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Partial least squares structural equation modeling (PLS-SEM) in the AI Era: Innovative methodological guide and framework for business research

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Abstract

Partial Least Squares Structural Equation Modeling (PLS-SEM) serves as a comprehensive methodological framework, critically addressing theoretical underpinnings, rigorous analytical approaches, and state-of-the-art modeling techniques vital for contemporary business research. The methodological discussion includes detailed exploration of reflective and formative measurement models, structural model specification, reliability, and validity assessments, alongside advanced analytical methods such as Confirmatory Tetrad Analysis (CTA-PLS) and Importance-Performance Matrix Analysis (IPMA). Advanced algorithms including bootstrapping and blindfolding procedures are elaborated, emphasizing predictive relevance and methodological precision. Partial Least Squares Structural Equation Modeling further offers robust analytical capabilities to evaluate modern AI-driven innovations, facilitating sophisticated assessment of user trust, perceived accuracy, and satisfaction with recommender systems, voice assistants, autonomous vehicles, AI-driven healthcare diagnostics, personalized educational platforms, and fraud detection technologies. Ethical considerations, reporting best practices, computational tools (SmartPLS, SEMinR), and Explainable AI (XAI) integration enhance the comprehensive nature of this framework. Furthermore, integration of cutting-edge analytical approaches such as moderation, mediation, Multi-Group Analysis (MGA), nonlinear modeling, machine learning integration, and quantum computing potential positions PLS-SEM as indispensable for contemporary business and technology research, ultimately promoting actionable scholarly insights and ensuring maximum methodological impact.

Keywords: Partial Least Squares Structural Equation Modeling; PLS-SEM; Reflective and Formative Models; CTA-PLS; IPMA; AI Product Innovations; Machine Learning; Quantum Computing; Explainable AI (XAI); Methodological Rigor; Predictive Analytics

1. Introduction

Partial Least Squares Structural Equation Modeling (PLS-SEM) is an advanced statistical technique widely used for analyzing and interpreting complex causal relationships among latent and observed variables. Central to this technique is the concept of latent variables (LVs), also known as constructs. Latent variables are theoretical constructs that are not directly observable but instead are measured through related observed variables or indicators (Al-Emran et al., 2023). Observed variables, in contrast, are concrete measurements obtained from survey instruments, experimental observations, or secondary data. The primary purpose of PLS-SEM is to precisely estimate the relationships among these latent constructs, effectively bridging theoretical frameworks with empirical evidence.

The technical robustness of PLS-SEM arises from its integration of principal component analysis (PCA) and multiple regression analysis. PCA facilitates the extraction of latent constructs from complex data structures by reducing dimensionality and revealing underlying patterns among indicators. Multiple regression further assesses and validates relationships among these constructs (Cepeda et al., 2024). The PLS-SEM computational process initiates with arbitrary

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values for latent variable scores, proceeding iteratively through outer and inner approximations. The outer approximation estimates outer weights, which indicate the relative contribution of individual indicators toward latent variables, and outer loadings, reflecting the correlation between latent constructs and their indicators. Subsequently, inner approximation evaluates the interrelationships among latent variables by calculating inner weights and loadings. Computationally, algorithms such as Nonlinear Iterative Partial Least Squares (NIPALS) and Ordinary Least Squares (OLS) ensure robust estimation and convergence to stable model parameters (Fordellone & Vichi, 2020). The strength and versatility of PLS-SEM have led to its widespread adoption across diverse academic disciplines, including management, psychology, economics, healthcare, education, information systems, and marketing. Its flexibility in handling non-normal data, tolerance of smaller sample sizes, and capability to model complex relationships underscore its significant methodological and practical advantages compared to traditional covariance-based SEM approaches.

1.1. Reflective vs Formative Measurement Models

A foundational aspect of employing PLS-SEM is distinguishing between reflective and formative measurement models. This differentiation substantially influences model specification, validation procedures, and interpretation of outcomes, underpinning the theoretical and empirical rigor of the research.

Reflective Measurement Models: Reflective models are conceptualized as latent variables causing observable indicators. Thus, indicators reflect the underlying latent construct and share a common conceptual meaning, rendering them interchangeable. Changes in a reflective latent construct directly manifest through corresponding variations in its indicators, highlighting the reflective nature of these measures (Chin, 2010). Reflective constructs typically include psychological states like satisfaction, perceived quality, attitudes, or trust.

Mathematically, reflective measurement models are defined as follows:

$$x=\Lambda\xi+\delta$$

Where: x represents the observed indicator variables.

Λ (lambda) represents the outer loadings or factor loadings, reflecting the relationship strength between indicators and latent variables.

ξ (xi) denotes the latent construct.

