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AN INTRODUCTION TO STRUCTURAL EQUATION MODELING

LEARNING OUTCOMES

1. Understand the meaning of structural equation modeling (SEM) and its relationship to multivariate data analysis.
2. Describe the basic considerations in applying multivariate data analysis.
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.

CHAPTER PREVIEW

Social science researchers have been using statistical analysis tools for many years to extend their ability to develop, explore, and confirm research findings. Application of first-generation statistical methods, such as factor analysis and regression analysis, dominated the research landscape through the 1980s. But since the early 1990s, second-generation methods have expanded rapidly and, in some disciplines, represent almost 50% of the statistical tools applied in empirical research. In this chapter, we explain the fundamentals of second-generation statistical methods and establish a foundation that will enable you to understand and apply one of the emerging second-generation tools, referred to as **partial least squares structural equation modeling** (**PLS-SEM**).

WHAT IS STRUCTURAL EQUATION MODELING?

Statistical analysis has been an essential tool for social science researchers for more than a century. Applications of statistical methods have expanded dramatically with the advent of computer hardware and software, particularly in recent years with widespread access to many more methods due to user-friendly interfaces with technology-delivered knowledge. Researchers initially relied on univariate and bivariate analysis to understand data and relationships. To comprehend more complex relationships associated with current research directions in the social science disciplines, it is increasingly necessary to apply more sophisticated multivariate data analysis methods.

Multivariate analysis involves the application of statistical methods that simultaneously analyze multiple variables. The variables typically represent measurements associated with individuals, companies, events, activities, situations, and so forth. The measurements are often obtained from surveys or observations that are used to collect primary data, but they may also be obtained from databases consisting of secondary data. Exhibit 1.1 displays some of the major types of statistical methods associated with multivariate data analysis.

EXHIBIT 1.1 ■ Organization of Multivariate Methods

	Primarily Exploratory	Primarily Confirmatory
First-generation techniques	• Cluster analysis • Exploratory factor analysis • Multidimensional scaling	• Analysis of variance • Logistic regression • Multiple regression • Confirmatory factor analysis (CFA)
Second-generation techniques	• Partial least squares structural equation modeling (PLS-SEM)	• Covariance-based structural equation modeling (CB-SEM)

The statistical methods often used by social scientists are typically called **first-generation techniques** (Fornell, 1982, 1987). These techniques, shown in the upper part of Exhibit 1.1, include regression-based approaches, such as multiple regression, logistic regression, and analysis of variance, but also techniques, such as exploratory and confirmatory factor analysis, cluster analysis, and multidimensional scaling. When applied to a research question, these methods can be used to either confirm a priori established theories or identify data patterns and relationships. Specifically, they are **confirmatory** when testing the hypotheses of existing theories and concepts, and **exploratory** when they search for patterns in the data in case there is no or only little prior knowledge on how the variables are related.

It is important to note that the distinction between confirmatory and exploratory is not always as clear-cut as it seems. For example, when running a regression analysis, researchers usually select the dependent and independent variables based on established theories and concepts. The goal of the regression analysis is then to test these theories and concepts. However, the technique can also be used to explore whether additional independent variables prove valuable for extending the concept being tested. The findings typically focus first on which independent variables are statistically significant predictors of the single dependent variable (more confirmatory) and then on which independent variables are, relatively speaking, better predictors of the dependent variable (more exploratory). In a similar fashion, when exploratory factor analysis is applied to a data set, the method searches for relationships between the variables in an effort to reduce a large number of variables to a smaller set of composite factors (i.e., linear combinations of variables). The final set of composite factors is a result of exploring relationships in the data and reporting the relationships that are found (if any). Nevertheless, while the technique is exploratory in nature (as the name already suggests), researchers often have theoretical knowledge that may, for example, guide their decision on how many composite factors to extract from the data (Sarstedt & Mooi, 2019; Chapter 8.3.3). In contrast, the confirmatory factor analysis is specifically designed for testing and substantiating an a priori determined factor(s) and its assigned indicators.

First-generation techniques have been widely applied by social science researchers, and they have significantly shaped the way we see the world today. In particular, methods such as multiple regression, logistic regression, and analysis of variance have been used to empirically test relationships among variables. However, what is common to these techniques is that they share three limitations, namely (1) the postulation of a simple model structure, (2) the assumption that all variables can be considered observable, and (3) the conjecture 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 great number of intervening variables can only be estimated piecewise rather than simultaneously, which can have severe consequences for the results' quality (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 or entity" (Bagozzi & Philipps, 1982, p. 465), can only be considered after prior stand-alone validation by means of, for example, a confirmatory factor analysis. The ex post inclusion of measures of theoretical concepts, however, comes with various limitations.

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 measurement error, which can be systematic or random (Chapter 4). First-generation techniques are, strictly speaking, only applicable when there is 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. As the social sciences, 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 indicator variables. 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 and chapters in greater detail.

There are two types of SEM methods: **covariance-based structural equation modeling (CB-SEM)** and partial least squares structural equation modeling (PLS-SEM; also called **PLS path modeling**). CB-SEM is primarily used to confirm (or reject) theories (i.e., a set of systematic relationships between multiple variables that can be tested empirically). It does this by determining how well a proposed theoretical model can estimate the covariance matrix for a sample data set. 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). We explain these differences in more detail later in the chapter.

PLS-SEM is evolving rapidly as a statistical modeling technique. Over the last decades, there have been numerous introductory articles on the method (e.g., Chin, 1998; Haenlein & Kaplan, 2004; 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 (Exhibit 1.2). 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).

