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Joseph F. Hair Jr. · G. Tomas M. Hult ·  
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# Partial Least Squares Structural Equation Modeling (PLS-SEM) Using R

A Workbook

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# **Partial Least Squares Structural Equation Modeling (PLS-SEM) Using R**


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## Preface

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In 2021, the third edition of our introductory book *A Primer on Partial Least Squares Structural Equation Modeling (PLS-SEM)* was published (Hair, Hult, Ringle, & Sarstedt, 2022). The book covers the latest developments in the field, including recent advances in model evaluation (e.g., inference testing in discriminant validity assessment, predictive power assessments using  $PLS_{\text{predict}}$ , and model comparisons), improved guidelines for minimum sample sizes, and new complementary methods and concepts such as necessary condition analysis and endogeneity. The book has been highly successful as evidenced in its citation count of more than 24,000 times according to Google Scholar (as of August 2021), and the translations into seven other languages, including in German (Hair et al., 2017), Italian (Hair et al., 2020), and Spanish (Hair et al., 2019). One of the book's features that has likely contributed to its popularity is our strong focus on pedagogical elements, most notably our reliance on a single running case study and the commercial SmartPLS 3 software (Ringle, Wende, & Becker, 2015), which stands out due to its frictionless design, allowing novice researchers to quickly specify and estimate PLS path models (Memon et al., 2021; Sarstedt & Cheah, 2019).

While SmartPLS constitutes the most frequently used software to conduct PLS-SEM analyses (Ghasemy, Teeroovengadum, Becker, & Ringle, 2020; Hair, Hollingsworth, Randolph, & Chong, 2017; Usakli & Kucukergin 2018), research has brought forward several packages for the R environment such as *csem* (Rademaker et al., 2020), *SEMinR* (Ray et al., 2021), and *semPLS* (Monecke & Leisch, 2012; Monecke & Leisch, 2013), whose use has recently gained traction. Among the R packages available on CRAN, Ray et al.'s (2021) *SEMinR* package brings a particularly friendly syntax to creating and estimating structural equation models using functions named appropriately for the facets of PLS path models that applied researchers are familiar with: “multi-item” versus “single-item,” “constructs,” “paths,” and so on. The package also gives users intuitive functions for generating higher-order constructs and interaction terms, the flexibility to quickly implement and insert their own extensions such as missing data imputation methods or visualizations, and generate reports and figures for research output. It was logical, therefore, to prepare a version of the book that shares the methodological concepts and also features the R software as a method for estimating PLS path models. This book caters this aim.

We designed the text as a workbook for readers who have already been exposed to PLS-SEM by reading textbooks (e.g., Hair et al., 2022; Henseler, 2021; Ramayah, Cheah, Chuah, Ting, & Memon, 2016; Mehmetoglu & Venturini, 2021; Wong, 2019) or seminal articles (e.g., Chin, 1998; Hair, Ringle, & Sarstedt, 2011; Hair, Risher, Ringle, & Sarstedt, 2019; Henseler, Ringle, & Sinkovics, 2009; Sarstedt, Ringle, & Hair, 2022; Tenenhaus, Esposito Vinzi, Chatelin, & Lauro, 2005) on the method. Nevertheless, to enable readers with little background in PLS-SEM to quickly grasp the concepts, each chapter offers a concise overview of relevant topics and metrics relevant for executing PLS-SEM and interpreting the results. Accompanied by a rich set of references for further reading, rules of thumb in

every chapter provide guidelines on best practices in the application of PLS-SEM. The focus, however, is on the in-depth description of the case study, which gives readers the “how-tos” of using SEMinR to obtain solutions and to report their results. Correspondingly, the workbook puts less emphasis on aspects related to model design and measurement model specification but, instead, introduces the R environment and particularly the SEMinR package in detail.

Nevertheless, the workbook incorporates many of the new features that have been introduced in the third edition of the *Primer on Partial Least Squares Structural Equation Modeling (PLS-SEM)* (Hair et al., 2022) and offers unique contents tailored to the SEMinR package. These include the following:

- An overview of the latest research on the nature of composite-based modeling, which is the conceptual foundation for PLS-SEM
- Details on the distinction between PLS-SEM and CB-SEM as well as the research goals and the model constellations, which are favorable toward the use of PLS-SEM
- Application of PLS-SEM with secondary (archival) data
- Guidelines for determining minimum sample sizes using the inverse square root method
- Detailed coverage of internal consistency reliability using  $\rho_{\alpha}$  and inference testing in discriminant validity assessment
- Latest research on bootstrapping settings and assessment
- Analyzing a model’s out-of-sample predictive power using the  $PLS_{\text{predict}}$  procedure
- Metrics for model comparisons (e.g., the Bayesian information criterion)
- Coverage of the latest literature on PLS-SEM

All examples in the edition apply to the newest version of the SEMinR package, which is available free of charge in CRAN (► <https://CRAN.R-project.org/package=seminr>; see also ► Chap. 3). The book chapters and learning support supplements are organized around the learning outcomes shown at the beginning of each chapter. Moreover, each chapter includes a single concise summary for the learning outcomes. The website ► <https://www.pls-sem.com> includes a series of support materials to facilitate learning and applying the PLS-SEM method and using the SEMinR package.

Visit ► <https://www.pls-sem.com> for access to R markdown documents, which weave together descriptions and code that can be easily copied into the R console.

Additionally, the PLS-SEM Academy (► <https://www.pls-sem-academy.com>) offers video-based online courses based on this book. The courses include basic contents such as model specification and evaluation as well as advanced topics, including mediation, higher-order constructs, moderation, measurement invariance, multigroup analysis, and nonlinear effects.

Besides several hours of online video material presented by world-renowned instructors, the PLS-SEM Academy provides comprehensive lecturing slides that

illustrate all analyses step-by-step. While the case study descriptions draw on the SmartPLS software, the concepts are fully applicable to the R software-based analyses using the SEMinR package. Registered users can claim course certificates after successful completion of each end of section exam.

#### Discounted PLS-SEM Academy Access

The PLS-SEM Academy offers all owners of this book a 15% discount on the purchase of access to its course offerings. All you have to do is send a photo of yourself with the book in your hand, your name and address to the e-mail address [support@pls-sem-academy.com](mailto:support@pls-sem-academy.com). A short time later you will receive a 15% discount code which you can use on the website ► <https://www.pls-sem-academy.com>. We hope you enjoy perfecting your PLS-SEM skills with the help of these courses and wish you every success in obtaining the certificates.

We would like to acknowledge the many insights and suggestions provided by the colleagues, students, and PLS-SEM users worldwide. Most notably, we thank Nicole Beachum (University of Alabama, Birmingham), Jan-Michael Becker (BI Norwegian Business School), Zakariya Belkhamza (Ahmed Bin Mohammed Military College), Charla Brown (Troy University), Roger Calantone (Michigan State University), Fabio Cassia (University of Verona), Gabriel Cepeda Carrión (University of Seville), Jacky Jun Hwa Cheah (Universiti Putra Malaysia), Adamantios Diamantopoulos (University of Vienna), Markus Eberl (Kantar), George Franke (University of Alabama), Anne Gottfried (University of Texas, Arlington), Siegfried P. Gudergan (University of Waikato), Saurabh Gupta (Kennesaw State University), Karl-Werner Hansmann (University of Hamburg), Dana Harrison (East Tennessee State University), Sven Hauff (Helmut Schmidt University), Mike Hollingsworth (Old Dominion University), Philip Holmes (Pensacola Christian College), Chris Hopkins (Auburn University), Lucas Hopkins (Florida State University), Maxwell K. Hsu (University of Wisconsin), Heungsun Hwang (McGill University), Ida Rosnita Ismail (Universiti Kebangsaan Malaysia), April Kemp (Southeastern Louisiana University), David Ketchen (Auburn University), Ned Kock (Texas A&M University), Marcel Lichters (TU Chemnitz), Benjamin Liengaard (Aarhus University), Chein-Hsin Lin (Da-Yeh University), Yide Liu (Macau University of Science and Technology), Francesca Magno (University of Bergamo), Lucy Matthews (Middle Tennessee State University), Jay Memmott (University of South Dakota), Mumtaz Ali Memon (NUST Business School), Adam Merkle (University of South Alabama), Ovidiu I. Moisesescu (Babeş-Bolyai University), Zach Moore (University of Louisiana at Monroe), Arthur Money (Henley Business School), Christian Nitzl (Universität der Bundeswehr München), Torsten Pieper (University of North Carolina), Dorian Proksch (University of Twente), Lacramioara Radomir (Babeş-Bolyai University), Arun Rai (Georgia State University), Sascha Raithel (Freie Universität Berlin), S. Mostafa Rasoolimanesh (Taylor's University), Lauren Rich (University of West Florida), Nicole



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Visit the companion site for this book at ► <https://www.pls-sem.com>.

