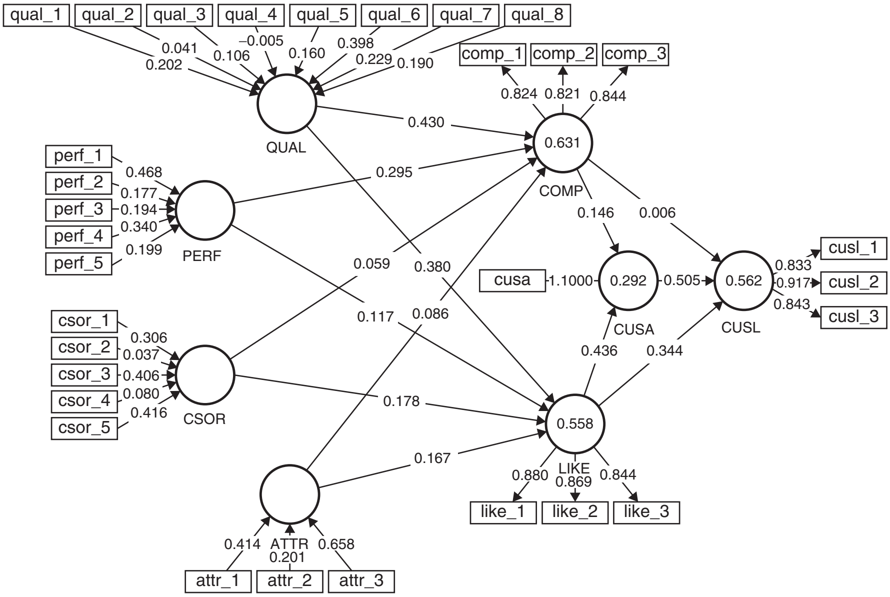

Fig. 6 Corporate reputation model and PLS-SEM results

Results Evaluation

Reflective Measurement Model Assessment

The evaluation of the PLS-SEM results begins with an assessment of the reflective measurement models (i.e., *COMP*, *CUSL*, and *LIKE*). Table 3 shows the results and evaluation criteria outcomes. We find that all three reflective measurement models meet the relevant assessment criteria. More specifically, all the outer loadings are above 0.70, indicating that all indicators exhibit a sufficient level of reliability (i.e., >0.50). Further, all AVE values are above 0.50, providing support for the measures' convergent validity. Composite reliability has values of 0.865 and higher, which is clearly above the expected minimum level of 0.70. Moreover, the Cronbach's alpha values range between 0.776 and 0.831, which is acceptable. Finally, all ρ_A values meet the 0.70 threshold. These results suggest that the construct measures of *COMP*, *CUSL*, and *LIKE* exhibit sufficient levels of internal consistency reliability.

Finally, we assess the discriminant validity by using the HTMT criterion. All the results are clearly below the conservative threshold of 0.85 (Table 4). Next, we run the bootstrapping procedure with 5,000 samples and use the no sign changes option, BCa bootstrap confidence intervals, and two-tailed testing at the 0.05 significance level (which corresponds to a 95% confidence interval). The results show that none of the HTMT confidence intervals includes the value 1, suggesting that all the HTMT values are significantly different from 1. We thus conclude that discriminant validity has been established.

Table 3 PLS-SEM assessment results of reflective measurement models

		Convergent validity			Internal consistency reliability		
		Loadings	Indicator reliability	AVE	Composite reliability ρ_c	Reliability ρ_A	Cronbach's alpha
Latent variable	Indicators	>0.70	>0.50	>0.50	>0.70	>0.70	0.70–0.90
COMP	***comp_1***	0.824	0.679	0.688	0.869	0.786	0.776
	comp_2	0.821	0.674				
	comp_3	0.844	0.712				
CUSL	***cusl_1***	0.833	0.694	0.748	0.899	0.839	0.831
	cusl_2	0.917	0.841				
	cusl_3	0.843	0.711				
LIKE	***like_1***	0.880	0.774	0.747	0.899	0.836	0.831
	like_2	0.869	0.755				
	like_3	0.844	0.712				

