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Emerging opportunities for information systems researchers to expand their PLS-SEM analytical toolbox

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Abstract

Purpose – Rigorous applications of analytical tools in information systems (IS) research are important for developing new knowledge and innovations in the field. Emerging tools provide building blocks for future inquiry, practice and innovation. This article summarizes the findings of an analysis of the adoption and reporting of partial least squares structural equation modeling (PLS-SEM) analytical tools by Industrial Management & Data Systems authors in the most recent five-year period.

Design/methodology/approach – Selected emerging advanced PLS-SEM analytical tools that have experienced limited adoption are highlighted to broaden awareness of their value to IS researchers.

Findings – PLS-SEM analytical tools that facilitate understanding increasingly complex theoretical models and deliver improved prediction assessment are now available. IS researchers should explore the opportunities to apply these new tools to more fully describe the contributions of their research.

Research limitations/implications – Findings demonstrate the increasing acceptance of PLS-SEM as a useful alternative research methodology within IS. PLS-SEM is a preferred structural equation modeling (SEM) method in many research settings and will become even more widely applied when IS researchers are aware of and apply the new analytical tools.

Practical implications – Emerging PLS-SEM methodological developments will help IS researchers examine new theoretical concepts and relationships and publish their work. Researchers are encouraged to engage in more complete analyses by applying the applicable emerging tools.

Originality/value – Applications of PLS-SEM for prediction, theory testing and confirmation have increased in recent years. Information system scholars should continue to exercise sound practice by applying these new analytical tools where applicable. Recommended guidelines following Hair *et al.* (2019; 2022) are included.

Keywords PLS-SEM, Information systems, Emerging analytical tools

Paper type General review

Introduction

Information system scholars are constantly trying to explain and predict relationships between technology, people and context. One of the most commonly used analytical methods is structural equation modeling (SEM), specifically partial least squares structural equation modeling (PLS-SEM), a method developed more than 50 years ago (Wold, 1966). Despite the

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long tradition of PLS-SEM in the field of information systems (IS), it is important for researchers in the field to become familiar with new methodological developments to ensure improved and more robust empirical research.

The PLS-SEM method can solve problems and explore path models involving complex relationships between multi-item composites (Gefen *et al.*, 2011). In addition, PLS-SEM is increasingly used not only to empirically evaluate theories but also to demonstrate methodological improvements (Ciavolino *et al.*, 2022). Two types of research on PLS-SEM have emerged: (1) the ongoing discussions about the appropriate use of the method and (2) numerous methodological developments in recent years. The limited adoption of recently emerging advanced PLS-SEM analytical tools, as reported in Sabol *et al.* (2023), is highlighted to expand awareness of the value of these new analytical tools for IS researchers and also to encourage IS researchers to adopt new methods to increase the likelihood of improved solutions and to advance our knowledge base (Bergh *et al.*, 2022).

The focus of this paper is to help IS researchers become aware of recent developments in PLS-SEM and how they can be applied, which will lead to a better understanding of research questions and facilitate new research in the IS field (Colquitt and Zapata-Phelan, 2007). To this end, we summarize selected recent PLS-SEM analytical capabilities and features identified in a recent assessment of PLS-SEM methods used by IS researchers (Sabol *et al.*, 2023). These developments include PLS-SEM extensions for prediction, theory testing and confirmation. We also introduce IS researchers to an emerging alternative composite (component)-based SEM method, generalized structured component analysis (GSCA; Hwang and Takane, 2004, 2014).

Essential PLS-SEM analytical tools and metrics

While numerous additional extensions for PLS-SEM applications have been developed in recent years, several others should be considered essential for the future as they facilitate the increasingly rigorous requirements for exploring and evaluating the full potential of PLS-SEM and IS research topics. The relevant essential PLS-SEM extensions and evaluation tools, as identified in our recent review (Sabol *et al.*, 2023), include (1) out-of-sample prediction, (2) mediation, (3) moderation, (4) conditional mediation analysis, and (5) model comparison and evaluation.

Out-of-sample prediction. The method of PLS is a causal-predictive approach to SEM. While researchers using PLS-SEM increasingly focus on the predictive nature of their analyses, model evaluation assessment in the past has relied exclusively on metrics that assess the structural model explanatory power, such as R^2 and blindfolding, now identified as in-sample prediction (Danks and Ray, 2018).

Systematic reviews of analytical methodologies have called for improved robustness measures (Becker *et al.*, 2023) to more accurately assess the predictive capabilities of SEM models. For example, until recently researchers have very seldom included holdout sample prediction procedures in their analysis to confirm the predictive performance of their models (Hair *et al.*, 2022; Sabol *et al.*, 2023). Easy-to-apply and interpret software options are, however, now available to calculate and report these metrics.

Recent research by Shmueli *et al.* (2019) proposed a holdout sample-based procedure that generates case-level predictions on both an item and construct level, referred to as PLSpredict, and executes out-of-sample prediction. Hair and Sarstedt (2021) define and clarify how out-of-sample prediction facilitates both explanation and prediction. Manley *et al.* (2021) and Shmueli *et al.* (2019) both provide an overview of an empirical application of the metric and provide guidelines for interpreting PLSpredict results.

To apply PLSpredict, first identify the ultimate target outcome construct(s). Next, evaluate the PLSpredict Q^2 statistic which compares the prediction errors for the path model to the simple mean predictions. If the Q^2 prediction is positive, the prediction error of the PLS-SEM model provides better predictive performance than simply using the indicator mean values. A second prediction metric utilizes a linear regression model (LM) calculated using sum scores as a benchmark. Model predictions for the LM and PLS-SEM models are compared using the root mean squared error (RMSE) statistic for each model. In this comparison, if the RMSE errors of the PLS prediction are smaller than the benchmark LM errors, the predictive power of the PLS-SEM model is superior (see Shmueli *et al.*, 2019; Manley *et al.*, 2021 for additional details).