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# An Introduction to Structural Equation Modeling

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### Learning Objectives

After reading this chapter, you should:

1. Understand the principles of structural equation modeling (SEM)
2. Describe the basic elements of a structural equation model
3. Comprehend the basic concepts of partial least squares structural equation modeling (PLS-SEM)
4. Explain the differences between covariance-based structural equation modeling (CB-SEM) and PLS-SEM and when to use each of the approaches

## 1.1 What Is Structural Equation Modeling?

First-generation multivariate data analysis techniques, such as multiple regression, logistic regression, and analysis of variance, belong to the core set of statistical methods employed by researchers to empirically test hypothesized relationships between variables of interest. Numerous researchers in various scientific disciplines have applied these methods to generate findings that have significantly shaped the way we see the world today. These techniques have three important limitations in common, namely (1) the postulation of a simple model structure, (2) requiring that all variables can be considered observable, and (3) the assumption that all variables are measured without error (Haenlein & Kaplan, 2004).

With regard to the first limitation, multiple regression analysis and its extensions postulate a simple model structure involving one layer of dependent and independent variables. Causal chains, such as “A leads to B leads to C” or more complex nomological networks involving a large number of intervening variables, can only be estimated piecewise with these methods rather than simultaneously, which can have severe consequences for the quality of the results (Sarstedt, Hair, Nitzl, Ringle, & Howard, 2020).

With regard to the second limitation, regression-type methods are restricted to processing observable variables, such as age or sales (in units or dollars). Theoretical concepts, which are “abstract, unobservable properties or attributes of a social unit of entity” (Bagozzi & Philipps, 1982, p. 465), can only be considered after prior stand-alone validation by means of, for example, a confirmatory factor analysis (CFA). The ex post inclusion of measures of theoretical concepts, however, comes with various shortcomings.

With regard to the third limitation and related to the previous point, one has to bear in mind that each observation of the real world is accompanied by a certain degree of **measurement error**, which can be systematic or random. First-generation techniques are, strictly speaking, only applicable when measured variables contain neither systematic nor random error. This situation is, however, rarely encountered in reality, particularly when the aim is to estimate relationships among measures of theoretical concepts. Since the social sciences, and many other fields of scientific inquiry, routinely deal with theoretical concepts, such as perceptions, attitudes, and intentions, these limitations of first-generation techniques are fundamental.

To overcome these limitations, researchers have increasingly been turning to **second-generation techniques**. These methods, referred to as **structural equation modeling (SEM)**, enable researchers to simultaneously model and estimate complex relationships among multiple dependent and independent variables. The concepts under consideration are typically unobservable and measured indirectly by multiple indicators. In estimating the relationships, SEM accounts for measurement error in observed variables. As a result, the method obtains a more precise measurement of the theoretical concepts of interest (Cole & Preacher, 2014). We will discuss these aspects in the following sections in greater detail.

Two popular methods dominate SEM in practice: **covariance-based SEM (CB-SEM)** and **partial least squares SEM (PLS-SEM)**, also called **PLS path modeling**. CB-SEM is primarily used to confirm (or reject) theories and their underlying hypotheses. This approach confirms/rejects hypotheses by determining how closely a proposed theoretical model can reproduce the covariance matrix for an observed **sample** dataset. In contrast, PLS has been introduced as a “causal–predictive” approach to SEM (Jöreskog & Wold, 1982, p. 270), which focuses on explaining the variance in the model’s dependent variables (Chin et al., 2020).

PLS-SEM is evolving rapidly as a statistical modeling technique. Over the last few decades, there have been numerous introductory articles on this methodology (e.g., Chin, 1998; Haenlein & Kaplan, 2004; Hair et al., 2020; Hair, Howard, & Nitzl, 2020; Hair, Risher, Sarstedt, & Ringle, 2019; Nitzl & Chin, 2017; Rigdon, 2013; Roldán & Sánchez-Franco, 2012; Tenenhaus, Esposito Vinzi, Chatelin, & Lauro, 2005; Wold, 1985) as well as review articles examining how researchers across different disciplines have used the method (■ Table 1.1). In light of the increasing maturation of the field, researchers have also started exploring the knowledge infrastructure of methodological research on PLS-SEM by analyzing the structures of authors, countries, and co-citation networks (Hwang, Sarstedt, Cheah, & Ringle, 2020; Khan et al., 2019).

The remainder of this chapter first provides a brief introduction of measurement and structural theory as a basis for presenting the PLS-SEM method. In describing the PLS-SEM method’s characteristics, we also discuss distinguishing features vis-à-vis CB-SEM. Finally, we outline considerations when using PLS-SEM and highlight situations that favor its use compared to CB-SEM.

## 1.2 Principles of Structural Equation Modeling

### 1.2.1 Path Models with Latent Variables

**Path models** are diagrams used to visually display the hypotheses and variable relationships that are examined when SEM is applied (Hair, Page, & Brunsveld, 2020; Hair, Ringle, & Sarstedt, 2011). An example of a path model is shown in ■ Fig. 1.1.

**Constructs** (i.e., variables that are not directly measurable), also referred to as **latent variables**, are represented in path models as circles or ovals ( $Y_1$  to  $Y_4$ ). The **indicators**, also called items or manifest variables, are the directly measured vari-