Table 4 HTMT values

	COMP	CUSA	CUSL	LIKE
COMP				
CUSA	0.465 [0.364;0.565]			
CUSL	0.532 [0.421;0.638]	0.755 [0.684;0.814]		
LIKE	0.780 [0.690;0.853]	0.577 [0.489;0.661]	0.737 [0.653;0.816]	

Note: The values in the brackets represent the lower and the upper bounds of the 95% confidence interval

The *CUSA* construct is not included in the reflective (and subsequent formative) measurement model assessment, because it is a single-item construct. For this construct indicator data and latent variable scores are identical. Consequently, *CUSA* does not have a measurement model, which can be assessed using the standard evaluation criteria.

Formative Measurement Model Assessment

The formative measurement model assessment initially focuses on the constructs' convergent validity by conducting a redundancy analysis of each construct (i.e., *ATTR*, *CSOR*, *PERF*, and *QUAL*). The redundancy analysis draws on global single items, which summarize the essence each formatively measured construct purports to measure. These single items have been included in the original questionnaire. For example, respondents had to answer the statement, "Please assess to which degree [the company] acts in socially conscious ways," measured on a scale of 0 (not at all) to 10 (extremely). This question can be used as an endogenous single-item construct to validate the formative measurement of corporate social responsibility (*CSOR*). For this purpose, we need to create a new PLS path model for each formatively measured construct that predicts the global measure as an endogenous single-item construct as shown in Fig. 7. All the path relationships between the formatively measured construct and its global single-item measure (i.e., 0.874, 0.857, 0.811, and 0.805) are above the critical value of 0.70. We thus conclude that convergent validity of the formatively measured constructs has been established.

Next, we assess whether critical levels of collinearity substantially affect the formative indicator weight estimates. We find that the highest *VIF* value (i.e., 2.269 of the formative indicator *qual_3*) is clearly below the threshold value of 5, suggesting that collinearity is not at a critical level. Testing the indicator weights' significance draws on the bootstrapping procedure (5,000 samples, no sign changes option, bootstrap confidence intervals (BCa), two-tailed testing at the 0.05 significance level.) and produces the 95% BCa confidence intervals as shown in Table 5. The results show that most of the indicator weights are significant, with the exception of *csor_2*, *csor_4*, *qual_2*, *qual_3*, and *qual_4*, whose indicator weight confidence intervals include the value 0. However, these indicators exhibit statistically significant loadings above the 0.50 threshold, providing support for their absolute contribution to the constructs. In addition, prior research has substantiated the relevance of these indicators for the measurement of the *CSOR* and *QUAL* constructs (Eberl 2010; Schwaiger 2004; Sarstedt et al. 2013). Therefore, we retain the nonsignificant, but relevant, indicators in the formative measurement models.