EXHIBIT 1.2 ■ Review Articles on PLS-SEM Usage

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

Until the first edition of this book, published in 2014, there was no comprehensive textbook that explained the fundamental aspects of the method, particularly in a way that can be comprehended by the non-statistician. In recent years, a growing number of follow-up textbooks (e.g., Garson, 2016; Henseler, 2020; Ramayah, Cheah, Chuah, Ting, & Memon, 2016; Wong, 2019) and edited books on the method (e.g., Avkiran & Ringle, 2018; Esposito Vinzi, Chin, Henseler, & Wang, 2010; Latan & Noonan, 2017) have been published, which helped to further popularize PLS-SEM. This third edition of our book expands and clarifies the nature and role of PLS-SEM in social science research and hopefully makes researchers aware of a tool that will enable them to pursue research opportunities in many new and different ways.

CONSIDERATIONS IN USING STRUCTURAL EQUATION MODELING

Depending on the underlying research question and the empirical data available, researchers must select an appropriate multivariate analysis method. Regardless of whether a researcher is using first- or second-generation multivariate analysis methods, several considerations are necessary in deciding to use multivariate analysis, particularly SEM. Among the most important are the following five elements: (1) composite variables, (2) measurement, (3) measurement scales, (4) coding, and (5) data distributions.

Composite Variables

A **composite variable** (also referred to as a **variate**) is a linear combination of several variables that are chosen based on the research problem at hand (Hair, Black, Babin, & Anderson, 2019). The process for combining the variables involves calculating a set of weights, multiplying the weights (e.g., w_1 and w_2) times the associated data observations for the variables (e.g., x_1 and x_2), and summing them. The mathematical formula for this linear combination with five variables is shown as follows (note that the composite value can be calculated for any number of variables):

$$\textit{Composite value} = w_1 \cdot x_1 + w_2 \cdot x_2 + \ldots + w_5 \cdot x_5,$$

where x stands for the individual variables and w represents the weights. All x variables (e.g., questions in a questionnaire) have responses from many respondents that can be arranged in a data matrix. Exhibit 1.3 shows such a data matrix, where i is an index that stands for the number of responses (i.e., cases). A composite value is calculated for each of the i respondents in the sample.

EXHIBIT 1.3 ■ Data Matrix

Case	x_1	x_2	. . .	x_5	Composite Value
1	x_{11}	x_{21}	. . .	x_{51}	v_1
. . .	. . .	. . .	. . .	. . .	. . .
i	x_{1i}	x_{2i}	. . .	x_{5i}	v_i

Measurement

Measurement is a fundamental concept in conducting social science research. When we think of **measurement**, the first thing that comes to mind is often a ruler, which could be used to measure someone's height or the length of a piece of furniture. But there are many other examples of measurement in life. When you drive, you use a speedometer to measure the speed of your vehicle, a heat gauge to measure the temperature of the engine, and a gauge to determine how much fuel remains in your tank. If you are sick, you use a thermometer to measure your temperature, and when you go on a diet, you measure your weight on a bathroom scale.

Measurement is the process of assigning numbers to a variable based on a set of rules (Hair, Page, & Brunsveld, 2020). The rules are used to assign the numbers to the variable in a way that accurately represent the variable. With some variables, the rules are easy to follow, while with other variables, the rules are much more difficult to apply. For example, if the variable is gender, then it is easy to assign a 1 for females and a 0 for males. Similarly, if the variable is age or height, it is again easy to assign a number. But what if the variable is satisfaction or trust? Measurement in these situations is much more difficult because the phenomenon that is supposed to be measured is abstract, complex, and not directly observable. We therefore talk about the measurement of **latent variables** or **constructs**.

We cannot directly measure abstract concepts such as satisfaction or trust. However, we can measure indicators of what we have agreed to call satisfaction or trust, for example, in a brand, product, or company. Specifically, when concepts are difficult to measure, one approach is to measure them indirectly by using a set of directly observable and measurable **indicators** (also called **items** or **manifest variables**). Each indicator represents a single separate aspect of a larger abstract concept. For example, if the concept is restaurant satisfaction, then the several indicators that could be used to measure this might be the following:

1. The taste of the food was excellent.
2. The speed of service met my expectations.

3. The waitstaff was very knowledgeable about the menu items.
4. The background music in the restaurant was pleasant.
5. The meal was a good value compared with the price.

By combining several indicators to form a scale (or index; Chapter 2), we can indirectly measure the overall concept of restaurant satisfaction. Usually, researchers use several items to form a multi-item scale, which indirectly measures a concept, as in the restaurant satisfaction example above. The several measures are combined to form a single **composite score** (i.e., the score of the variate). In some instances, the composite score is a simple summation of the several measures. In other instances, the scores of the individual measures are combined to form a composite score by using a linear weighting process. The logic of using several individual variables to measure an abstract concept such as restaurant satisfaction is that the measure will be more accurate. The anticipated improved accuracy is based on the assumption that using several items to measure a single concept is more likely to represent all the different aspects of that concept. This involves reducing **measurement error**, which is the difference between the true value of a variable and the value obtained by a measurement. There are many sources of measurement error, including poorly worded questions in a survey, misunderstanding of the scaling approach, and incorrect application of a statistical method. Indeed, all measurements used in multivariate analysis are likely to contain some measurement error. The objective, therefore, is to reduce the measurement error as much as possible.

Rather than using multiple items, researchers sometimes opt for the use of **single-item constructs** to measure concepts such as satisfaction or purchase intention. For example, we may use only "Overall, I'm satisfied with this restaurant" to measure restaurant satisfaction instead of all five items described above. While this is a good way to make the questionnaire shorter, it also reduces the quality of your measurement. We discuss the fundamentals of measurement and measurement evaluation in the following chapters.