■ **Table 1.1** Review articles on the use of PLS-SEM

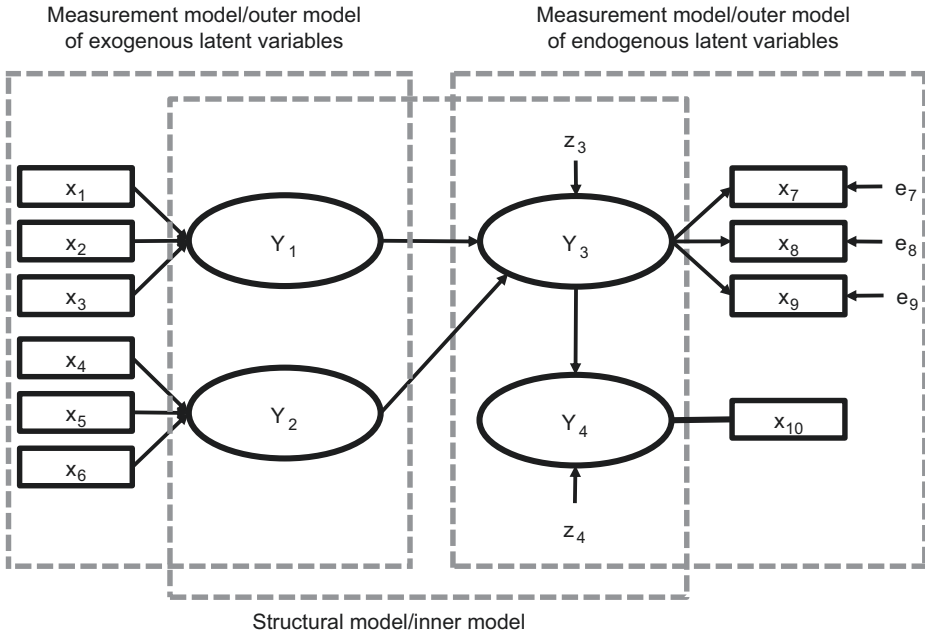
Disciplines	References
Accounting	Lee, Petter, Fayard, and Robinson (2011) Nitzl (2016)
Construction management	Zeng, Liu, Gong, Hertogh, and König (2021)
Entrepreneurship	Manley, Hair, Williams, and McDowell (2020)
Family business	Sarstedt, Ringle, Smith, Reams, and Hair (2014)
Higher education	Ghasemy, Teeroovengadum, Becker, & Ringle, (2020)
Hospitality and tourism	Ali, Rasoolimanesh, Sarstedt, Ringle, and Ryu (2018) do Valle, P. O., and Assaker, G. (2016) Usakli and Kucukergin (2018)
Human resource management	Ringle et al. (2020)
International business research	Richter, Sinkovics, Ringle, and Schlägel (2016)
Knowledge management	Cepeda Carrión, Cegarra-Navarro, and Cillo (2019)
Management	Hair, Sarstedt, Pieper, and Ringle (2012)
Marketing	Hair, Sarstedt, Ringle, and Mena (2012)
Management information systems	Hair, Hollingsworth, Randolph, and Chong (2017) Ringle et al. (2012)
Operations management	Bayonne, Marin-Garcia, and Alfalla-Luque (2020) Peng and Lai (2012)
Psychology	Willaby, Costa, Burns, MacCann, and Roberts (2015)
Software engineering	Russo and Stol (2021)
Supply chain management	Kaufmann and Gaeckler (2015)

Source: Hair, Hult, Ringle, & Sarstedt (2022), Chap. 1; used with permission by Sage

ables that contain the raw data. They are represented in path models as rectangles ( $x_1$  to  $x_{10}$ ). Relationships between constructs, as well as between constructs and their assigned indicators, are depicted as arrows. In PLS-SEM, the arrows are always single headed, thus representing directional relationships. Single-headed arrows are considered predictive relationships and, with strong theoretical support, can be interpreted as causal relationships.

A PLS path model consists of two elements. First, there is a **structural model** (also called the **inner model** in the context of PLS-SEM) that links together the constructs (circles or ovals). The structural model also displays the relationships (paths) between the constructs. Second, there are the **measurement models** (also referred to as the **outer models** in PLS-SEM) of the constructs that display the relationships between the constructs and the indicator variables (rectangles). In

■ Fig. 1.1, there are two types of measurement models: one for the **exogenous**



■ Fig. 1.1 A simple path model. (Source: Hair et al., 2022, Chap. 1; used with permission by Sage)

**latent variables** (i.e., those constructs that only explain other constructs in the model) and one for the **endogenous latent variables** (i.e., those constructs that are being explained in the model). Rather than referring to measurement models of exogenous and endogenous latent variables, researchers often refer to the measurement model of one specific latent variable. For example,  $x_1$  to  $x_3$  are the indicators used in the measurement model of  $Y_1$ , while  $Y_4$  only includes the  $x_{10}$  indicator in the measurement model.

The **error terms** (e.g.,  $e_7$  or  $e_8$ ; ■ Fig. 1.1) are connected to the (endogenous) constructs and (reflectively) measured variables by single-headed arrows. Error terms represent the unexplained variance when path models are estimated (i.e., the difference between the model's in-sample prediction of a value and an observed value of a manifest or latent variable). Error terms  $e_7$  to  $e_9$  in ■ Fig. 1.1 are connected to those indicators whose relationships point from the construct ( $Y_3$ ) to the indicators (i.e., reflectively measured indicators).

In contrast, the formatively measured indicators  $x_1$  to  $x_6$ , where the relationship goes from the indicator to the construct ( $Y_1$  and  $Y_2$ ), do not have error terms (Sarstedt, Hair, Ringle, Thiele, & Gudergan, 2016). Finally, for the single-item construct  $Y_4$ , the direction of the relationships between the construct and the indicator is not relevant, as construct and item are equivalent. For the same reason, there is no error term connected to  $x_{10}$ . The structural model also contains error terms. In ■ Fig. 1.1,  $z_3$  and  $z_4$  are associated with the endogenous latent variables  $Y_3$  and  $Y_4$  (note that error terms on constructs and measured variables are labeled differently). In contrast, the exogenous latent variables ( $Y_1$  and  $Y_2$ ) that only explain

other latent variables in the structural model do not have an error term, regardless of whether they are specified reflectively or formatively.

### 1.2.2 Testing Theoretical Relationships

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Path models are developed based on theory and are often used to test theoretical relationships. **Theory** is a set of systematically related hypotheses developed following the scientific method that can be used to explain and predict outcomes. Thus, hypotheses are individual conjectures, whereas theories are multiple hypotheses that are logically linked together and can be tested empirically. Two types of theory are required to develop path models: measurement theory and structural theory. Measurement theory specifies which indicators and how these are used to measure a certain theoretical concept. In contrast, structural theory specifies how the constructs are related to one another in the structural model.

Testing theory using PLS-SEM follows a two-step process (Hair, Black, Babin, & Anderson, 2019). We first test the measurement theory to confirm the reliability and validity of the measurement models. After the measurement models are confirmed, we move on to testing the structural theory. The logic is that we must first confirm the measurement theory before testing the structural theory, because structural theory cannot be confirmed if the measures are unreliable or invalid.

### 1.2.3 Measurement Theory

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**Measurement theory** specifies how the latent variables (constructs) are measured. Generally, there are two different ways to measure unobservable variables. One approach is referred to as reflective measurement, and the other is formative measurement. Constructs  $Y_1$  and  $Y_2$  in ■ Fig. 1.1 are modeled based on a **formative measurement model**. Note that the directional arrows are pointing from the indicator variables ( $x_1$  to  $x_3$  for  $Y_1$  and  $x_4$  to  $x_6$  for  $Y_2$ ) to the construct, indicating a predictive (causal) relationship in that direction.

In contrast,  $Y_3$  in ■ Fig. 1.1 is modeled based on a **reflective measurement model**. With reflective indicators, the direction of the arrows is from the construct to the indicator variables, indicating the assumption that the construct “causes” the measurement (more precisely, the covariation) of the indicator variables. As indicated in ■ Fig. 1.1, reflective measures have an error term associated with each indicator, which is not the case with formative measures. The latter are assumed to be error-free (Diamantopoulos, 2006). Finally, note that  $Y_4$  is measured using a single item rather than multi-item measures. Therefore, the relationship between construct and indicator is undirected.

Deciding whether to measure the constructs reflectively versus formatively and whether to use multiple items or a single-item measure is fundamental when developing path models. Hair, Hult, Ringle, and Sarstedt (2022; Chap. 2) explain these approaches to modeling constructs in more detail.

### 1.2.4 Structural Theory

**Structural theory** shows how the latent variables are related to one another (i.e., it shows the constructs and their path relationships in the structural model). The location and sequence of the constructs are either based on theory or the researcher's experience and accumulated knowledge or both. When path models are developed, the sequence is from left to right. The variables on the left side of the path model are independent variables, and any variable on the right side is a dependent variable. Moreover, variables on the left are shown as sequentially preceding and predicting the variables on the right. However, when variables are in the middle of the path model (between the variables that serve only as independent or dependent variables –  $Y_3$ ; ■ Fig. 1.1), they serve as both independent and dependent variables in the structural model.