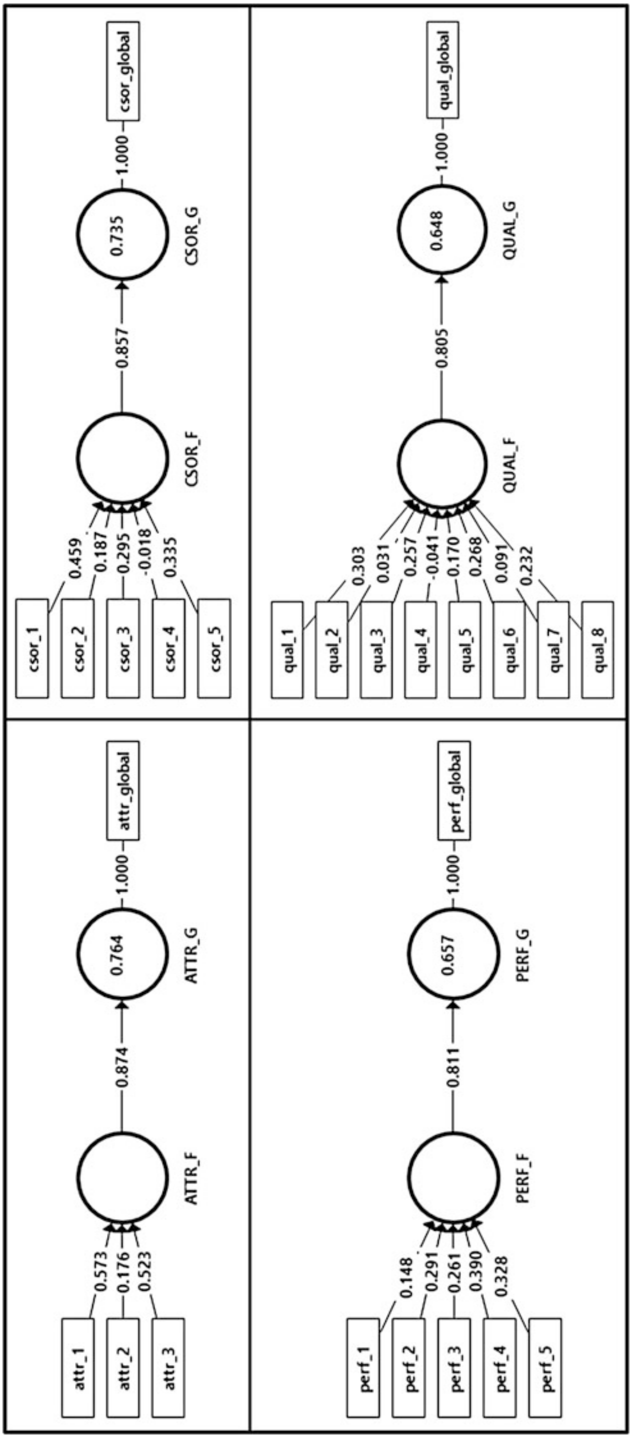

Fig. 7 Redundancy analysis

Table 5 Formative indicator weights and significance testing results

Formative constructs	Formative indicators	Outer weights (Outer loadings)	95% BCa confidence interval	Significant (p <0.05)?
ATTR	***attr_1***	0.414 (0.755)	[0.273, 0.554]	Yes
	attr_2	0.201 (0.506)	[0.073, 0.332]	Yes
	attr_3	0.658 (0.891)	[0.516, 0.761]	Yes
CSOR	***csor_1***	0.306 (0.771)	[0.145, 0.458]	Yes
	csor_2	0.037 (0.571)	[−0.082, 0.167]	*No*
	csor_3	0.406 (0.838)	[0.229, 0.550]	Yes
	csor_4	0.080 (0.617)	[−0.063, 0.219]	*No*
	csor_5	0.416 (0.848)	[0.260, 0.611]	Yes
PERF	***perf_1***	0.468 (0.846)	[0.310, 0.582]	Yes
	perf_2	0.177 (0.690)	[0.044, 0.311]	Yes
	perf_3	0.194 (0.573)	[0.069, 0.298]	Yes
	perf_4	0.340 (0.717)	[0.205, 0.479]	Yes
	perf_5	0.199 (0.638)	[0.070, 0.350]	Yes
QUAL	***qual_1***	0.202 (0.741)	[0.103, 0.332]	Yes
	qual_2	0.041 (0.570)	[−0.074, 0.148]	*No*
	qual_3	0.106 (0.749)	[−0.004, 0.227]	*No*
	qual_4	−0.005 (0.664)	[−0.119, 0.081]	*No*
	qual_5	0.160 (0.787)	[0.045, 0.267]	Yes
	qual_6	0.398 (0.856)	[0.275, 0.501]	Yes
	qual_7	0.229 (0.722)	[0.094, 0.328]	Yes
	qual_8	0.190 (0.627)	[0.060, 0.303]	Yes

The results of the reflective and formative measurement model assessment suggest that all construct measures exhibit satisfactory levels of reliability and validity. We can therefore proceed with the assessment of the structural model.