Measurement Scales

A **measurement scale** is a tool with a predetermined number of closed-ended responses that can be used to obtain an answer to a question. There are four types of measurement scales, each representing a different level of measurement—nominal, ordinal, interval, and ratio. Nominal scales are the lowest level of scales because they are the most restrictive in terms of the type of analysis that can be carried out. A **nominal scale** assigns numbers that can be used to identify and classify objects (e.g., people, companies, products) and is also referred to as a **categorical scale**. For example, if a survey asked a respondent to identify his or her profession and the categories are doctor, lawyer, teacher, engineer, and so forth, the question has a nominal scale. Nominal scales can have two or more categories, but each category must be mutually exclusive, and all possible categories must be included. A number could be assigned to identify each category, and the numbers could be used to count the responses in each category, or the modal response or percentage in each category.

If we have a variable measured on an **ordinal scale**, we know that if the value of that variable increases or decreases, this gives meaningful information. For example, if we code customers' use of a product as nonuser = 0, light user = 1, and heavy user = 2, we know that if the value of the use variable increases, the level of use also increases. Therefore, when an attribute or characteristic is measured on an ordinal scale, the values provide information about the order of our observations. However, we cannot assume that the differences in the order are equally spaced. That is, we do not know if the difference between "nonuser" and "light user" is the same as between "light user" and "heavy user," even though the differences in the values (i.e., 0–1 and 1–2) are equal. Therefore, it is not appropriate to calculate arithmetic means or variances for ordinal data.

If an attribute or characteristic is measured with an **interval scale**, we have precise information on the rank order at which something is measured and, in addition, we can interpret the magnitude of the differences in values directly. For example, if the temperature is 80°F, we know that if it drops to 75°F, the difference is exactly 5°F. This difference of 5°F is the same as the increase from 80°F to 85°F. This exact "spacing" is called **equidistance**, and equidistant scales are necessary for certain analysis techniques, such as SEM. What the interval scale does not give us is an absolute zero point. If the temperature is 0°F, it may feel cold, but the temperature can drop further. The value of 0 therefore does not mean that there is no temperature at all (Sarstedt & Mooi, 2019; Chapter 3.6). The value of interval scales is that almost any type of mathematical computations can be carried out, including the mean and standard deviation. Moreover, you can convert and extend interval scales to alternative interval scales. For example, instead of degrees Fahrenheit (°F), many countries use degrees Celsius (°C) to measure the temperature. While 0°C marks the freezing point, 100°C depicts the boiling point of water. You can convert temperature from Fahrenheit into Celsius by using the following equation: Degrees Celsius (°C) = (degrees Fahrenheit (°F) – 32) · 5 / 9. In a similar way, you can convert data (via rescaling) on a scale from 1 to 5 into data on a scale from 0 to 100: (([data point on the scale from 1 to 5] – 1) / (5 – 1)) · 100.

A **ratio scale** provides the most information. If something is measured on a ratio scale, we know that a value of 0 means that a particular characteristic for a variable is not present. For example, if a customer buys no products (value = 0), then he or she really buys no products. Or, if we spend no money on advertising a new product (value = 0), we really spend no money. Therefore, the zero point or origin of the variable is equal to 0. The measurement of length, mass, and volume as well as time elapsed uses ratio scales. With ratio scales, all types of mathematical computations are possible.

Coding

The assignment of numbers to categories in a manner that facilitates measurement is referred to as **coding**. In survey research, data are often precoded. Precoding is assigning numbers ahead of time to answers (e.g., scale points) that are specified on a questionnaire. For example, a 10-point agree–disagree scale typically would assign the number 10 to the highest endpoint "agree" and a 1 to the lowest endpoint "disagree," and the points between would be coded 2 to 9. Postcoding is assigning numbers to categories of responses after data are collected. The responses might be to an open-ended question in a quantitative survey or to an interview response in a qualitative study.

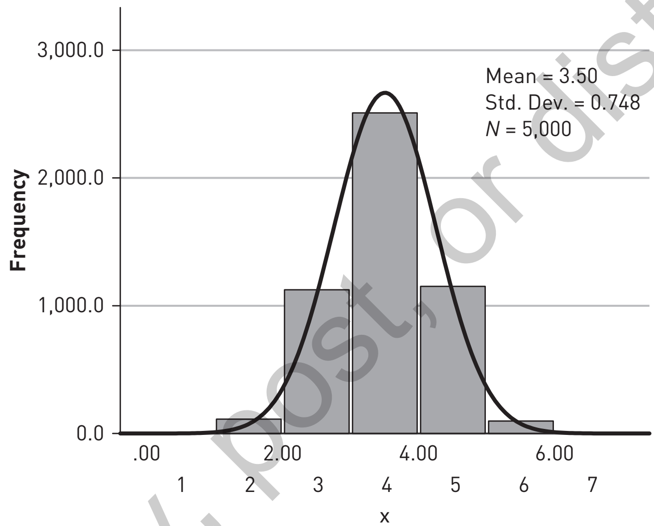
Coding is very important in the application of multivariate analysis because it determines when and how various types of scales can be used. For example, variables measured with interval and ratio scales can always be used with multivariate analysis. However, when using ordinal scales such as Likert scales (which is common within an SEM context), researchers have to pay special attention to the coding to fulfill the requirement of equidistance. For example, when using a typical 7-point Likert scale with the categories (1) *fully disagree*, (2) *disagree*, (3) *somewhat disagree*, (4) *neither agree nor disagree*, (5) *somewhat agree*, (6) *agree*, and (7) *fully agree*, the inference is that the "distance" between categories 1 and 2 is the same as between categories 3 and 4. In contrast, the same type of Likert scale but using the categories (1) *fully disagree*, (2) *disagree*, (3) *neither agree nor disagree*, (4) *somewhat agree*, (5) *agree*, (6) *strongly agree*, and (7) *fully agree* is unlikely to be equidistant, as there are only two categories below the neutral category "neither agree nor disagree," whereas four categories score above the neutral category. This would clearly bias any result in favor of a better outcome. A suitable Likert scale, as in our first example above, will present symmetry of Likert items about a middle category that have clearly defined linguistic qualifiers for each category. In such symmetric scaling, equidistant attributes will typically be more clearly observed or, at least, inferred. When a Likert scale is perceived as symmetric and equidistant, it will behave more like an interval scale. So, while a Likert scale is ordinal, if it is well presented, then it is likely that the Likert scale can approximate an interval-level measurement, and the corresponding variables can be used in SEM.