When latent variables only serve as independent variables, they are called exogenous latent variables ( $Y_1$  and  $Y_2$ ). When latent variables only serve as dependent variables ( $Y_4$ ) or as both independent and dependent variables ( $Y_3$ ), they are called endogenous latent variables (■ Fig. 1.1). Any latent variable that has only single-headed arrows going out of it is an exogenous latent variable. In contrast, endogenous latent variables can have either single-headed arrows going both into and out of them ( $Y_3$ ) or only going into them ( $Y_4$ ). Note that the exogenous latent variables  $Y_1$  and  $Y_2$  do not have error terms, since these constructs are the entities (independent variables) that are explaining the dependent variables in the path model.

### 1.3 PLS-SEM and CB-SEM

There are two main approaches to estimating the relationships in a structural equation model (Hair et al., 2011; Hair, Black, et al., 2019). One is CB-SEM, and the other is PLS-SEM, the latter being the focus of this book. Each is appropriate for a different research context, and researchers need to understand the differences in order to apply the correct method (Marcoulides & Chin, 2013; Rigdon, Sarstedt, & Ringle, 2017). Finally, some researchers have argued for using regressions based on sum scores, instead of some type of indicator weighting as is done by PLS-SEM. The sum scores approach offers practically no value compared to the PLS-SEM weighted approach and in fact can produce erroneous results (Hair et al., 2017). For this reason, in the following sections, we only briefly discuss sum scores and instead focus on the PLS-SEM and CB-SEM methods.

A crucial conceptual difference between PLS-SEM and CB-SEM relates to the way each method treats the latent variables included in the model. CB-SEM represents a **common factor-based SEM** method that considers the constructs as common factors that explain the covariation between its associated indicators. This approach is consistent with the measurement philosophy underlying reflective measurement, in which the indicators and their covariations are regarded as manifestations of the underlying construct. In principle, CB-SEM can also accommodate formative measurement models, even though the method follows a common

factor model estimation approach. To estimate this model type, however, researchers must follow rules that require specific constraints on the model to ensure model identification (Bollen & Davies, 2009; Diamantopoulos & Riefler, 2011), which means that the method can calculate estimates for all model parameters. As Hair, Sarstedt, Ringle, and Mena (2012, p. 420) note, “[t]hese constraints often contradict theoretical considerations, and the question arises whether model design should guide theory or vice versa.”

PLS-SEM, on the other hand, assumes the concepts of interest can be measured as composites (Jöreskog & Wold, 1982), which is why PLS is considered a **composite-based SEM** method (Hwang et al., 2020). Model estimation in PLS-SEM involves linearly combining the indicators of a measurement model to form composite variables. The composite variables are assumed to be comprehensive representations of the constructs, and, therefore, valid proxies of the conceptual variables being examined (e.g., Hair & Sarstedt, 2019). The composite-based approach is consistent with the measurement philosophy underlying formative measurement, but this does not imply that PLS-SEM is only capable of estimating formatively specified constructs. The reason is that the estimation perspective (i.e., forming composites to represent conceptual variables) should not be confused with the measurement theory perspective (i.e., specifying measurement models as reflective or formative). The way a method like PLS-SEM estimates the model parameters needs to be clearly distinguished from any measurement theoretical considerations on how to operationalize constructs (Sarstedt et al., 2016). Researchers can include reflectively and formatively specified measurement models that PLS-SEM can straightforwardly estimate.

In following a composite-based approach to SEM, PLS relaxes the strong assumption of CB-SEM that all of the covariation between the sets of indicators is explained by a common factor (Henseler et al., 2014; Rigdon, 2012; Rigdon et al., 2014). At the same time, using weighted composites of indicator variables facilitates accounting for measurement error, thus making PLS-SEM superior compared to multiple regression using **sum scores**, where each indicator is weighted equally.

It is important to note that the composites produced by PLS-SEM are not assumed to be identical to the theoretical concepts, which they represent. They are explicitly recognized as approximations (Rigdon, 2012). As a consequence, some scholars view CB-SEM as a more direct and precise method to empirically measure theoretical concepts (e.g., Rönkkö, McIntosh, & Antonakis, 2015), while PLS-SEM provides approximations. Other scholars contend, however, that such a view is quite shortsighted, since common factors derived in CB-SEM are also not necessarily equivalent to the theoretical concepts that are the focus of the research (Rigdon, 2012; Rigdon et al., 2017; Rossiter, 2011; Sarstedt et al., 2016). Rigdon, Becker, and Sarstedt (2019a) show that common factor models can be subject to considerable degrees of metrological uncertainty. **Metrological uncertainty** refers to the dispersion of the measurement values that can be attributed to the object or concept being measured (JCGM/WG1, 2008). Numerous sources contribute to metrological uncertainty such as definitional uncertainty or limitations related to the measurement scale design, which go well beyond the simple standard errors



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produced by CB-SEM analyses (Hair & Sarstedt, 2019). As such, uncertainty is a validity threat to measurement and has adverse consequences for the replicability of study findings (Rigdon, Sarstedt, & Becker, 2020). While uncertainty also applies to composite-based SEM, the way researchers treat models in CB-SEM analyses typically leads to a pronounced increase in uncertainty (Rigdon & Sarstedt, 2021). More precisely, in an effort to improve model fit, researchers typically reduce the number of indicators per construct, which in turn increases uncertainty (Hair, Matthews, Matthews, & Sarstedt, 2017; Rigdon et al., 2019a). These issues do not necessarily imply that composite models are superior, but they cast considerable doubt on the assumption of some researchers that CB-SEM constitutes the gold standard when measuring unobservable concepts. In fact, researchers in various fields of science show increasing appreciation that common factors may not always be the right approach to measure concepts (e.g., Rhemtulla, van Bork, & Borsboom, 2020; Rigdon, 2016). Similarly, Rigdon, Becker, and Sarstedt (2019b) show that using sum scores can significantly increase the degree of metrological uncertainty, which questions this measurement practice.

Apart from differences in the philosophy of measurement, the differing treatment of latent variables and, more specifically, the availability of **construct scores** also have consequences for the methods' areas of application. Specifically, while it is possible to estimate latent variable scores within a CB-SEM framework, these estimated scores are not unique. That is, an infinite number of different sets of latent variable scores that will fit the model equally well are possible. A crucial consequence of this **factor (score) indeterminacy** is that the correlations between a common factor and any variable outside the factor model are themselves indeterminate (Guttman, 1955). That is, they may be high or low, depending on which set of factor scores one chooses. As a result, this limitation makes CB-SEM grossly unsuitable for **prediction** (e.g., Dijkstra, 2014; Hair & Sarstedt, 2021). In contrast, a major advantage of PLS-SEM is that it always produces a single specific (i.e., determinate) score for each composite of each observation, once the indicator weights/loadings are established. These determinate scores are proxies of the theoretical concepts being measured, just as factors are proxies for the conceptual variables in CB-SEM (Rigdon et al., 2017; Sarstedt et al., 2016).

Using these proxies as input, PLS-SEM applies ordinary least squares regression with the objective of minimizing the error terms (i.e., the residual variance) of the endogenous constructs. In short, PLS-SEM estimates coefficients (i.e., path model relationships) with the goal of maximizing the  $R^2$  values of the endogenous (target) constructs. This feature achieves the (in-sample) prediction objective of PLS-SEM (Hair & Sarstedt, 2021), which is therefore the preferred method when the research objective is theory development and explanation of variance (prediction of the constructs). For this reason, PLS-SEM is also regarded a **variance-based SEM** approach. Specifically, the logic of the PLS-SEM approach is that all of the indicators' variance should be used to estimate the model relationships, with particular focus on prediction of the dependent variables (e.g., McDonald, 1996). In contrast, CB-SEM divides the total variance into three types – common, unique, and error variance – but utilizes only common variance (i.e., the variance shared

with other indicators in the same measurement model) for the model estimation (Hair, Black, et al., 2019). That is, CB-SEM only explains the covariation between measurement and structural model indicators (Jöreskog, 1973) and does not focus on predicting dependent variables (Hair, Matthews, et al., 2017).