Structural Model Assessment

Following the structural model assessment procedure (Fig. 3), we first need to check the structural model for collinearity issues by examining the *VIF* values of all sets predictor constructs in the structural model. As all *VIF* values are below the threshold of 5, we can conclude that collinearity is not a critical issue. When analyzing the path coefficient estimates of the structural model (Table 6), we start with the key target construct *CUSL* on the right-hand side of the PLS path model (Fig. 6). The construct *CUSA* (0.505) has the strongest effect on *CUSL*, followed by *LIKE* (0.344), while the effect of *COMP* (0.006) is very close to zero. Bootstrapping results substantiate that the effects of *CUSA* and *LIKE* on *CUSL* are significant, while *COMP* does not have a significant effect at the 5% probability of error level. Moreover, *COMP* has a significant but relatively small effect on *CUSA* (0.146),

Table 6 Path coefficients of the structural model and significance testing results

	Path coefficient	95% BCa confidence interval	Significant (p <0.05)?	f^2 effect size	q^2 effect size
ATTR* → *COMP	0.086	[−0.013, 0.187]	No	0.009	<0.001
ATTR* → *LIKE	0.167	[0.032, 0.273]	Yes	0.030	0.016
COMP* → *CUSA	0.146	[0.033, 0.275]	Yes	0.018	0.006
COMP* → *CUSL	0.006	[−0.111, 0.113]	No	<0.001	−0.002
CSOR* → *COMP	0.059	[−0.036, 0.156]	No	0.005	−0.005
CSOR* → *LIKE	0.178	[0.084, 0.288]	Yes	0.035	0.018
CUSA* → *CUSL	0.505	[0.428, 0.580]	Yes	0.412	0.229
LIKE* → *CUSA	0.436	[0.312, 0.544]	Yes	0.159	0.151
LIKE* → *CUSL	0.344	[0.241, 0.453]	Yes	0.138	0.077
PERF* → *COMP	0.295	[0.172, 0.417]	Yes	0.082	0.039
PERF* → *LIKE	0.117	[−0.012, 0.254]	No	0.011	0.003
QUAL* → *COMP	0.430	[0.295, 0.560]	Yes	0.143	0.052
QUAL* → *LIKE	0.380	[0.278, 0.514]	Yes	0.094	0.050

while the effect of *LIKE* is relatively strong (0.436). We also find that the model explains 56.2% of *CUSL's* variance (i.e., $R^2 = 0.562$), which is relatively high considering that the model only considers the effects of customer satisfaction and the rather abstract concept of corporate reputation as predictors of customer loyalty. With a value of 0.292, R^2 of *CUSA* is clearly lower but still satisfactory, considering that only *LIKE* and *COMP* predict customer satisfaction in this model.

When analyzing the key predictors of *LIKE*, which has a substantial R^2 value of 0.558, we find that *QUAL* has the strongest significant effect (0.380), followed by *CSOR* (0.178), and *ATTR* (0.167); *PERF* (0.117) has the weakest effect on *LIKE*, which is not significant at the 5% level (Table 6). Corporate reputation's cognitive dimension *COMP* also has a substantial R^2 value of 0.631. Analyzing this construct's predictors shows that *QUAL* (0.430) and *PERF* (0.295) have the strongest significant effects. On the contrary, the effects of *ATTR* (0.086) and *CSOR* (0.059) on *COMP* are not significant at the 5% level. Analyzing the exogenous constructs' total effects on *CUSL* shows that *QUAL* has the strongest total effect (0.248), followed by *CSOR* (0.105), *ATTR* (0.101), and *PERF* (0.089). These results suggest that companies should focus on marketing activities that positively influence the customers' perception of the quality of their products and services.

Table 6 also shows the f^2 effect sizes. Relatively high f^2 effect sizes occur for the relationships *CUSA* ➔ *CUSL* (0.412), *LIKE* ➔ *CUSA* (0.159), *QUAL* ➔ *COMP* (0.143), and *LIKE* ➔ *CUSL* (0.138). These relationships also have particularly strong path coefficients of 0.30 and higher. Interestingly, the relationship between *QUAL* and *LIKE* has a strong path coefficient of 0.380 but only a weak f^2 effect size of 0.094. All the other f^2 effect sizes in the structural model are weak and, if below 0.02, negligible.