Data Distributions

When researchers collect quantitative data, the answers to the questions asked are reported as a distribution across the available (predefined) response categories. For example, if responses are requested using a 7-point agree–disagree scale, then a distribution of the answers in each of the possible response categories (1, 2, 3, . . . , 7) can be calculated and displayed in a table or chart.

Exhibit 1.4 shows an example of the frequencies of a corresponding variable *x*. As can be seen, most respondents indicated a 4 on the 7-point scale, followed by 3 and 5, and finally (barely visible), 1 and 7. Overall, the frequency count approximately follows a bell-shaped, symmetric curve around the mean value of 4. This bell-shaped curve is the normal distribution, which many statistical methods require for their analyses.

EXHIBIT 1.4 ■ Distribution of Responses



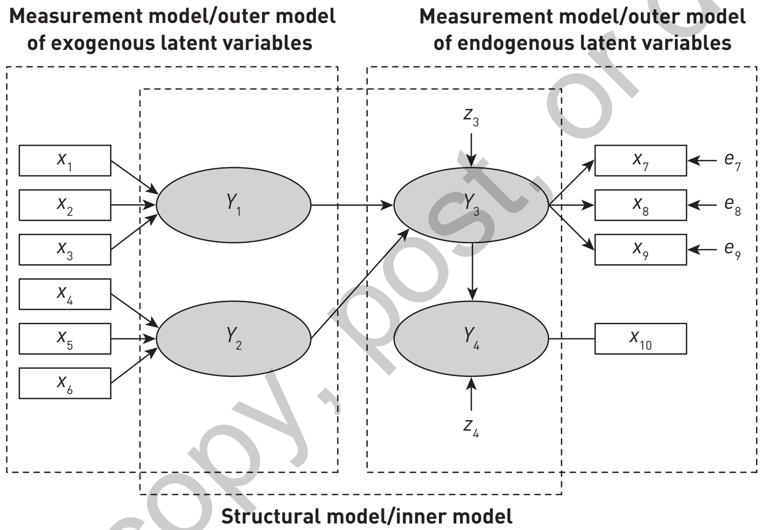
While many different types of distributions exist (e.g., normal, binomial, Poisson), researchers working with SEM generally only need to distinguish normal from nonnormal distributions. Normal distributions are usually desirable, especially when working with CB-SEM. In contrast, PLS-SEM generally makes no assumptions about the data distributions. However, for reasons discussed in later chapters, it is worthwhile to consider the distribution when working with PLS-SEM. To assess whether the data follow a normal distribution, researchers can apply statistical tests such as the Kolmogorov–Smirnov test and Shapiro–Wilk test (Sarstedt & Mooi, 2019; Chapter 6.3.3.3). In addition, researchers can examine two measures of distributions—skewness and kurtosis (Chapter 2)—which allow assessing to what extent the data deviate from normality (Hair, Black, Babin, & Anderson, 2019).

PRINCIPLES OF STRUCTURAL EQUATION MODELING

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 Exhibit 1.5.

EXHIBIT 1.5 ■ A Simple Path Model



Constructs (i.e., variables that are not directly measured) 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 variables 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 shown 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, a construct's **measurement model** (also referred to as the **outer model** in PLS-SEM) displays the relationships between the construct and its indicator variables (rectangles). In Exhibit 1.5, there are two types of measurement models: one for the **exogenous latent variables** (i.e., those constructs that 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 has only the x_{10} indicator in the measurement model.

The **error terms** (e.g., e_7 or e_8; Exhibit 1.5) 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). In Exhibit 1.5, error terms e_7 to e_9 are on those indicators whose relationships point from the construct (Y_3) to the indicator (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 Exhibit 1.5, 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.

Testing Theoretical Relationships

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 construct. In contrast, **structural theory** specifies how the constructs are related to each other 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.

Measurement Theory

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 Exhibit 1.5 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 the exhibit 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 Exhibit 1.5, 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 vs. formatively and whether to use multiple items or a single-item measure are fundamental when developing path models. We therefore explain these two approaches to modeling constructs as well as their variations in more detail in Chapter 2.

Structural Theory

Structural theory shows how the latent variables are related to each other (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 the 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) they may also serve as both independent and dependent variables in the structural model.

When latent variables serve only as independent variables, they are called exogenous latent variables (Y_1 and Y_2). When latent variables serve only as dependent variables (Y_4) or as both independent and dependent variables (Y_3), they are called endogenous latent variables. Any latent variable that has only single-headed arrow 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.