### ! Attention

PLS-SEM is similar but not equivalent to **PLS regression**, another popular multivariate data analysis technique (Abdi, 2010; Wold, Sjöström, & Eriksson, 2001). PLS regression is a regression-based approach that explores the linear relationships between multiple independent variables and a single or multiple dependent variable(s). PLS regression differs from regular regression, however, because, in developing the regression model, the method derives composite factors from the multiple independent variables by means of principal component analysis. PLS-SEM, on the other hand, relies on prespecified networks of relationships between constructs as well as between constructs and their measures (see Mateos-Aparicio, 2011, for a more detailed comparison between PLS-SEM and PLS regression).

## 1.4 Considerations When Applying PLS-SEM

### 1.4.1 Key Characteristics of the PLS-SEM Method

Several considerations are important when deciding whether or not to apply PLS-SEM. These considerations also have their roots in the method's characteristics. The statistical properties of the PLS-SEM algorithm have important features associated with the characteristics of the data and model used. Moreover, the properties of the PLS-SEM method affect the evaluation of the results. Four critical issues are relevant to the application of PLS-SEM (Hair et al., 2011; Hair, Risher, et al., 2019): (1) data characteristics, (2) model characteristics, (3) model estimation, and (4) model evaluation. ■ Table 1.2 summarizes the key characteristics of the PLS-SEM method. An initial overview of these issues is provided in this chapter. For a more detailed explanation, see Hair et al. (2022).

PLS-SEM works efficiently with small sample sizes and complex models (Cassel, Hackl, & Westlund, 1999; Hair, Sarstedt, & Ringle, 2019). In addition, different from maximum likelihood-based CB-SEM, which requires normally distributed data, PLS-SEM makes no distributional assumptions (i.e., it is nonparametric). PLS-SEM can easily handle reflective and formative measurement models, as well as single-item constructs, with no identification problems. It can therefore be applied in a wide variety of research situations. When applying PLS-SEM, researchers also benefit from high efficiency in parameter estimation, which is manifested in the method's greater **statistical power** in comparison to that of CB-SEM. Greater statistical power means that PLS-SEM is more likely to render a specific relationship significant when it is in fact present in the population. The same holds for the comparison with regression using sum score data, which is also characterized by lower statistical power than PLS-SEM (Hair, Hollingsworth, et al., 2017).

**Table 1.2** Key characteristics of PLS-SEM

<i>Data characteristics</i>	
Sample size	No identification issues with small sample sizes Achieves high levels of statistical power with small sample sizes Larger sample sizes increase the precision (i.e., consistency) of PLS-SEM estimations
Distribution	No distributional assumptions; PLS-SEM is a nonparametric method Influential outliers and collinearity may influence the results
Missing values	Highly robust as long as missing values are below a reasonable level (less than 5%)
Scale of measurement	Works with metric data and quasi-metric (ordinal) scaled variables The standard PLS-SEM algorithm accommodates binary-coded variables, but additional considerations are required when they are used as control variables and moderators and in the analysis of data from discrete choice experiments
<i>Model characteristics</i>	
Number of items in each construct's measurement model	Handles constructs measured with single- and multi-item measures
Relationships between constructs and their indicators	Easily incorporates reflective and formative measurement models
Model complexity	Handles complex models with many structural model relationships
Model setup	No causal loops (no circular relationships) are allowed in the structural model
<i>Model estimation</i>	
Objective	Aims at maximizing the amount of unexplained variance in the dependent measures (i.e., the $R^2$ values)
Efficiency	Converges after a few iterations (even in situations with complex models and/or large sets of data) to the optimum solution (i.e., the algorithm is very efficient)
Nature of constructs	Viewed as proxies of the latent concept under investigation, represented by composites
Construct scores	Estimated as linear combinations of their indicators (i.e., they are determinate) Used for predictive purposes Can be used as input for subsequent analyses Not affected by data limitations and inadequacies
Parameter estimates	Structural model relationships are generally underestimated, and measurement model relationships are generally overestimated compared to solutions obtained using data from common factor models Unbiased and consistent when estimating data from composite models High levels of statistical power compared to alternative methods, such as CB-SEM and multiple regression with sum scores

■ **Table 1.2** (continued)

<i>Model evaluation</i>	
Evaluation of the overall model	The concept of fit – as defined in CB-SEM – does not apply to PLS-SEM. Efforts to introduce model fit measures have generally proven unsuccessful
Evaluation of the measurement models	Reflective measurement models are assessed on the grounds of indicator reliability, internal consistency reliability, convergent validity, and discriminant validity Formative measurement models are assessed on the grounds of convergent validity, indicator collinearity, and the significance and relevance of indicator weights
Evaluation of the structural model	Collinearity among sets of predictor constructs Significance and relevance of path coefficients Criteria available to assess the model's in-sample (i.e., explanatory) power and out-of-sample predictive power ( $PLS_{predict}$ )
Additional analyses	Methodological research has substantially extended the original PLS-SEM method by introducing advanced modeling, assessment, and analysis procedures. Some examples include: Confirmatory tetrad analysis Confirmatory composite analysis Discrete choice modeling Endogeneity assessment Higher-order constructs Latent class analysis Measurement model invariance Mediation analysis Model selection Moderating effects, including moderated mediation Multigroup analysis Necessary condition analysis Nonlinear effects

Source: Adapted and extended from Hair et al. (2011). Copyright © 2011 by M.E. Sharpe, Inc. Reprinted by permission of the publisher (Taylor & Francis Ltd., ► <http://www.tandfonline.com>)

There are, however, several limitations of PLS-SEM. In its basic form, the technique cannot be applied when structural models contain causal loops or circular relationships between the latent variables (i.e., non-recursive models). Early extensions of the basic PLS-SEM algorithm that have not yet been implemented in standard PLS-SEM software packages, however, enable the handling of circular relationships (Lohmöller, 1989). Furthermore, since PLS-SEM does not have an established global goodness-of-fit measure, its use for theory testing and confirmation is more limited in certain situations. Recent research has attempted to promote common goodness-of-fit measures within a PLS-SEM framework (Schuberth, Henseler, & Dijkstra, 2018) but with very limited success. The concept of model fit – as defined in CB-SEM – is not applicable to PLS-SEM because of the methods'

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different functioning principles (Hair, Sarstedt, & Ringle, 2019). Instead, PLS-SEM-based model estimation and assessment follow a causal–predictive paradigm, in which the objective is to test the predictive power of a model, derived from theory and logic. As such, the method strikes a balance between machine learning methods, which are fully predictive in nature and CB-SEM, which focuses on confirmation and model fit (Richter, Cepeda Carrión, Roldán, & Ringle, 2016). Its causal–predictive nature makes PLS-SEM particularly appealing for research in fields that aim to derive recommendations for practice. For example, recommendations in managerial implication sections in business research journals always include predictive statements (“our results suggest that managers should...”). Making such statements requires a prediction focus on model estimation and evaluation (Sarstedt & Danks, 2021). PLS-SEM perfectly emphasizes this need as the method sheds light on the mechanisms (i.e., the structural model relationships) through which the predictions are generated (Hair, 2020; Hair & Sarstedt, 2019, 2021).