A recent contribution by Sharma *et al.* (2023) extended the cross-validated predictive ability test (CVPAT) developed by Liengaard *et al.* (2021). This updated method evaluates the predictive capability of a theoretical model, both overall and for each dependent composite (construct). To do so, the predictive performance of a proposed model is compared to naïve benchmarks such as sum scores and linear model predictions, and the results confirm whether the model meets the minimum requirements for predictive accuracy.

Mediation. Mediation models describe how, or by what means, an independent variable (composite) affects a dependent variable through one or more potential intervening variables or mediators (Zhao *et al.*, 2010; Cheah *et al.*, 2021). Nitzl *et al.* (2016) indicate that the primary objective of researchers in mediation analysis is causal explanation, while Rucker and Preacher (2019) believe the central issue in mediation is whether an indirect path exists. Finally, Rasoolimanesh *et al.* (2021) distinguish between implicit and explicit procedures to analyze mediation and conclude the explicit procedures most appropriate for PLS-SEM.

When mediation analysis is conducted, several recommendations should be considered. When assessing mediation effects, avoid applying the Hayes' PROCESS routine that is based on PLS-SEM latent variable sum scores. Table 1 provides a comparison and contrast between PLS-SEM and PROCESS. Moreover, Hair *et al.* (2024a) recently provided additional evidence against using sum scores versus applying differentiated weights produced by PLS-SEM or other composite-based SEM methods (e.g. GSCA). For example, applying sum scores often leads to inaccuracies in estimating parameters in structural and measurement models as well as lower out-of-sample predictive accuracy. In addition, the traditional Baron and Kenny approach should now be avoided since it requires assessing the direct, indirect and total effects separately in a multiple regression model using sum scores and is thereby likely to distort the results (Nitzl *et al.*, 2016).

Researchers should always include and interpret the direct effect between the independent and the dependent variables (Nitzl *et al.*, 2016). Unfortunately, quite a few studies do not evaluate the direct effect of the model (Rasoolimanesh *et al.*, 2021). This approach is a problem

Table 1.
Arguments why PLS-SEM is more adequate than PROCESS to test mediation

PLS-SEM	PROCESS
Uses raw data to calculate weighted latent variable construct scores	Uses raw data to calculate unweighted latent variable sum scores
Uses direct estimations from the PLS-SEM algorithm obtained from the original dataset	Includes measurement error and assumes the indicators are equally weighted (Sarstedt *et al.*, 2020; Hair *et al.*, 2022)
Includes bootstrapping based on individually weighted constructs This approach provides more reliable and valid results	Does not include a bootstrapping process based on individually weighted composites (Sarstedt *et al.*, 2020)
Includes common and specific variance in obtaining results and does not require additional ad hoc regressions	Uses total variance and requires additional ad hoc regressions

Source(s): Authors' own creation/work since not considering the direct effect can overlook a notable bias in estimating the indirect effect, which may be inflated due to not controlling for the impact of the direct effect of the independent variable(s) on the dependent. When the direct effect is not considered, the probability of encountering a Type I error may increase (Yzerbyt *et al.*, 2018). Some researchers recommend including effect size measures in mediation analysis to complement p-values evaluation and better assess the magnitude of effects (Lachowicz *et al.*, 2018; Ogbeibu and Gaskin, 2023; Rucker and Preacher, 2019). The benefits of using effect sizes operate as a complementary role in hypothesis testing. We recommend examining the effect size $\boldsymbol{\nu}$**,** as proposed by Lachowicz *et al.* (2018). Gaskin *et al.* (2023) have recently proposed the following $\boldsymbol{\nu}$ effect size thresholds: 0.01 (small), 0.04 (medium) and 0.09 (large). In sum, PLS-SEM is, therefore, the method of choice for evaluating mediation (see Shiau *et al.*, 2020, for a good illustration).

Further considerations regarding PLS-SEM and mediation are noted by Danks (2021) and Ogbeibu and Gaskin (2023) who have recently proposed a mediation analysis assessment by adopting a prediction approach. With this aim in mind, Danks (2021) proposed a new metric that quantifies the predictive contribution of the mediator (PCM), which provides evidence of the predictive validity of mediated relationships. Finally, Sarstedt and Moisescu (2024) view mediation analysis as a form of model comparison. As a first step, they propose the use of the Bayesian Information Criterion (BIC) (Sharma *et al.*, 2019, 2021) and Akaike weights (Danks *et al.*, 2020) to support the inclusion of mediators in a model. They then recommend, as a second step, using a combination of Akaike weights and bootstrapping to measure the level of uncertainty in the model effects caused by the mediator. This approach adds a new perspective to evaluating mediation models as it helps assess the potential generalizability of the research results (Rigdon *et al.*, 2023).

In conclusion, PLS-SEM is an excellent tool for streamlining mediation and assessing the direct, indirect and total effects of mediation. Moreover, at the same time, the method removes measurement errors while other methods do not (Sarstedt *et al.*, 2020; Hair *et al.*, 2022).

Moderation. Moderating effects emerge from variables whose variation influences the strength (increasing or decreasing) or direction (positive or negative) of a relationship between an exogenous and an endogenous variable (Hair *et al.*, 2022). Moderators can be either categorical (e.g. part-time vs full-time workers or adopters vs non-adopters) or continuous (e.g. income, age and interval or ratio measured constructs). In addition, either single-item variables or multi-item composites are suitable as moderators. The choice of moderators should be based on a sound theoretical foundation from a broad literature review or qualitative research and considering a set of contingencies described by Memon *et al.* (2019). Note, too, that quite small moderating effects are often statistically significant.