PLS-SEM, CB-SEM, AND REGRESSIONS BASED ON SUM SCORES

There are two main approaches to estimating the relationships in a structural equation model (Hair, Black, Babin, & Anderson, 2019; Hair, Ringle, & Sarstedt, 2011). One is CB-SEM, 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 done by PLS-SEM. The sum scores approach offers practically no value compared to the PLS-SEM weighted approach. For this reason, in the following, 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 (Diamantopoulos, Riefler, & Roth, 2008). 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, "these 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 the method is regarded as a **composite-based SEM** method (Hwang et al., 2020). Model estimation in PLS-SEM involves combining the indicators based on a linear method to form composite variables (Chapter 3). 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, Hair, Ringle, Thiele, & Gudergan, 2016). Researchers can include reflectively and formatively specified measurement models, which PLS-SEM estimates without any limitations.

In following a composite-based approach to SEM, PLS relaxes the strong assumptions 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 with multiple regression using **sum scores**. If multiple regression with sum scores is used, the researcher assumes an equal weighting of indicators, which means that each indicator contributes equally to forming the composite (Hair & Sarstedt, 2019; Henseler et al., 2014). Referring to our descriptions on composite variables at the very beginning of this chapter, this would imply that all indicator weights w are set to 1. As noted earlier, the resulting mathematical formula for a linear combination with five variables would be as follows:

$$\textit{Composite value} = 1 \cdot x_1 + 1 \cdot x_2 + \ldots + 1 \cdot x_5.$$

For example, if a respondent has the scores 4, 5, 4, 6, and 7 on the five variables, the corresponding composite value would be 26. While easy to apply, regressions using sum scores equalize any differences in the individual item weights. Such differences are, however, common in research reality, and ignoring them entails substantial biases in the parameter estimates (e.g., Hair, Hollingsworth, Randolph, & Chong, 2017). Furthermore, learning about individual item weights offers important insights, as the researcher learns about each item's importance for forming the composite in a certain context (i.e., its relationships with other composites in the structural model). When measuring customer satisfaction, for example, the researcher learns which aspects covered by the individual items are of particular importance for the shaping of satisfaction.

It is important to note that the composites produced by PLS-SEM are not assumed to be identical to the constructs, which they replace. 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 as common factors derived in CB-SEM are also not necessarily equivalent to the theoretical concepts that are the focus of research (Rigdon, 2012; Rigdon, Sarstedt, & Ringle, 2017; Rossiter, 2011; Sarstedt, Hair, Ringle, Thiele, & Gudergan, 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 considered in 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. More precisely, in an effort to improve model fit, researchers typically restrict the number of indicators per construct, which in turn increases uncertainty (Hair, Matthews, Matthews, & Sarstedt, 2017; Rigdon, Becker, & Sarstedt, 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 casts additional doubt on this measurement practice.

Apart from differences in the philosophy of measurement, the differing treatment of latent variables and, more specifically, the availability of latent variable scores also has 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., Hair & Sarstedt, 2021a; Dijkstra, 2014). In contrast, a major advantage of PLS-SEM is that it always produces a single specific (i.e., determinate) composite score for each case, once the weights are established. These determinate scores are proxies of the concepts being measured, just as factors are proxies for the conceptual variables in CB-SEM (Rigdon, Sarstedt, & Ringle, 2017; Sarstedt, Hair, Ringle, Thiele, & Gudergan, 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** (i.e., the amount of explained variance) of the (target) endogenous constructs. This feature achieves the (in-sample) prediction objective of PLS-SEM, 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 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) in the model estimation (Hair, Black, Babin, & Anderson, 2019). That is, CB-SEM only explains the covariation between the indicators (Jöreskog, 1973) and does not focus on predicting dependent variables (Hair, Matthews, Matthews, & Sarstedt, 2017).

Note that 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, it 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).

CONSIDERATIONS WHEN APPLYING PLS-SEM

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. There are four critical issues relevant to the application of PLS-SEM (Hair, Ringle,

& Sarstedt, 2011; Hair, Risher, Sarstedt, & Ringle, 2019): (1) data characteristics, (2) model characteristics, (3) model estimation, and (4) model evaluation. Exhibit 1.6 summarizes the key characteristics of the PLS-SEM method. An initial overview of these issues is provided in this chapter, and a more detailed explanation is provided in later chapters of the book, particularly as they relate to the PLS-SEM algorithm and evaluation of results.

EXHIBIT 1.6 ■ Key Characteristics of PLS-SEM

	Data Characteristics
Sample size	• Neglectable 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 also accommodates binary coded variables, but additional considerations are required when they are used as control variables, moderators, and in the analysis of data from discrete choice experiments
	Model Characteristics
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

(Continued)

EXHIBIT 1.6 ■ (Continued)

Model Characteristics	
Model complexity	• Handles complex models with many structural model relationships
Model setup	• No causal loops (no circular relationships) are allowed in the structural model
Model Estimation	
Objective	• Aims at maximizing the amount of unexplained variance in the dependent measures (i.e., maximizes 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 when solutions are 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
Model Evaluation	
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

(Continued)

EXHIBIT 1.6 ■ (Continued)

Model Evaluation	
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 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: o Confirmatory tetrad analysis o Discrete choice modeling o Endogeneity assessment o Higher-order constructs o Latent class analysis o Measurement model invariance o Mediation analysis o Model selection o Moderating effects o Multigroup analysis o Necessary condition analysis o Nonlinear effects

Source: Adapted and extended from Hair, J. F., Ringle, C. M., & Sarstedt, M. (2011). PLS-SEM: Indeed a silver bullet. *Journal of Marketing Theory and Practice*, *19*(2), 139–151. Copyright © 2011 by M. E. Sharpe, Inc. Reprinted with permission of the publisher (Taylor & Francis Ltd., http://www.tandfonline.com).