δ denotes measurement errors, reflecting the unexplained variance.

Formative Measurement Models, in contrast, conceptualize indicators as directly causing or forming the latent variable. In formative measurement, each indicator uniquely contributes to the latent construct, and thus the indicators are not interchangeable (Becker et al., 2023). Formative constructs are typically composite indices, such as socioeconomic status, innovation capability indices, or aggregate performance metrics.

The mathematical representation for formative models is given by:

$$\xi = w_1x_1 + w_2x_2 + w_3x_3 + \cdots + w_nx_n + \zeta$$

Where:

ξ represents the latent construct.
xi denotes observed indicators.
wi are the indicator weights determining the contribution of each observed variable.
ζ is the measurement error term.

A detailed comparative analysis between reflective and formative models is presented in the table 1 below: Understanding the theoretical distinctions between reflective and formative measurement models is essential for appropriate model specification, validation, and effective interpretation of PLS-SEM research outcomes. The criteria presented in the comparison table between reflective and formative measurement models are derived from fundamental theoretical distinctions and critical methodological considerations inherent in model specification (Benitez et al., 2019). First, the criterion concerning the direction of causality differentiates whether the latent construct influences the indicators (reflective) or whether the indicators form the latent construct (formative). Second, indicator interchangeability addresses whether indicators measure a shared concept (reflective) or individually contribute unique aspects to the construct's definition (formative). Third, indicator correlation is included to highlight that reflective indicators generally demonstrate high intercorrelations due to their shared underlying cause, whereas formative indicators do not necessarily correlate, as each captures distinct dimensions of the construct (Cheah, Amaro, & Roldán, 2022). Additionally, the criterion concerning the removal of indicators illustrates that deleting a reflective indicator typically does not substantially alter the latent construct’s meaning; however, eliminating a formative indicator fundamentally changes the construct's conceptual domain. Lastly, the choice of statistical evaluation methods reflects differences in assessing reflective (e.g., indicator loadings, AVE, and composite reliability) versus formative constructs (e.g., indicator weight significance and variance inflation factor [VIF]). These criteria ensure accurate specification, robust measurement validity, and methodological integrity within PLS-SEM research.

Table 1 Criteria Evaluation Between Reflective & Formative measurement models

Criterion	**Reflective Measurement Models**	**Formative Measurement Models**
Direction of causality	Latent construct → Indicators	Indicators → Latent construct
Indicator interchangeability	Interchangeable	Not interchangeable
Nature of indicators	Manifestations of underlying latent constructs	Distinct dimensions forming latent construct
Indicator correlation	Highly correlated	Not necessarily correlated
Statistical evaluation criteria	Factor Loadings, AVE, Composite Reliability	Weights significance, VIF (multicollinearity)
Effect of dropping indicators	Minimal impact on construct meaning	Significant alteration of construct meaning
Typical examples	Satisfaction, attitudes, perceived quality	Socioeconomic indices, innovation indices

1.2. Research Objective

This research article aims to provide an in-depth, technically rigorous examination of Partial Least Squares Structural Equation Modeling (PLS-SEM), thoroughly outlining its theoretical underpinnings, methodological advancements, critical analytical techniques, and practical applications. The article carefully articulates foundational theories and methodological innovations, emphasizing significant analytical procedures such as the distinction between reflective and formative measurement models. Key algorithms essential to PLS-SEM such as bootstrapping, blindfolding, and predictive relevance analyses are elaborated clearly, ensuring methodological precision (Durdyev et al., 2018). Additionally, the article extends beyond theoretical foundations to practical applications, illustrating how PLS-SEM can be effectively utilized in the analysis of advanced AI product innovations, including recommender systems, voice assistants, autonomous vehicles, AI-powered healthcare diagnostics, and personalized educational platforms. By exploring these contemporary applications, the paper aims to enhance researchers' understanding of PLS-SEM’s versatility and practical efficacy (Danks, Sharma, & Sarstedt, 2020). Ultimately, this article provides scholars and practitioners with an authoritative methodological guide for rigorous and impactful research involving complex structural equation models within innovative AI contexts.

2. Theoretical foundations of PLS-SEM

Partial Least Squares Structural Equation Modeling (PLS-SEM) was originally conceptualized and introduced by Herman Wold in the early 1980s as a statistical method tailored for econometric modeling. Wold aimed to address limitations inherent in traditional covariance-based Structural Equation Modeling (CB-SEM), particularly emphasizing the technique’s robustness for handling complex models, limited sample sizes, and data lacking normal distribution. Initially applied within econometrics, PLS-SEM quickly transcended its original discipline and became extensively utilized in various fields such as psychology, marketing, management, organizational behavior, and information systems, reflecting its methodological flexibility and broad applicability (Avkiran, 2018).