Moderation with categorical variables is generally associated with multigroup analysis (MGA). This type of analysis is a good illustration of the heterogeneity many datasets contain (Sarstedt *et al.*, 2011). Before carrying out an MGA, measurement invariance should be tested using the Measurement Invariance for Composites procedure (Henseler *et al.*, 2016; Hair *et al.*, 2022). Recent guidelines for carrying out MGA are available in Cheah *et al.* (2020) and Hair *et al.* (2022). These guidelines include a new permutation-based test that enables the entire model to be compared between two or more groups (Klesel *et al.*, 2022; Cheah *et al.*, 2023). In addition, Liengaard (2024) proposed a new invariance testing method for reflective constructs which expands the possibilities of measurement invariance testing to longitudinal studies.

Moderator analysis with a continuous variable is also possible with PLS-SEM (Hair *et al.*, 2022). To do so, researchers execute the analysis using interaction effects. Since the results of the continuous variable approach to moderation are usually equivalent to or better than those of the multigroup comparison approach, we recommend using the continuous variable approach. The only exception to this guideline is when the moderating variable is categorical, and the researcher wants to develop a quick overview of moderating effects; in such cases, the

MGA approach should be applied. In addition, a recent proposal by Becker *et al.* (2023) outlines a method for specifying and evaluating categorical moderators using the interaction approach.

The recommended approach for continuous variable moderation in PLS-SEM is the two-stage approach. The two-stage approach is used whenever any of the variables that create the interaction term are composites (most commonly in PLS) (Becker *et al.*, 2018). To analyze moderation effects, the direct coefficients of the exogenous (independent) variable and of the moderating variable (coefficients *b* and *c*), as well as the ratio of the moderating term (*d*), should be examined. The moderation hypothesis is supported if the parameter *d* is significant via bootstrapping. To determine the strength (significance) of the moderating effects, the f^2 ratio (effect size) is used. A simple slope analysis of the results is useful for interpreting and showing the moderation results. This graphical illustration is available in most software packages (Hair *et al.*, 2022).

Conditional mediation (CoMe). Including mediation and moderation analyses in the same study has previously been challenging for IS research. The combination of these two theoretical options has typically been labeled as moderated mediation or mediated moderation. The most recent PLS-SEM methodological developments have focused on moderated mediation. The literature has referred to this type of analysis as conditional mediating effect analysis (CoMe) (Edwards and Lambert, 2007; Hayes, 2018; Preacher *et al.*, 2007).

This analysis approach integrates mediation and moderation analyses to examine and test hypotheses about how mediated relationships vary as a function of context, boundaries or individual differences (Cheah *et al.*, 2021). CoMe analysis can be a crucial element of empirical studies that seek to advance theory in IS. Unfortunately, thus far, applications of CoMe analysis are limited, including the IS area. This lack of applications is particularly true for the PLS-SEM method. The conceptual fundamentals and guidelines for CoMe analysis within a PLS-SEM context are summarized in Cheah *et al.* (2021). The article also includes an illustrative application of CoMe analysis including detailed step-by-step procedures summarizing how to execute, report and interpret CoMe analysis with PLS-SEM.

Mediation and conditional process analyses have become popular approaches for examining the mechanisms by which effects operate in structural models and the factors that influence them. As noted earlier, when estimating mediation models, researchers often extend their SEM analyses to include the PROCESS macro. This duality is surprising, considering research has long acknowledged the limitations of regression analyses when estimating models with latent variables (Sarstedt *et al.*, 2020). Much of the confusion regarding the efficacy of PLS-SEM for mediation analyses results from a previous singular focus on factor-based SEM methods. Indeed, the tandem application of CB-SEM (covariace-based structural equation modelling) and PROCESS for mediation analysis is not necessary (Sarstedt *et al.*, 2020). Specifically, composite-based SEM methods overcome the limitations of both regression and factor-based SEM analyses when estimating even highly complex mediation models. Moreover, composite-based SEM methods such as PLS-SEM, including the CoMe approach, are the preferred and superior approach when estimating mediation and conditional process models, and reporting the PROCESS approach with PLS-SEM creates confusion (Sarstedt *et al.*, 2020).

Theoretical model comparisons. Information system researchers as well as social sciences scholars in general often develop forward-looking theories and methodologies. As noted above, predictive modeling is based on theoretical models proposed to predict unseen or new data (data not included in the analytical process to obtain a solution). In addition, the models complement and extend the retrospective nature of causal-explanatory modeling currently dominating the field of predictive modeling. The PLS path modeling is an excellent tool for building and exploring theories that provide insights for both explanation and prediction. A recent enhancement of PLS-SEM is the addition of a statistical test to assess whether a proposed or alternative theoretical model offers significantly better out-of-sample predictive power than a benchmark or established model. This out-of-sample prediction assessment tool for comparison is essential for theory development and validation and for selecting a model on which to base managerial and policy decisions.

Sharma *et al.* (2019) initially proposed model selection criteria drawn from information theory. When these criteria are applied, researchers can compare and evaluate multiple models simultaneously and choose a parsimonious yet well-fitting model. To do so, the BIC and the Geweke-Meese (GM) criteria are applied based on their high model selection accuracy and user-friendliness. Sharma *et al.* (2021) later analyzed the performance of these model selection criteria to select the best predictive model from among a group of competing models. The approach explored whether and when the in-sample measures belonging to the model selection criteria can substitute for out-of-sample criteria that require a holdout sample. Their findings demonstrated the BIC and the GM criteria were functional substitutes for out-of-sample criteria when the overall sample was small. Both criteria could also be used for prediction-oriented model selection purposes.