PLS-SEM works efficiently with small sample sizes and complex models (Cassel, Hackl, & Westlund, 1999; Chin, 2010). 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** compared to 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 based on sum scores, which lags behind PLS-SEM in terms of statistical power (Hair, Hult, Ringle, Sarstedt, & Thiele, 2017).

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 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' differing functioning principles (see Chapter 6 for details). Instead, PLS-SEM-based model estimation and assessment follows a causal–predictive paradigm, where the aim is to test the predictive power in the confinements of a model carefully developed on the ground of theory and logic. The underlying causal–predictive logic follows what Gregor (2006) refers to as **explaining and predicting (EP) theories**. EP theories imply an understanding of the underlying causes and prediction as well as description of theoretical constructs and their relationships. According to Gregor (2006, p. 626), this type of theory "corresponds to commonly held views of theory in both the natural and social sciences." Numerous seminal theories and models such as Oliver's (1980) expectation–disconfirmation theory or the various technology acceptance models (e.g., Davis, 1989; Venkatesh, Morris, Davis, & Davis, 2003) follow an EP–theoretic approach in that they aim to explain *and* predict. PLS-SEM is perfectly suited to investigate models derived from EP theories as 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 implications sections that populate business research journals always come in the form of predictive statements ("our results suggest that managers should . . ."). Making such statements requires a prediction focus in model estimation and evaluation. PLS-SEM perfectly emphasizes this need as the method sheds light on the mechanisms (i.e., the structural model relationships) through which the predictions were generated (Hair, 2020; Hair & Sarstedt, 2019, 2021b).

In early writing, researchers noted that PLS estimation is "deliberately approximate" to factor-based SEM (Hui & Wold 1982, p. 127), a characteristic that has come to be known as the **PLS-SEM bias** (e.g., Chin, Marcoulin, & 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), which manifests itself in measurement model estimates that are higher, while structural model estimates that are lower compared to the prespecified values. 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 these 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, biases can be expected in such an assessment (Lohmöller, 1989; Schlittgen, Sarstedt, & Ringle, 2020; Schneeweiß, 1991). Not surprisingly, the very same issues apply when composite models are used to estimate CB-SEM results. In fact, Sarstedt, Hair, Ringle, Thiele, and Gudergan (2016) show that the biases produced by CB-SEM are far more severe than those of PLS-SEM, when applying the method to the wrong type of model (i.e., estimating composite models with CB-SEM vs. estimating common factor models with PLS-SEM). When acknowledging the different nature of the construct measures, most of the criticism voiced by critics of the PLS-SEM method (Rönkkö, McIntosh, Antonakis, & Edwards, 2016) are no longer an issue (Cook & Forzani, 2020). 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 (≥0.70), there is practically no difference between the two methods in terms of parameter accuracy (e.g., Reinartz, Haenlein, & Henseler, 2009; Sarstedt, Hair, Ringle, Thiele, & Gudergan, 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 procedures. Examples include different types of robustness checks (Sarstedt, Ringle et al., 2020), discrete choice modeling (Hair, Ringle et al., 2018), necessary condition analysis (Richter, Schubring, Hauff, Ringle, & Sarstedt, 2020), out-of-sample prediction metrics (Hair, 2020), endogeneity assessment (Hult et al., 2018), and higher-order constructs (Sarstedt, Hair, Cheah, Becker, & Ringle, 2019). Chapter 8 and Hair, Sarstedt, Ringle, and Gudergan (2018) offer an introduction into several of these advanced issues.

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

Data Characteristics

Data characteristics, such as **minimum sample size requirements**, nonnormal 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, Sarstedt, Mitchell, & Gudergan, 2020). While some of the arguments are consistent with the method's capabilities, others are not. In the following sections, we discuss these and related data characteristics.

Minimum Sample Size Requirements

Small sample size is probably the most often misused argument for using PLS-SEM, with some researchers considering 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 (e.g., less than 100) to obtain results representing the effects that exist in a population of several million elements or individuals. No multivariate analysis technique, including PLS-SEM, has this kind of "magic" capabilities (Petter, 2018).

PLS-SEM can certainly be used 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 sampling error (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 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 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 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). Subsequent simulation studies by, for example, Hair, Hult, Ringle, Sarstedt, and Thiele (2017) and Reinartz, Haenlein, and Henseler (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 solutions can be obtained with PLS-SEM when other methods such as CB-SEM do not converge or provide inadmissible solutions. For instance, problems often are encountered when using CB-SEM on complex models, especially when the sample size is limited. Finally, CB-SEM suffers from identification and convergence issues when formative measures are involved (e.g., Diamantopoulos & Riefler, 2011).

Unfortunately, some researchers believe that sample size considerations do not play a role in the application of PLS-SEM. This idea has been fostered by the often-cited **10 times 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 use the most complex regression in the (formative) measurement models and structural model of a PLS path model as 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. Therefore, the results for the technically required minimum sample size depend on only one path coefficient and do not depend on the size of the most complex regression in the model. Assuming a common power level of 80% and significance levels of 1%, 5%, and 10%, the minimum sample size (n_{min}) is given by the following equations, where p_{min} is the value of the path coefficient with the minimum magnitude in the PLS path model, which is expected to be statistically significant:

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

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

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

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 stands out due to its ease of use as 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 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, either depending on whether the model produces overall weak or strong effects or depending on the smallest relevant (to be detected) effect.