In early writing, researchers noted that PLS estimation is “deliberately approximate” to factor-based SEM (Hui & Wold, 1982, p. 127), a characteristic previously referred to as the **PLS-SEM bias** (e.g., Chin, Marcolin, & Newsted, 2003). A number of studies have used simulations to demonstrate the alleged PLS-SEM bias (e.g., Goodhue, Lewis, & Thompson, 2012; McDonald, 1996; Rönkkö & Evermann, 2013). According to prior research on the PLS-SEM bias, measurement model estimates are biased upward, whereas structural model estimates are biased downward compared to CB-SEM results. The studies conclude that parameter estimates will approach what has been labeled the “true” parameter values when both the number of indicators per construct and sample size increase (Hui & Wold, 1982). However, all the abovementioned simulation studies used CB-SEM as the benchmark against which the PLS-SEM estimates were evaluated with the assumption that they should be the same. Because PLS-SEM is a composite-based approach, which uses the total variance to estimate parameters, differences can be expected in such an assessment (Lohmöller, 1989; Schneeweiß, 1991). Not surprisingly, the very same issues apply when composite models are used to estimate CB-SEM results. In fact, Sarstedt et al. (2016) show that the bias produced by CB-SEM is far more severe than that of PLS-SEM, when applying the method to the wrong type of model (i.e., estimating composite models with CB-SEM versus estimating common factor models with PLS-SEM). Apart from these conceptual concerns, simulation studies show that the differences between PLS-SEM and CB-SEM estimates, when assuming the latter as a standard of comparison, are very small, provided that measurement models meet minimum recommended standards in terms of measurement quality (i.e., reliability and validity). Specifically, when the measurement models have four or more indicators and indicator loadings meet the common standards ( $\geq 0.70$ ), there are practically no differences between the two methods in terms of parameter accuracy (e.g., Reinartz, Haenlein, & Henseler, 2009; Sarstedt et al., 2016). Thus, the extensively discussed PLS-SEM bias is of no practical relevance for the vast majority of applications (e.g., Binz Astrachan, Patel, & Wanzenried, 2014).

Finally, methodological research has substantially extended the original PLS-SEM method by introducing advanced modeling, assessment, and analysis proce-

dures. Examples include different types of robustness checks (Sarstedt et al., 2020), higher-order constructs (Sarstedt, Hair, Cheah, Becker, & Ringle, 2019), discrete choice modeling (Hair, Sarstedt, & Ringle, 2019), necessary condition analysis and related methods (Rasoolimanesh, Ringle, Sarstedt, & Olya, 2021; Richter, Schubring, Hauff, Ringle, & Sarstedt, 2020), and out-of-sample prediction metrics (Hair, 2020). Hair, Sarstedt, Ringle, and Gudergan (2018) offer an introduction into several of these advanced topics.

In the following, we discuss aspects related to data characteristics (e.g., minimum sample size requirements) and model characteristics (e.g., model complexity).

### 1.4.2 Data Characteristics

Data characteristics, such as minimum sample size requirements, non-normal data, and scales of measurement (i.e., the use of different scale types), are among the most often stated reasons for applying PLS-SEM across numerous disciplines (e.g., Ghasemy, Teeroovengadum, Becker, & Ringle, 2020; Hair, Sarstedt, Ringle, & Mena, 2012; Ringle et al., 2020). While some of the arguments are consistent with the method's capabilities, others are not. In the following sections, we discuss these and also aspects related data characteristics.

#### 1.4.2.1 Minimum Sample Size Requirements

Small sample size is likely the most often abused reason stated for using PLS-SEM, with some researchers obtaining model solutions with unacceptably low sample sizes (Goodhue et al., 2012; Marcoulides & Saunders, 2006). These researchers oftentimes believe there is some “magic” in the PLS-SEM approach that allows them to use a very small sample to obtain results representing the effects that exist in large populations of several million elements or individuals. No multivariate analysis technique, including PLS-SEM, has this kind of “magic” inferential capability (Petter, 2018).

PLS-SEM can certainly obtain solutions with smaller samples, but the population's nature determines the situations in which small sample sizes are acceptable (Rigdon, 2016). For example, in business-to-business research, populations are often restricted in size. Assuming that other situational characteristics are equal, the more heterogeneous the population, the larger the sample size needed to achieve an acceptable accuracy (Cochran, 1977). If basic sampling theory guidelines are not considered (Sarstedt, Bengart, Shaltoni, & Lehmann, 2018), questionable results are produced.

In addition, when applying multivariate analysis techniques, the technical dimension of the sample size becomes relevant. Adhering to the minimum sample size guidelines ensures the results of a statistical method, such as PLS-SEM, have adequate statistical power. In these regards, an analysis based on an insufficient sample size may not reveal an effect that exists in the underlying population (which results in committing a type II error). Moreover, executing statistical analyses based on minimum sample size guidelines will ensure the results of the statistical method are robust and the model is generalizable to another sample from that

same population. Thus, an insufficient sample size may lead to PLS-SEM results that differ from those of another larger sample. In the following, we focus on the PLS-SEM method and its technical requirements of the minimum sample size.

The overall complexity of a structural model has little influence on the **minimum sample size requirements** for PLS-SEM. The reason is the PLS-SEM algorithm does not compute all relationships in the structural model at the same time. Instead, it uses ordinary least squares regressions to estimate the model's partial regression relationships. Two early studies systematically evaluated the performance of PLS-SEM with small sample sizes and concluded that the method performed well (e.g., Chin & Newsted, 1999; Hui & Wold, 1982). More recently, simulation studies by Hair et al. (2017) and Reinartz et al. (2009) indicate that PLS-SEM is the method of choice when the sample size is small. Moreover, compared with its covariance-based counterpart, PLS-SEM has higher levels of statistical power in situations with complex model structures and smaller sample sizes. Similarly, Henseler et al. (2014) show that results can be obtained with PLS-SEM when other methods do not converge or provide inadmissible solutions. For example, problems often are encountered when using CB-SEM on complex models, especially when the sample size is limited. Finally, CB-SEM encounters identification and convergence issues when formative measures are involved (e.g., Diamantopoulos & Riefler, 2011).

Unfortunately, some researchers believe sample size considerations do not play a role in the application of PLS-SEM. This idea has been fostered by the often-cited 10-time rule (Barclay, Higgins, & Thompson, 1995), which suggests the sample size should be equal to 10 times the number of independent variables in the most complex regression in the PLS path model (i.e., considering both measurement and structural models). This rule of thumb is equivalent to saying the minimum sample size should be 10 times the maximum number of arrowheads pointing at a latent variable anywhere in the PLS path model. While this rule offers a rough guideline, the minimum sample size requirement should consider the statistical power of the estimates. To assess statistical power, researchers can consider power tables (Cohen, 1992) or power analyses using programs, such as G\*Power (Faul, Erdfelder, Buchner, & Lang, 2009), which is available free of charge at ► <http://www.gpower.hhu.de/>. These approaches do not explicitly consider the entire model but instead use the most complex regression in the (formative) measurement models and structural model of a PLS path model as a point of reference for assessing the statistical power. In doing so, researchers typically aim at achieving a power level of 80%. However, the minimum sample size resulting from these calculations may still be too small (Kock & Hadaya, 2018).

Addressing these concerns, Kock and Hadaya (2018) proposed the **inverse square root method**, which considers the probability that the ratio of a path coefficient and its standard error will be greater than the critical value of a test statistic for a specific significance level. The results depend, therefore, on only one path coefficient and are dependent neither on the size of the most complex regression in the (formative) models nor on the size of the overall model. Assuming a common power level of 80% and significance levels of 1%, 5%, and 10%, the minimum sam-



ple size ( $n_{\min}$ ) is given by the following equations, respectively, where  $p_{\min}$  is the value of the path coefficient with the minimum magnitude in the PLS path model:

$$\text{Significance level} = 1\%: n_{\min} > \left( \frac{3.168}{|p_{\min}|} \right)^2.$$

$$\text{Significance level} = 5\%: n_{\min} > \left( \frac{2.486}{|p_{\min}|} \right)^2.$$

$$\text{Significance level} = 10\%: n_{\min} > \left( \frac{2.123}{|p_{\min}|} \right)^2.$$

For example, assuming a significance level of 5% and a minimum path coefficient of 0.2, the minimum sample size is given by

$$n_{\min} > \left( \frac{2.486}{0.2} \right)^2 = 154.505.$$

This result needs to be rounded to the next integer, so the minimum sample size is 155.