Nevertheless, selecting one model over others based on model selection criteria can sometimes lead to a false sense of confidence due to the slight changes in criterion values. Danks *et al.* (2020) proposed Akaike weights to overcome this limitation. Their approach confirmed that Akaike weights derived from BIC and GM are well suited for separating incorrectly specified models from correctly specified models. Furthermore, Akaike weights based on AIC facilitate the development of model-averaged predictions under conditions of model selection uncertainty. For example, Rigdon *et al.* (2023) proposed an approach to quantify the uncertainty of competitive models based on Akaike weights and bootstrapping. The uncertainty perspective provides a new dimension to assess such models, indicating evidence for or against their generalizability. The proposed approach has been adapted by Sarstedt and Moisescu (2024) to the PLS-SEM domain so that it can be applied to mediation analysis as a model selection approach.

When out-of-sample prediction metrics are relevant to the research objectives, criteria based on PLSpredict are useful. Specifically, the RMSE and mean absolute deviation (MAD) metrics, also referred to as mean absolute error (MAE), are applied for this type of prediction-oriented assessment and model comparisons. In addition, when evaluating PLSpredict error results, researchers should focus on the prediction error of the key (ultimate) endogenous construct(s) of a theoretical model. To do so, you first review the Q^2_{predict} statistic (>0.0) and also the distribution of the RMSE error statistic. If the prediction distribution is relatively symmetrical, the RMSE error is evaluated. However, if the distribution is highly non-symmetric, the MAE prediction statistic should be used. The process involves comparing the RMSE (or MAE) values with the LM naïve benchmark, which are the errors produced by an LM to generate predictions (Danks and Ray, 2018). Finally, another powerful tool available to researchers when comparing competitive models from a predictive perspective is the CVPAT (Liengaard *et al.*, 2021; Sharma *et al.*, 2023), which will be discussed in more detail in the next section.

Emerging analytical tools and metrics

Numerous analytical enhancements are emerging that expand opportunities for additional PLS-SEM analyses. These opportunities will lead to an improved understanding of measurement and path model relationships, exploration of more complex theories and ultimately theoretical model confirmation. The new options also provide additional reasons to apply PLS-SEM, not available with other methods, to explain SEM relationships. The relevant emerging PLS-SEM extensions and evaluation tools include (1) CVPAT; (2) higher-order constructs (HOCs); and (3) necessary condition analysis (NCA). In addition, the emerging methodological composite-based alternative to PLS-SEM, GSCA, is explained and compared to SEM. Other emerging PLS-SEM advanced options not included in this article, which we suggest you consider if appropriate for your research, are latent class analysis (Sarstedt *et al.*, 2022a, b, c; Becker *et al.*, 2013) and discrete choice modeling (Hair *et al.*, 2019).

Cross-validated predictive ability test (CVPAT). Liengaard *et al.* (2021) developed the CVPAT. This test executes an inferential test to determine whether the predictive capabilities of alternative models are superior to those of the initially proposed model. Unlike information-theoretic model selection criteria, whose objective is to balance model fit and predictive power in the context of PLS-SEM, CVPAT focuses exclusively on the predictive power of a model (Hair *et al.*, 2020). More recently, Sharma *et al.* (2023) proposed several extensions to broaden the capabilities of CVPAT. These new features facilitate (1) comparison of a single proposed model with a naïve benchmark to ensure it meets minimum predictive accuracy, and (2) comparison of two models by focusing on the prediction accuracy of individual constructs rather than all constructs simultaneously.

Higher-order constructs (HOCs). HOCs enable researchers to model constructs on a higher-level of abstraction, with lower-order dimensions presented as subdimensions (lower-order constructs) (LOCs) representing more concrete measures/concepts. The conceptualizations of these complex constructs, also referred to as hierarchical component models (HCMs), are a type of data structure that represents hierarchical relationships within the constructs. HCMs have become an increasingly visible trend in applications of PLS-SEM (Sabol *et al.*, 2023). Unfortunately, researchers too often confuse the validation of HOCs when assessing their reliability and validity. Sarstedt *et al.* (2019) describe the logic and justifications for HOCs as well as how to evaluate and validate the results when using PLS-SEM to model HOCs and LOCs. Cataldo *et al.* (2024) update and extend methodological issues encountered when modeling HOCs. These two papers enable IS researchers to update and improve the design and assessment of HOCs in their research.

There are three well-known approaches for specifying HOCs: (1) the extended repeated indicator approach, (2) the embedded two-stage approach and (3) the disjoint two-stage approach (Sarstedt *et al.*, 2019; Schuberth *et al.*, 2020). Although the three approaches are similar when estimating different parameters, Becker *et al.* (2023) recommend the two-stage approaches because they address issues that can arise in alternative model designs and are relatively simple to include when using contemporary PLS-SEM software. All three of these approaches use composites as the constructs in both the lower-order dimension (LOC) and the HOC.

The increasing application of these hierarchical models is based on their usefulness in representing both complex concepts and relationships as well as several other advantages, particularly reducing multicollinearity issues in structural model relationships. By reducing the number of relationships in the structural model, PLS-SEM structural relationships become easier to understand and are more parsimonious (Becker *et al.*, 2012; Sarstedt *et al.*, 2019). Moreover, in situations characterized by collinearity among the constructs, a HOC reduces this issue and may solve discriminant validity problems (Ringle *et al.*, 2022).

Four types of HOCs are suggested, as shown in Figure 1. The type of HOC specification varies but the two most often applied types of HOCs are Type I: Reflective-Reflective and Type II: Reflective-Formative. The other two types appear in publications much less often. HOCs are almost always modeled with two levels, but, theoretically, HOCs can be extended to additional layers representing third-, fourth- and fifth-order models. An example of a third-order HOC can be found in Patel *et al.* (2016).