Second, by relying on model estimates, the inverse square root method follows a retrospective approach. Such an assessment 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. 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. Exhibit 1.7 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 as 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.

EXHIBIT 1.7 ■ Minimum Sample Sizes for Different Levels of Minimum Path Coefficients (p_{min}) and Significance Levels

p_{min}	Significance level		
	1%	5%	10%
0.05–0.1	1,004	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

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, EM (expectation–maximization algorithm), and nearest neighbor (e.g., Hair, Black, Babin, & Anderson, 2019) generally result in only slightly different PLS-SEM estimates. 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.

Nonnormal Data

The use of PLS-SEM has two other key advantages related to 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 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 nonnormal distributional properties (Hair, Hult, Ringle, Sarstedt, & Thiele, 2017; Reinartz, Haenlein, & Henseler, 2009). It must be remembered, however, that influential 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, Babin, & Anderson, 2019).

Scales of Measurement

The PLS-SEM algorithm generally requires variables to be measured on a **metric scale** (ratio or interval measurement) 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; Chapter 3.6) and with binary coded data. The use of binary coded data is often a means of including categorical control variables 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 predict a binary dependent variable requires specific designs and estimation routines (Hair, Ringle et al., 2019).

Secondary Data

Secondary data are data that have already been gathered, often for a different research purpose and some time ago (Sarstedt & Mooi, 2019; Chapter 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 relationships in situations that have little clearly defined theory (Hair, Risher, Sarstedt, & Ringle, 2019; Hair, Hollingsworth, Randolph, & Chong, 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 cannot be analyzed with the CB-SEM method. In contrast, due to its less stringent requirements on the data, 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 (also see Gefen, Rigdon, & Straub, 2011).

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 typically 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, 2017b). Such artifacts typically are reported in the form of formative indices whose estimation dictates the use of PLS-SEM.

Exhibit 1.8 summarizes key considerations related to data characteristics.

EXHIBIT 1.8 ■ Data Considerations When Applying PLS-SEM

- The 10 times rule is not a reliable indication of sample size requirements in PLS-SEM. Statistical power analyses provide a more reliable minimum sample size estimate. Researchers can also draw on the inverse square root method as a more conservative way of assessing minimum sample size requirements.
- When the construct measures meet recommended guidelines in terms of reliability and validity, results from CB-SEM and PLS-SEM are generally very similar.
- PLS-SEM can handle extremely nonnormal data (e.g., data with high levels of skewness).
- Due to its flexibility in handling different data and measurement types, PLS-SEM is the method of choice when analyzing secondary data.
- 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.

Model Characteristics

PLS-SEM is very flexible in its modeling properties. In its basic form, the PLS-SEM algorithm requires all models to be without 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 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 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 be used in such situations since it 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 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, 2014a), but due to PLS-SEM's multistage estimation process (Chapter 3), 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 a high level of collinearity exists 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 (Chapter 3). Exhibit 1.9 summarizes rules of thumb for PLS-SEM model characteristics.

EXHIBIT 1.9 ■ 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.

GUIDELINES FOR CHOOSING BETWEEN PLS-SEM AND CB-SEM

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, Hollingsworth, Randolph, & Chong, 2017; Hair, Sarstedt, & Ringle, 2019).

Summarizing the previous discussions and drawing on Hair, Risher, Sarstedt, and Ringle (2019), Exhibit 1.10 displays the rules of thumb that can be 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 philosophies of measurement. Neither of the techniques is generally superior to the other, and neither of them is appropriate for all situations (Petter, 2018). 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 confirmation (Hair, Howard, & Nitzl, 2020). It is important that researchers understand the different applications each approach was developed for—and to 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).

EXHIBIT 1.10 ■ 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;
- 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 PLS-SEM also works very well with large sample sizes;
- distribution issues are a concern, such as lack of normality; or
- the research requires latent variable scores for follow-up analyses.

Use CB-SEM when

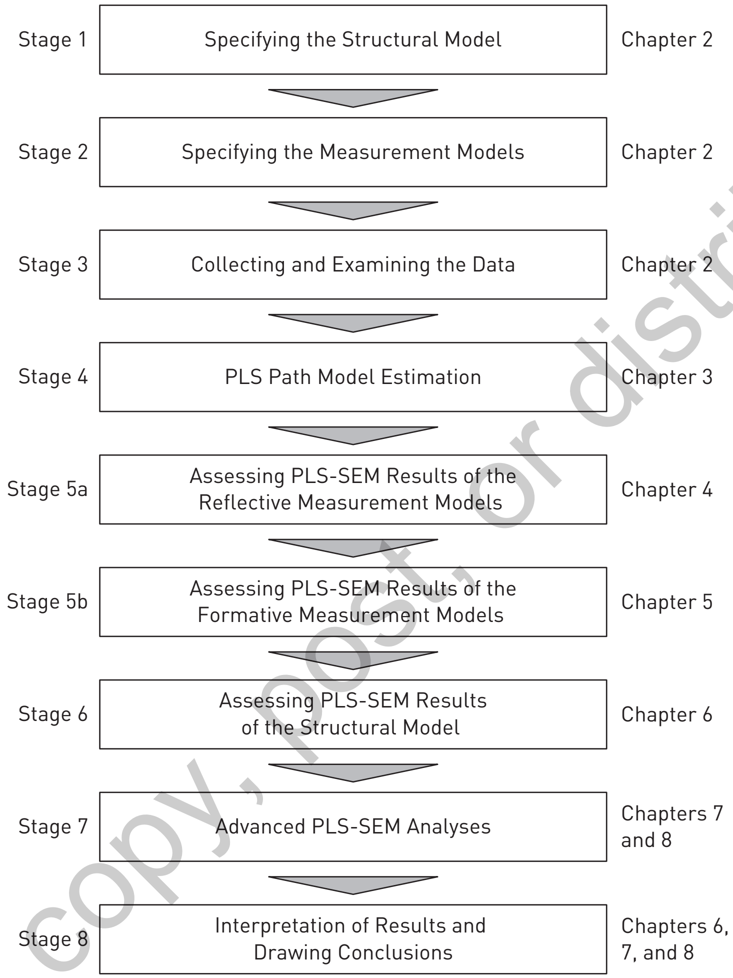
- the goal is theory testing and confirmation;
- error terms require additional specification, such as the covariation;
- the structural model has circular relationships; or
- the research requires a global goodness-of-fit criterion.