The inverse square root method is rather conservative, in that it slightly overestimates the sample size required to render an effect significant at a given power level. Most importantly, the method is characterized by its ease of use, since it can be readily implemented.

Nevertheless, two considerations are important when using the inverse square root method. First, by using the smallest statistical path coefficient as the point of reference, the method can be misleading as researchers will not expect marginal effects to be significant. For example, assuming a 5% significance level and a minimum path coefficient of 0.01 would require a sample size of 61,802! Hence, researchers should choose a higher path coefficient as input, depending on whether the model produces either overall weak or strong effects or the smallest relevant (to be detected) effect.

Second, by relying on model estimates, the inverse square root method follows a retrospective approach. As a result, this assessment approach can be used as a basis for additional data collection or adjustments in the model. If possible, however, researchers should follow a prospective approach by trying to derive the minimum expected effect size prior to data analysis. To do so, researchers can draw on prior research involving a comparable conceptual background or models with similar complexity or, preferably, the results of a pilot study, which tested the hypothesized model using a smaller sample of respondents from the same population. For example, if the pilot study produced a minimum path coefficient of 0.15, this value should be chosen as input for computing the required sample size for the main study.



**Table 1.3** Minimum sample sizes for different levels of minimum path coefficients ( $p_{\min}$ ) and a power of 80%

$p_{\min}$	Significance level		
	1%	5%	10%
0.05–0.1	1004	619	451
0.11–0.2	251	155	113
0.21–0.3	112	69	51
0.31–0.4	63	39	29
0.41–0.5	41	25	19

Source: Hair et al. (2022), Chap. 1; used with permission by Sage

In most cases, however, researchers have only limited information regarding the expected effect sizes, even if a pilot study has been conducted. Hence, it is reasonable to consider ranges of effect sizes rather than specific values to determine the sample size required for a specific study. Table 1.3 shows the minimum sample size requirement for different significance levels and varying ranges of  $p_{\min}$ . In deriving the minimum sample size, it is reasonable to consider the upper boundary of the effect range as reference, since the inverse square root method is rather conservative. For example, when assuming that the minimum path coefficient expected to be significant is between 0.11 and 0.20, one would need approximately 155 observations to render the corresponding effect significant at 5%. Similarly, if the minimum path coefficient expected to be significant is between 0.31 and 0.40, then the recommended sample size would be 39.

#### 1.4.2.2 Missing Value Treatment

As with other statistical analyses, missing values should be dealt with when using PLS-SEM. For reasonable limits (i.e., less than 5% values missing per indicator), **missing value treatment** options, such as mean replacement, the EM (expectation–maximization) algorithm, and nearest neighbor (e.g., Hair, Black, et al., 2019), generally result in only slightly different PLS-SEM estimates (Grimm & Wagner, 2020). Alternatively, researchers can opt for deleting all observations with missing values, which decreases variation in the data and may introduce biases when certain groups of observations have been deleted systematically.

#### 1.4.2.3 Non-normal Data

The use of PLS-SEM has two other key advantages associated with data characteristics (i.e., distribution and scales). In situations where it is difficult or impossible to meet the stricter requirements of more traditional multivariate techniques (e.g., normal data distribution), PLS-SEM is always the preferred method. PLS-SEM's greater flexibility is described by the label “soft modeling,” coined by Wold (1982), who developed the method. It should be noted, however, that “soft” is attributed

only to the distributional assumptions and not to the concepts, models, or estimation techniques (Lohmöller, 1989). PLS-SEM's statistical properties provide very robust model estimations with data that have normal as well as extremely non-normal (i.e., skewness and/or kurtosis) distributional properties (Hair, Hollingsworth, et al., 2017; Hair, Matthews, et al., 2017; Reinartz et al., 2009). It must be remembered, however, that influential observations, outliers, and collinearity do influence the ordinary least squares regressions in PLS-SEM and researchers should evaluate the data and results for these issues (Hair, Black, et al., 2019).

#### 1.4.2.4 Scales of Measurement

The PLS-SEM algorithm generally requires variables to be measured on a **metric scale (ratio scale or interval scale)** for the measurement model indicators. But the method also works well with ordinal scales with equidistant data points (i.e., quasi-metric scales; Sarstedt & Mooi, 2019; Chap. 3.6) and with binary-coded data. The use of binary-coded data is often a means of including categorical control variables (Hair et al., 2022) or moderators in PLS-SEM models. In short, binary indicators can be included in PLS-SEM models but require special attention. For example, using PLS-SEM in discrete choice experiments, where the aim is to explain or to predict a binary dependent variable, requires specific designs and estimation routines (Hair, Ringle, Gudergan, Fischer, Nitzl, & Menictas, 2019).

#### 1.4.2.5 Secondary Data

**Secondary data** are data that have already been gathered, often for a different research purpose some time ago (Sarstedt & Mooi, 2019; Chap. 3.2.1). Secondary data are increasingly available to explore real-world phenomena. Research based on secondary data typically focuses on a different objective than in a standard CB-SEM analysis, which is strictly confirmatory in nature. More precisely, secondary data are mainly used in exploratory research to propose causal–predictive relationships in situations that have little clearly defined theory (Hair, Matthews, et al., 2017; Hair, Hollingsworth, et al., 2017). Such settings require researchers to place greater emphasis on examining all possible relationships rather than achieving model fit (Nitzl, 2016). By its nature, this process creates large, complex models that can hardly be analyzed with the CB-SEM method. In contrast, due to its less stringent data requirements, PLS-SEM offers the flexibility needed for the interplay between theory and data (Nitzl, 2016). Or, as Wold (1982, p. 29) notes, “soft modeling is primarily designed for research contexts that are simultaneously data-rich and theory-skeletal.” Furthermore, the increasing popularity of secondary data analysis (e.g., by using data that stem from company databases, social media, customer tracking, national statistical bureaus, or publicly available survey data) shifts the research focus from strictly confirmatory to predictive and causal–predictive modeling. Such research settings are a perfect fit for the prediction-oriented PLS-SEM approach and even more so when assessing out-of-sample prediction (Shmueli, et al., 2019).

PLS-SEM also proves valuable for analyzing secondary data from a measurement theory perspective. First, unlike survey measures, which are usually crafted to confirm a well-developed theory, measures used in secondary data sources are typ-

**Table 1.4** Data considerations when applying PLS-SEM

- The 10-time rule is not a reliable indication of sample size requirements in PLS-SEM. While statistical power analyses provide a more reliable minimum sample size estimate, researchers should primarily draw on the inverse square root method, which is superior in terms of precision and ease of use
- When the construct measures meet recommended guidelines in terms of reliability and validity, results from CB-SEM and PLS-SEM are generally similar
- PLS-SEM can handle extremely non-normal data (e.g., data with high levels of skewness)
- Most missing value treatment procedures (e.g., mean replacement, pairwise deletion, EM, and nearest neighbor) can be used for reasonable levels of missing data (less than 5% missing per indicator) with limited effect on the analysis results
- PLS-SEM works with metric, quasi-metric, and categorical (i.e., dummy-coded) scaled data, although there are certain limitations. Processing of data from discrete choice experiments requires specific designs and estimation routines
- Due to its flexibility in handling different data and measurement types, PLS-SEM is the method of choice when analyzing secondary data

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ically not created and refined over time for confirmatory analyses. Thus, achieving model fit is very unlikely with secondary data measures in most research situations when using CB-SEM. Second, researchers who use secondary data do not have the opportunity to revise or refine the measurement model to achieve fit. Third, a major advantage of PLS-SEM when using secondary data is that it permits the unrestricted use of single-item and formative measures. This is extremely valuable for research involving secondary data, because many measures included in corporate databases are artifacts, such as financial ratios and other firm-fixed factors (Henseler, 2017). Such artifacts typically are reported in the form of formative indices whose estimation dictates the use of PLS-SEM.

■ Table 1.4 summarizes key considerations related to data characteristics.