There are two fundamental considerations in setting up HOCs. First, their formulation must be based on theoretical considerations or qualitative research. For example, employee work environment typically is formulated as a single layer consisting of independent variables (constructs) such as supervision, compensation, teamwork and other considerations like

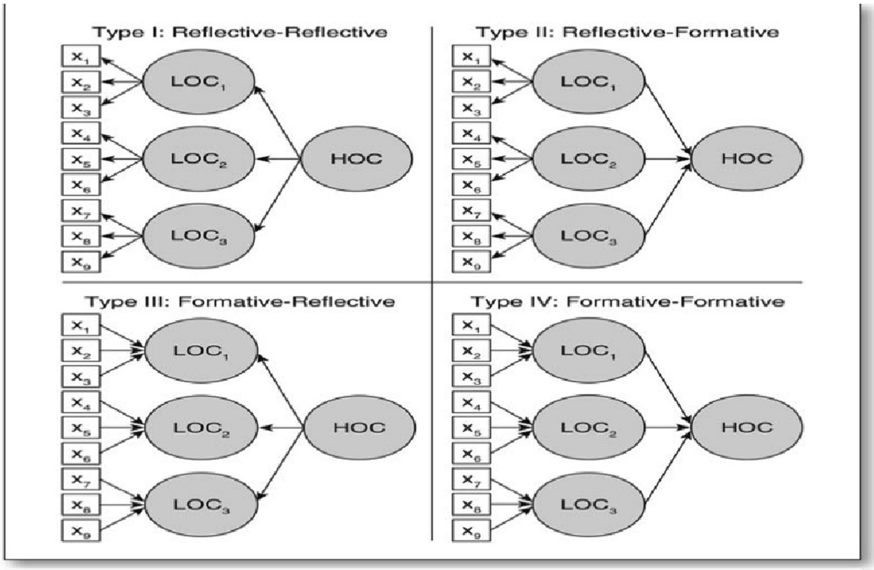

Figure 1. Types of higher-order constructs

Source(s): Hair *et al.*, (2024). Advanced Issues in Partial Least Squares Structural Equation Modeling, 2nd edition, Sage Publications, Los Angeles, CA. Reprinted with permission

physical environment, including lighting, temperature and equipment to support employees' work. A justification for converting the work environment from a single layer to two layers (a HOC and multiple LOCs) would be if multicollinearity becomes an issue between the work environment components (independent variables (IVs)). In short, if you conceptualize the work environment as a single HOC with multiple LOCs, this will reduce the problem of multicollinearity. This approach works well if the IVs are based on established theory.

If the theoretical justification is limited, however, logic and/or informed judgment supports conceptualizing HOCs. For example, an alternative approach would be to conduct qualitative research to support the specification of a HOC. The qualitative research could also clarify whether the HOC-LOC relationships should be specified as reflective or formative. This is an example of the benefit of PLS-SEM being acceptable for exploratory research as well as causal-predictive designs.

Guenther *et al.* (2023) recently added a predictive perspective when modeling HOCs. They propose utilizing the disjoint two-stage technique and BIC (Sharma *et al.*, 2019, 2021) or CVPAT (Sharma *et al.*, 2023). Researchers can then confirm that the model's predictive power is higher with the HOC and exhibits reduced multicollinearity, compared to not including the HOC in the structural model.

This overview of the benefits of HOCs is limited. For researchers considering this type of conceptualization for their measurement models (composites), HOC conceptualization is often useful in obtaining improved solutions. To learn more, see Hair *et al.* (2024a, b), *Advanced Issues in Partial Least Squares Structural Equation Modeling*, 2nd edition, for a much more extensive description and explanation of HOCs.

Necessary condition analysis (NCA). When applying PLS-SEM, researchers have generally relied on the concept of sufficiency logic when interpreting their PLS-SEM results. This type of logic focuses on producing the best possible outcomes (explained variance and predictive power) when interpreting PLS-SEM results. Specifically, this logic is applied when statements such as *X increases Y* and *a higher X is associated with a higher Y* are included in evaluating the results. Based on this logic, researchers assume each antecedent construct in the structural model is sufficient (but not necessary) for producing changes in the dependent construct.

More recently, researchers have also proposed considering the necessity of logic for interpreting causal relationships (Richter and Hauff, 2022). The concept of necessity logic focuses on examining antecedent constructs that are necessary for a predictive relationship but, overall, may not contribute sufficiently to influence the dependent construct. In other words, necessary antecedents are first needed to produce the outcome, whereas sufficient antecedents can influence the outcome. More specifically, a necessary condition variable cannot be compensated for by other antecedent constructs. Thus, not including the variable in the model will prevent the anticipated outcome from being achieved. As an example of necessary condition considerations, Richter *et al.* (2020) applied both NCA and PLS to understand the causal relationships between antecedents of technology use. Their results identified ease of use and compatibility as necessary but insufficient conditions for technology use. That is, the results did not identify either construct as having a significant impact on technology use. What their findings did reveal, however, is critical levels of compatibility are required to achieve a relevant level of technology use but "increasing compatibility to higher levels does not further increase technology use."

In Richter *et al.* (2020), step-by-step guidelines are provided for researchers to apply NCA logic with PLS-SEM models along with suggestions on how to interpret model results. They also included the code for the open-source software *R* platform to perform NCA. New software options for conducting NCA and PLS-SEM are now available in SmartPLS 4.1 (Ringle *et al.*, 2022). More recently, Richter *et al.* (2024) updated the application of NCA with PLS-SEM, and Sukhov *et al.* (2023) provided an example of expanding the application of NCA and PLS-SEM.