Source: Adapted from Hair, J. F., Risher, J. J., Sarstedt, M., & Ringle, C. M. (2019). When to use and how to report the results of PLS-SEM. *European Business Review*, *31*(1), 2–24.

ORGANIZATION OF REMAINING CHAPTERS

The remaining chapters provide more detailed information on PLS-SEM, including specific examples of how to use software to estimate simple and complex PLS path models. In doing so, the chapters follow a multistage procedure that should be used as a blueprint when conducting PLS-SEM analyses (Exhibit 1.11).

EXHIBIT 1.11 ■ A Systematic Procedure for Applying PLS-SEM



Specifically, the process starts with the specification of structural and measurement models, followed by the examination of data (Chapter 2). Next, we discuss the PLS-SEM algorithm and provide an overview of important considerations when running the analyses (Chapter 3). On the basis of the results of the computation, researchers then have to evaluate the results. To do so, researchers must know how to assess both reflective and formative measurement models (Chapters 4 and 5). When the data for the measures are considered reliable and valid (based on established criteria), researchers can then evaluate the structural model (Chapter 6). Chapter 7 covers the handling of mediating and moderating effects whose analysis has become standard in PLS-SEM research. On the basis of the results of Chapters 6 and 7, researchers interpret their findings and draw their final conclusions. Finally, Chapter 8 offers a brief overview of advanced techniques.

Summary

- **Understand the meaning of structural equation modeling (SEM) and its relationship to multivariate data analysis.** 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. Whereas CB-SEM considers the constructs as common factors, PLS-SEM considers the constructs as composites based on total variance, linearly formed by sets of indicator variables.
- **Describe the basic considerations in applying multivariate data analysis.** Several considerations are necessary when applying multivariate analysis, including the following five: (1) composite variables, (2) measurement, (3) measurement scales, (4) coding, and (5) data distributions. A composite variable (also called a variate) is a linear combination of several indicators that are chosen based on the research problem at hand. Measurement is the process of assigning numbers to a variable based on a set of rules. Multivariate measurement involves using several variables to indirectly measure a concept to improve measurement accuracy. The anticipated improved accuracy is based on the assumption that using several variables (indicators) to measure a single concept is more likely to represent all the different aspects of the concept and thereby result in a more valid measurement of the concept. The ability to identify measurement error using multivariate measurement also helps researchers obtain more accurate measurements. Measurement error is the difference between the true value of a variable and the value obtained by a measurement. A measurement scale is a tool with a predetermined number of closed-ended responses that can be used to obtain an answer to a question. There are four types of measurement scales: nominal, ordinal, interval, and ratio. When researchers collect quantitative data using scales, the answers to the questions can be shown as a distribution across the available (predefined) response

categories. The type of distribution must always be considered when working with SEM.

- **Comprehend the basic concepts of partial least squares structural equation modeling (PLS-SEM).** Path models are diagrams used to visually display the hypotheses and variable relationships that are examined when structural equation modeling is applied. Four basic elements must be understood when developing path models: (1) constructs, (2) measured variables, (3) relationships, and (4) error terms. Constructs (or latent variables) measure theoretical concepts that are not directly observable. They are represented in path models as circles or ovals. Measured variables are directly measured observations (raw data), generally referred to as either indicators or manifest variables, and are represented in path models as rectangles. Relationships represent hypotheses in path models and are shown as arrows that are single-headed, indicating a predictive-causal relationship between the constructs. These relationships are derived from structural theory and logic. Depending on their role in the model, constructs are either exogenous or endogenous. Error terms represent the unexplained variance when path models are estimated and are present for endogenous constructs and reflectively measured indicators. Exogenous constructs and formative indicators do not have error terms. Measurement theory specifies how the constructs (latent variables) are measured. Latent variables can be specified as either reflective or formative.

- **Explain the differences between covariance-based structural equation modeling (CB-SEM) and PLS-SEM, and when to use each.** 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 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 require accounting for most distributional assumptions. Moreover, PLS-SEM can better handle formative measurement models and has advantages when sample sizes are relatively small and 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.

Review Questions

1. What is multivariate analysis?
2. Describe the difference between first- and second-generation multivariate methods.
3. What is structural equation modeling?
4. What is the key difference in the common factor model and the composite model?
5. What is the value of structural equation modeling in understanding relationships between variables?

Critical Thinking Questions

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

Key Terms

10 times rule 25
Categorical scale 8
Coding 10
Common factor-based SEM 15
Composite-based SEM 16
Composite scores 8
Composite variable 6
Confirmatory 3
Constructs 7
Covariance-based structural equation modeling (CB-SEM) 4

Suggested Readings

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