Finally, we determine the predictive relevance of the PLS path model by carrying out the blindfolding procedure using an omission distance $D = 7$. The resulting cross-validated redundancy Q^2 values are above zero for all endogenous constructs, providing support for the model's predictive accuracy. More precisely, *CUSL* and *COMP* have the highest Q^2 values (0.415), followed by *LIKE* (0.406) and, finally, *CUSA* (0.280). Further analysis of the q^2 shows that the relationships CUSA ➔ CUSL (0.229) and LIKE ➔ CUSA (0.151) have moderate q^2 effect sizes of 0.15 and higher. All other q^2 effect sizes are weak and, if below 0.02, negligible.

Conclusions

Most prior research discussing the benefits and limitations of PLS-SEM or analyzing its performance (e.g., in terms of parameter estimation) has not acknowledged that the method takes on a fundamentally different philosophy of measurement compared to factor-based SEM (e.g., Rigdon et al. 2017). Rather than assuming a common factor model structure, PLS-SEM draws on composite model logic to represent reflective and formative measurement models. The method linearly combines sets (or blocks) of indicators to form composites that represent the conceptual variables and assesses the extent to which these measures are valid and reliable (Tenenhaus et al. 2005). In other words, PLS-SEM is an approximation method that inherently recognizes that constructs and conceptual variables are not identical (Rigdon et al. 2017). For several reasons, factor indeterminacy being the most prominent one, this view of measurement is more reasonable than the common factor model logic assumed by factor-based SEM, which equates constructs and conceptual variables. As Rigdon (2016, p. 19) notes, "common factor proxies cannot be assumed to carry greater significance than composite proxies in regard to the existence or nature of conceptual variables."

PLS-SEM offers a good approximation of common factor models in situations where factor-based SEM cannot deliver results due to its methodological limitations in terms of model complexity, sample size requirements, or inclusion of composite variables in the model (Reinartz et al. 2009; Sarstedt et al. 2016b; Willaby et al. 2015). Dijkstra and Henseler's (2015b) PLSc allows researchers mimicking factor-based SEM results while benefiting from the original PLS-SEM method's flexibility in terms of model specification. However, such an analysis rests on the implicit assumption that factor-based SEM is the correct estimator that delivers the true results as a benchmark for SEM.

While standard PLS-SEM analyses provide important insights into the strength and significance of the hypothesized model relationships, more advanced modeling and estimating techniques shed further light on the nature of the proposed relationships. Research has brought forward a variety of complementary analysis techniques and procedures, which extend the methodological toolbox of researchers working with the method. Examples of these methods include the confirmatory tetrad analysis (CTA-PLS), which enables researchers to statistically test if the measurement model operationalization should rather build on effect or composite indicators (Gudergan et al. 2008), and latent class techniques, which allow assessing if unobserved heterogeneity affects the model estimates. Prominent examples of PLS-SEM-based latent class techniques include finite mixture partial least squares (Hahn et al. 2002; Sarstedt et al. 2011a), PLS genetic algorithm segmentation (Ringle et al. 2013, 2014), prediction-oriented segmentation (Becker et al. 2013b), and iterative reweighted regressions (Schlittgen et al. 2016). Further methods to account for heterogeneity in the structural model include the analysis of moderating effects (Henseler and Chin 2010), nonlinear effects (Henseler et al. 2012a), and the multigroup analysis (Sarstedt et al. 2011b), including testing for measurement invariance (Henseler et al. 2016b). A further complementary method, the importance-performance map analysis (IPMA), facilitates richer outcome discussions in that it extends the analysis of total effects in the model by adding a second results dimension to the analysis which incorporates the average values of the latent variables (Ringle and Sarstedt 2016). Hair et al. (2018) provide a more detailed overview and introduction to these complementary techniques for more advanced PLS-SEM analyses.

Cross-References

► Design and Process of Survey Research
► Factor Analysis
► Regression Analysis
► Structural Equation Modeling

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