Figure 2 represents the theoretical model proposed by Sukhov *et al.* (2023) in which they proposed and tested the relationships between the service quality attributes of functionality, information, security/safety, comfort and cost, and the dependent variable perceived accessibility. Applying PLS-SEM, they first confirmed the measurement models and then evaluated the structural model by examining both in-sample and out-of-sample prediction, as well as the CVPAT. Next, they executed NCA following the guidelines of Richter *et al.* (2020) and Sukhov *et al.* (2022). Results of the NCA indicated four of the five service quality

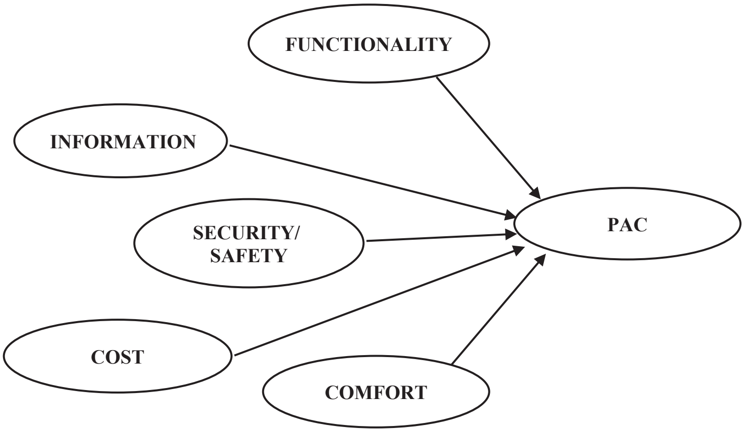

Figure 2.
Service quality attributes and perceived accessibility (PAC)

Source(s): Authors' own creation

attributes were necessary to achieve high levels of perceived accessibility; cost was not considered necessary. More specifically, for elderly respondents, comfort must be perceived as at an acceptable level, and functionality, information and security/safety must not be at a level of complete dissatisfaction to consider the perceived accessibility of their experience to be high (Sukhov *et al.* (2023). These analytical extensions demonstrate the value of more fully exploring expanded structural models, such as PLS-SEM, when simple models like multiple regression cannot fully explain relationships.

As a final note, Hauff *et al.* (2024) incorporate findings from an NCA to extend the application of importance-performance map analysis (IPMA) (Ringle and Sarstedt, 2016) in PLS-SEM. The combined importance-performance map analysis (cIPMA) approach was developed by incorporating two types of logic (sufficiency and necessity) into the performance dimension. The approach enables researchers and practitioners to improve decision-making and more effectively prioritize their efforts, which often leads to improved target outcomes.

Generalized structured component analysis (GSCA). An emerging methodological composite-based alternative to PLS-SEM is GSCA, a component-based structural equation modeling approach for analyzing complex inter-relationships between indicators and composites. GSCA obtains solutions using the alternating least squares (ALS) algorithm and optimizes a single criterion (Hwang and Takane, 2014). The established PLS-SEM method evaluates measurement and structural models representing the relationships between model components and indicators. It calculates a separate optimization criterion for both the measurement models and the structural model. In contrast, the emerging method of GSCA includes a third sub-model, the weighted relation model, which combines the three sub-models into a single overall model and specifies the components as weighted sums of their associated indicators. The addition of the third model enables the method to calculate an additional global optimization metric, similar to the CB-SEM goodness of fit metric (Hwang and Takane, 2004, 2014; Cho *et al.*, 2023).

There are other meaningful differences between GSCA and PLS-SEM researchers may want to apply. GSCA path models can include circular or bidirectional relationships between the components (non-recursive relationships) while PLS-SEM structural relationships are considered recursive. Moreover, with GSCA, it is possible for each indicator to be linked to multiple components (Hwang and Takane, 2014) while PLS-SEM indicators are generally linked to only one composite component (Hair *et al.*, 2021). To assist researchers in better understanding the differences between PLS-SEM and GSCA, we have included a table comparing the characteristics of the two approaches (see Table 2). Technically, GSCA can include PLS as a special case (Hwang and Cho, 2020). In practice, if the model is unidimensional, unidirectional and unconstrained, both methods will likely produce similar parameter estimates (Hwang and Cho, 2020).

Hwang *et al.* (2021) developed the integrated generalized structured component analysis (IGSCA). Their method facilitates the estimation of models comprising both components and factors inside a single framework. IGSCA is less likely to produce incorrect solutions and can estimate more complex models than consistent Partial Least Squares (PLSc) and is, therefore, the recommended approach. In addition, a simulation study demonstrated that IGSCA typically outperforms PLSc in various scenarios (Hwang *et al.*, 2021). While Hwang *et al.* (2023a) offer basic guidelines about using it, Hwang *et al.* (2023b) introduce the use of GSCA and IGSCA using GSCA Pro software.

In a practical way, Table 2 presents a summary of the most important differences in the execution of a path model in GSCA and in PLS-SEM. These differences are in the calculation of the components and their names, the possible relationships between the constructs (i.e. structural model), and the possibility of an indicator being related to several constructs (i.e. composites). The method of estimation also includes differences since GSCA is a full

		GSCA	PLS-SEM
Model Specification	Component Type	• Nomological • Canonical	• Reflective (Mode A) • Formative (Mode B)
	Measurement Model	• Unidimensional • Multidimensional	
	Structural Model	• Unidirectional • Bidirectional	• Unidirectional
Estimation	Method	• Full information • Least squares • Unconstrained and constrained estimation • Bayesian	• Limited information • Least squares • Unconstrained estimation
	Statistical Inference	• Bootstrapping • Bayesian	• Bootstrapping
Model Evaluation		• Overall assessment • Local assessment	• Local assessment

Source(s): Adapted from: Heungsun Hwang, A Gentle Introduction to Generalized Structured Component Analysis (GSCA), December 13, 2022, presentation at Instituto de Economia y Negocios de la Universidad de Sevilla – IUSEN. The table is authors' creation/work

Table 2.
Comparison of PLS-SEM and GSCA

information method and PLS-SEM is a limited information method (Latan *et al.*, 2023b). This enables GSCA to provide an overall assessment of the estimated model.