### 1.4.3 Model Characteristics

PLS-SEM is very flexible in its modeling properties. In its basic form, the PLS-SEM algorithm requires all models to not include circular relationships or loops of relationships between the latent variables in the structural model. Although causal loops are sometimes specified in business research, this characteristic does not limit the applicability of PLS-SEM, if such models are required as Lohmöller's (1989) extensions of the basic PLS-SEM algorithm allow for handling such model types. Other model specification requirements that constrain the use of CB-SEM, such as distribution and identification assumptions, are generally not relevant with PLS-SEM.

Measurement model difficulties are one of the major obstacles to obtaining a solution with CB-SEM. For instance, estimation of complex models with many latent variables and/or indicators is often impossible with CB-SEM. In contrast,

PLS-SEM can easily be applied in such situations, since this method is not constrained by identification and other technical issues. Consideration of reflective and formative measurement models is a key issue in the application of SEM (Bollen & Diamantopoulos, 2017). PLS-SEM can easily handle both formative and reflective measurement models and is (therefore) considered the primary approach when the hypothesized model incorporates formative measures. CB-SEM can accommodate formative indicators, but to ensure model identification, they must follow distinct specification rules (Diamantopoulos & Riefler, 2011). In fact, the requirements often prevent running the analysis as originally planned. In contrast, PLS-SEM does not have such requirements and handles formative measurement models without any limitation. This also applies to model settings in which endogenous constructs are measured formatively. The applicability of CB-SEM to such model settings has been subject to considerable debate (Cadogan & Lee, 2013; Rigdon, 2014), but due to PLS-SEM’s multistage estimation process (Tenenhaus et al., 2005), which separates measurement from structural model estimation, the inclusion of formatively measured endogenous constructs is not an issue in PLS-SEM (Rigdon et al., 2014). The only problematic issue is when high levels of collinearity exist between the indicator variables of a formative measurement model.

Different from CB-SEM, PLS-SEM facilitates easy specification of interaction terms to map moderation effects in a path model. This makes PLS-SEM the method of choice in simple moderation models and more complex conditional process models, which combine moderation and mediation effects (Sarstedt, Hair, et al., 2020). Similarly, higher-order constructs, which allow specifying a construct simultaneously on different levels of abstraction (Sarstedt et al., 2019), can readily be implemented in PLS-SEM.

Finally, PLS-SEM is capable of estimating very complex models. For example, if theoretical or conceptual assumptions support large models and sufficient data are available (i.e., meeting minimum sample size requirements), PLS-SEM can handle models of almost any size, including those with dozens of constructs and hundreds of indicator variables. As noted by Wold (1985), PLS-SEM is virtually without competition when path models with latent variables are complex in their structural relationships. ■ Table 1.5 summarizes rules of thumb for PLS-SEM model considerations.

■ Table 1.5 Model considerations when choosing PLS-SEM

- PLS-SEM offers much flexibility in handling different measurement model setups. For example, PLS-SEM can handle reflective and formative measurement models as well as single-item measures without additional requirements or constraints
- The method allows for the specification of advanced model elements, such as interaction terms and higher-order constructs
- Model complexity is generally not an issue for PLS-SEM. As long as appropriate data meet minimum sample size requirements, the complexity of the structural model is virtually unrestricted

Source: Hair et al. (2022), Chap. 1; used with permission by Sage)

## 1.5 Guidelines for Choosing Between PLS-SEM and CB-SEM

Summarizing the previous discussions and drawing on Hair, Risher, et al. (2019), ■ Table 1.6 displays the rules of thumb applied when deciding whether to use CB-SEM or PLS-SEM. As can be seen, PLS-SEM is not recommended as a universal alternative to CB-SEM. Both methods differ from a statistical point of view, are designed to achieve different objectives, and rely on different measurement philosophies. Neither of the techniques is generally superior to the other, and neither of them is appropriate for all situations (Petter, 2018). Hence, to answer the question of when to use PLS-SEM versus CB-SEM, researchers should focus on the characteristics and objectives that distinguish the two methods (Hair, Sarstedt, Ringle, & Mena, 2012). Broadly speaking, with its strong focus on model fit and in light of its extensive data requirements, CB-SEM is particularly suitable for testing a theory in the confinement of a concise theoretical model. However, if the primary research objective is prediction and explanation of target constructs (Rigdon, 2012), PLS-SEM should be given preference (Hair, Sarstedt, & Ringle, 2019; Hair, Hollingsworth, Randolph, & Chong, 2017).

In general, the strengths of PLS-SEM are CB-SEM's limitations and vice versa, although PLS-SEM is increasingly being applied for scale development and confir-

■ Table 1.6 Rules of thumb for choosing between PLS-SEM and CB-SEM

*Use PLS-SEM when*

- The analysis is concerned with testing a theoretical framework from a prediction perspective, particularly out-of-sample prediction
- The structural model is complex and includes many constructs, indicators, and/or model relationships
- The research objective is to better understand increasing complexity by exploring theoretical extensions of established theories (exploratory research for theory development)
- The path model includes one or more formatively measured constructs
- The research consists of financial ratios or similar types of artifacts
- The research is based on secondary data, which may lack a comprehensive substantiation on the grounds of measurement theory
- A small population restricts the sample size (e.g., business-to-business research), but note that PLS-SEM also works very well with large sample sizes
- Distribution issues are a concern, such as lack of normality
- The research requires latent variable scores for follow-up analyses

*Use CB-SEM when*

- The goal is theory testing and confirmation
- Error terms require additional specification, such as the covariation
- The structural model has circular relationships
- The research requires a global goodness-of-fit criterion

Source: Adapted from Hair, Risher, et al. (2019). Copyright © 2019 by Emerald Publishing. Reprinted by permission of the publisher (Emerald Publishing; ► <https://www.emeraldgroupublishing.com>)

mation (Hair, Howard, & Nitzl, 2020). It is important that researchers understand the different applications each approach was developed for and use them accordingly. Researchers need to apply the SEM technique that best suits their research objective, data characteristics, and model setup (Roldán & Sánchez-Franco, 2012).

### Summary

SEM is a second-generation multivariate data analysis method, which facilitates analyzing the relationships among constructs, each measured by one or more indicator variables. The primary advantage of SEM is its ability to measure complex model relationships while accounting for measurement error inherent in the indicators. There are two types of SEM methods – CB-SEM and PLS-SEM. The two method types differ in the way they estimate the model parameters and their assumptions regarding the nature of measurement. Compared to CB-SEM, PLS-SEM emphasizes prediction, while simultaneously relaxing the demands regarding the data and specification of relationships. PLS-SEM aims at maximizing the endogenous latent variables' explained variance by estimating partial model relationships in an iterative sequence of ordinary least squares regressions. In contrast, CB-SEM estimates model parameters, such that the discrepancy between the estimated and sample covariance matrices is minimized. Instead of following a common factor model logic in estimating concept proxies as CB-SEM does, PLS-SEM calculates composites of indicators that serve as proxies for the concepts under research. The method is not constrained by identification issues, even if the model becomes complex – a situation that typically restricts CB-SEM use – and does not rely on distributional assumptions. Moreover, PLS-SEM can better handle formative measurement models and has advantages when sample sizes are relatively small as well as when analyzing secondary data. Researchers should consider the two SEM approaches as complementary and apply the SEM technique that best suits their research objective, data characteristics, and model setup.

### ? Exercise

Please answer the following questions:

1. When would SEM methods be more advantageous than first-generation techniques in understanding relationships between variables?
2. Why should social science researchers consider using SEM instead of multiple regression?
3. What are the most important considerations in deciding whether to use CB-SEM or PLS-SEM?
4. Under what circumstances is PLS-SEM the preferred method over CB-SEM?
5. Why is an understanding of theory important when deciding whether to use PLS-SEM or CB-SEM?
6. Why is PLS-SEM's prediction focus a major advantage of the method?

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