Hair (2021) provides an excellent overview of these emerging prediction assessment tools for composite-based PLS-SEM and proposed out-of-sample prediction methodologies. A practical application of these approaches is demonstrated in Chin *et al.* (2020). In Table 3 an overview of the utility and recent developments in these emerging tools is presented.

Best practices recommendations on evaluating and reporting PLS-SEM results

PLS-SEM is a widely applied tool in the IS literature. The attractiveness of this analytical tool for IS scholars and practitioners can be attributed to several characteristics. First, as a limited

Tools	Utility	Recent developments and applications
CVPAT	Comparatively assesses the predictive accuracy of theoretical models	Sharma *et al.* (2023) expanded the application of CVPAT from simultaneous model comparison to include target construct comparison
HCM	Facilitates the simultaneous modeling of a construct's higher-order abstract dimension and its more concrete subdimensions	Using the disjoint two-stage approach makes it possible to apply PLS prediction or CVPAT (Becker *et al.*, 2023)
NCA	Examines whether predictor variables are essential for the prediction of an outcome variable and to what extent they are considered necessary	Sukhov *et al.* (2023) combine PLS-SEM and NCA with fsQCA* to improve methodological triangulation and expand causal logic research Hauff *et al.* (2024) created cIPMA by combining IPMA (PLS-SEM) and NCA to prioritize initiatives that could improve target outcomes
GSCA	Indicators can be linked to multiple components and path models can include circular or bidirectional relationships between the components	Cho *et al.* (2023) systematically compare GSCA and PLS providing evidence of the trade-offs between the methods' performance related to prediction and model fit

Note(s): Fuzzy set qualitative comparative analysis (fsQCA) is a methodology developed to combine case-oriented and variable-oriented quantitative analysis
Source(s): Authors' own creation/work

Table 3.
Emerging tools and recent developments

information approach, there are very few population characteristics or measurement scale assumptions when using PLS-SEM (Fornell and Bookstein, 1982). Therefore, nominal (control and dummy-coded), ordinal, interval and ratio scaled variables can be included in theoretical models when interpreted according to recommended guidelines for these measurement scale types. Second, PLS-SEM achieves high levels of statistical power with small sample sizes and complex models (Hair *et al.*, 2022). Moreover, the general PLS path modeling algorithm is based on ordinary least squares regression, ensuring that sample size requirements are minimally influenced by model complexity. Third, PLS-SEM is preferred over CB-SEM in many research contexts, particularly when the statistical objective is prediction (Hair *et al.*, 2022, 2024a, b), and the measures of the structural concepts in the proposed PLS-SEM model are considered composites. Fourth, PLS-SEM readily incorporates constructs/composites measured either reflectively or formatively, making the approach particularly appealing for many types of studies, including success factor studies (Hair *et al.*, 2022). Fifth, a primary reason for using PLS-SEM is the ability to evaluate the measurement model composites to reduce error and also to operationalize the composites as either reflective or formative (Hair *et al.*, 2017a, b, 2022). Sixth, researchers must communicate the purposes for using PLS-SEM, such as causal, predictive, descriptive, and/or exploratory, and should report their results consistent with these declared purposes. Moreover, if the purpose is causal, the focus must be on the statistical inference of hypotheses, explained variance of dependent variables (R^2) and effect sizes (f^2), and out-of-sample prediction (PLSpredict). Finally, researchers should also evaluate and test for endogeneity (Mithas *et al.*, 2022) when that is a relevant consideration (Hair *et al.*, 2019a), particularly in studies with causal purposes.

Researchers applying and evaluating PLS-SEM in their papers should note the following considerations when assessing and reporting the measurement and structural model results. Endogeneity occurs when one or more predictor constructs correlate with the dependent variable's error term, violating a key causal modeling assumption (Benitez *et al.*, 2016). To evaluate and treat endogeneity, researchers can (1) use control or instrumental variables in their analysis (Shiau *et al.*, 2024), or (2) when there are no control or instrumental variables, apply the Gaussian copula approach (Becker *et al.*, 2022; Hult *et al.*, 2018). If the purpose of the research is predictive modeling, however, then errors based on out-of-sample procedures are the main parameters to evaluate and report. For descriptive purposes, latent variable scores and their weights based on a nomological network are key elements to consider. In addition, the size of the structural path coefficients, identification of potential structural relationships and statistical significance are the parameters to consider in exploratory research.

Several user-friendly software packages with a graphical user interface and numerous expanded options for advanced analyses are available. The SmartPLS 4.1 (Ringle *et al.*, 2022) is the most widely applied PLS-SEM software, but PLS-graph, ADANCO, and WarpPLS are alternative packages. In addition, requiring coding are the SEMinR and cSEM packages as components of the R-software platform, whereas the plssem package belongs to the Stata environment. Finally, the *R* Primer workbook (Hair *et al.*, 2021) is a free download at https://link.springer.com/book/10.1007/978-3-030-80519-7. These resources will continue to enhance the attractiveness of PLS-SEM, but the method should always be applied in a rigorous way.

Our recent review of PLS-SEM applications in IS reveals there is limited awareness of all the methodological properties of PLS-SEM (Sabol *et al.*, 2023). Moreover, some assessment metrics and requirements continue to be misunderstood, and at times these issues have led to misapplications of the technique. Table 4 includes guidelines for best practices in the application and evaluation of the PLS-SEM for IS research. We believe following these guidelines will clearly enhance the quality of IS scholarly publications. Researchers should not forget the former criteria about the reason and purposes for applying PLS-SEM in their publications.

Criterion	Rules of thumb
Characteristics of the data	
Sample size	Apply the recently updated sample size determination approach developed by Kock and Hadaya (2018) as described in (Hair *et al.*, 2022) • In selected situations where the population is quite small, sample sizes <100 may be acceptable
Sample distribution	Very robust when applied to highly skewed data
Use of holdout sample	A minimum of 30 from the original sample, particularly for out-of-sample prediction
Number of missing values	PLS-SEM is robust with approximately 10% missing at random data
Missing value treatment	In general, delete responses case-wise or execute nearest neighbor or estimated model algorithm imputation
Measurement scale	All types of scales are OK, except the categorical scale for the ultimate dependent variable
Algorithm settings and software	
Starting values of weights for initial approximation of latent variable scores	Use 1 as an initial value for each outer weight
Weighting scheme	Use a path weighting scheme
Stop criterion	The sum of the outer weights' changes between two iterations $<10^{-5}$
Software	Report full citation as required by license agreements
Parameter settings	
Bootstrapping sign changes option	Use individual sign changes
Number of bootstrap samples	10,000 bootstrap samples. The minimum number must be greater than the number of observations
Size of bootstrap samples	Equal to the number of observations
Multigroup comparisons	Use a non-parametric approach to assess significance
Model characteristics	
Inner model description	The structural model should display all inner model relationships
Outer model description	Identify all measurement model indicators (questions)
Latent variable measurement mode	Evaluate measurement mode of constructs with CTA-PLS (confirmatory tetrad analysis)
Number of items on latent variable	In general, avoid single-item measures except for sales, profits, market share and similar concepts
Outer model evaluation of reflective measurement models	
Indicator loadings size	Standardized indicator loadings ≥0.708
Construct reliability	Composite reliability ≥0.70 (in exploratory research 0.60 to 0.70 is considered acceptable). It is not desirable to have reliability values higher than 0.95, which could indicate potentially undesirable response patterns
Convergent validity	AVE (average variance extracted) ≥ 0.50
Fornell-Larcker criterion	Avoid this metric since it often is not an adequate measure of discriminant validity. The AVE (convergent validity) of a latent construct should be equal to and greater than the construct's highest squared correlation with any other latent construct

(*continued*)

Table 4.
Best practices evaluating and reporting of PLS-SEM results

Criterion	Rules of thumb
HTMT	This is the preferred discriminant validity metric. Values lower than 0.85 for conceptually distinct constructs and below 0.90 for conceptually similar constructs. Note: confidence intervals should not include a value of 0.90
Outer model evaluation of formative measurement models	
Significance of weights	Report t-values, confidence intervals and p-values
Multicollinearity	Evaluate VIF (variance inflation factor) <3
Absolute versus relative indicator contributions	Report indicator weights and/or loadings; assess significance
Inner model evaluation (path models)	
Type of hypothesis and significance testing	If the alternative hypothesis related to the path coefficient is directional (i.e. includes a sign, positive or negative), then use a one-tailed test. If it is exploratory (i.e. no assumptions are made about the coefficient sign), use a two-tailed test (Diamantopoulos *et al.*, 2023; Kock, 2015)
R^2	Research context determines the acceptable level
Effect size f^2	0.02, 0.15, 0.35 for weak, moderate, strong effects
Mediation	To test a mediating effect, always include the direct effect between the independent and the dependent variable The report effect size for both direct and indirect relationships
Path coefficient estimates	Assess the sign, size and significance of coefficients and also confidence intervals
PLSpredict Q^2_{predict} statistic and Errors	RMSE and MAE errors should be smaller than LM errors
Conditional mediation (CoMe)	When relevant theory suggests, explore moderated mediation possibilities
Observed and unobserved heterogeneity	Consider categorical or continuous moderating variables using *a priori* information or FIMIX-PLS

Note(s): Latent variable constructs are also referred to as composite measurement models
Source(s): Authors' own creation; adapted from Hair *et al.* (2022, 2024a, b)

Table 4.

Finally, we strongly recommend researchers follow open science practices to improve research transparency. In line with this, Adler *et al.* (2023) suggested a PLS-SEM-specific template for preregistration that researchers can apply to promote transparency in their analyses. Doing so will ensure increased confidence in their findings.

Conclusions

The IS field should continue to exercise sound practices by improving the reporting of PLS-SEM assessment metrics and advanced analytical features. This paper heeds recent updated guidelines for awareness and application of accepted reporting practices. The numerous new options for additional PLS-SEM analyses and robustness tests will lead to an improved understanding of measurement and path model relationships, exploration of more complex theories, and ultimately theoretical model confirmation.

The new options also provide additional reasons to apply PLS-SEM to explain SEM relationships. The traditional CB-SEM approach has some unique situations where the method is considered the preferred SEM approach; for example, when the research objective is to evaluate and explain the relationships between all variables in the theoretical model. Overall, however, there are numerous situations where PLS-SEM is the preferred SEM approach, including continuous moderators, HOCs with only two first-order constructs, out-of-sample prediction, model comparisons (CVPAT), moderated mediation (CoMe), NCA, not to mention the availability, dependability and ease of use of the SmartPLS and R-software options. Moreover, the emerging GSCA methodology enables a fit index assessment if the application and understanding of theoretical model relationships are improved by this option.

In planning future research projects, we encourage IS researchers to become familiar with the rapidly increasing PLS-SEM analytical possibilities. The new options should be evaluated early in the research planning process so that they can be considered when specifying the research design as well as selecting the method of SEM. The last thing researchers want is to be unable to confirm/reject their research hypotheses because the necessary data were not collected, or they were not aware of the best method to analyze the data.

As a final thought, authors should remember that PLS-SEM and other structural model approaches differ, and these differences influence their selection. None of the various methods is superior overall to the other and neither method is appropriate for all situations. In general, the strengths of one approach offset the limitations of others, and vice versa, although numerous methodological developments are emerging much more rapidly for PLS-SEM than other methods. It is important for researchers to be aware of the different applications for which each approach was developed and the analytical features available, and to apply these methods accordingly.

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