At its core, PLS-SEM relies on several foundational theoretical concepts essential for understanding its application. The first is the concept of latent variables (LVs), which represent theoretical constructs that researchers cannot directly measure, such as customer attitudes, intentions, and perceived quality. Latent variables are inferred through observed variables (indicators), which provide quantifiable measures such as survey items, behavioral indicators, or objective data (Carrión, Nitzl, & Roldán, 2017). These indicators operationalize latent constructs within measurement models. Measurement models formally define how observed variables link to latent variables, clearly delineating construct measurement. Conversely, the structural model in PLS-SEM specifies theoretical relationships among latent constructs themselves, depicting a hypothesized network of cause-effect pathways. Furthermore, methodological innovations and variations, such as Consistent PLS (PLSc) and Factor-based PLS (PLSF), have been introduced to refine parameter estimation and align the strengths of variance-based PLS with traditional factor-model estimation methods, ensuring consistency and theoretical coherence in PLS-SEM research (Fong & Law, 2013).

2.1. Model Specification and Path Modeling Basics

In Partial Least Squares Structural Equation Modeling (PLS-SEM), model specification forms the foundational step that directly impacts the validity, interpretability, and applicability of analytical outcomes. Model specification begins with the conceptual representation of theoretical relationships, depicted graphically through a clearly structured path diagram. Such diagrams distinguish explicitly between latent variables (LVs) and observed indicators. Latent variables, representing abstract theoretical concepts, are conventionally illustrated as circles or ovals, whereas their measurable indicators (observed variables) are presented as rectangles (Cheah, Magno, & Cassia, 2024). Directional arrows illustrate the presumed causal relationships, clarifying how constructs are theoretically linked with their indicators and how constructs interrelate to one another.

The process of specification involves two critical interconnected components: the measurement model and the structural model. The measurement model explicitly defines relationships between latent variables and their observed indicators, identifying precisely how theoretical constructs are empirically operationalized. Proper measurement model specification requires careful consideration of the construct's conceptual nature, either reflective or formative to accurately reflect theoretical assumptions (Becker, Klein, & Wetzels, 2012). Conversely, the structural model delineates hypothesized causal relationships among latent variables, explicitly representing how constructs influence or depend upon each other.

Path modeling constitutes the analytical core of PLS-SEM, guiding the precise definition and quantification of relationships among latent variables within the structural model. It involves the specification of directional paths, which represent hypothesized theoretical relationships, clearly denoted by arrows connecting latent variables (Ashill, 2011). These paths are categorized according to distinct theoretical mechanisms. They are:

Direct Effects: These paths signify direct relationships between pairs of latent variables without mediators. A direct path between two latent constructs (e.g., perceived usefulness directly influencing user intention) is visually indicated by a straight, single-headed arrow (Dash & Paul, 2021).

Indirect Effects (Mediating Effects): Indirect paths represent relationships that occur through one or more intervening latent variables (mediators). In these cases, the impact from one latent variable on another operates through an intermediate construct, with the chain of mediation clearly outlined by sequential paths (Cho et al., 2022).

Moderating Effects: These paths depict interactions in which the strength or direction of the relationship between two latent variables changes depending upon another latent variable known as a moderator. Graphically, moderation is indicated by dashed lines intersecting existing paths, clearly highlighting conditional relationships (Barcia, Garcia-Castro, & Abad-Moran, 2022).

Mathematically, these relationships are quantified by estimating path coefficients, which represent both the direction (positive or negative) and magnitude (strength) of relationships between latent variables. The structural model in PLS-SEM can be mathematically represented by the following general equation:

$$\eta_i = \sum_j \beta_{ij}\eta_j + \sum_k \gamma_{ik}\xi_k + \zeta_i$$

Where:

ηi denotes endogenous latent variables (dependent variables).
ηj denotes other endogenous latent variables influencing
ξk represents exogenous latent variables (independent predictors).
βij signifies path coefficients indicating the strength and direction of relationships between endogenous latent variables.
γik symbolizes path coefficients between exogenous and endogenous latent variables.
ζi represents the residual or error term, indicating unexplained variance in the endogenous latent variable.

2.2. Validity and Reliability in PLS SEM

In the context of PLS-SEM, ensuring that constructs are measured accurately is paramount, and this involves a thorough understanding of various forms of validity and reliability. Validity generally refers to the extent to which a construct truly represents the concept it is intended to measure, while reliability pertains to the consistency and stability of the measurement (Bodoff & Ho, 2016). Both concepts are critical in establishing the credibility of any model. Reliability in PLS-SEM typically focuses on the internal consistency of the indicators used to measure a latent construct. Traditional measures such as Cronbach's alpha have been widely used to assess reliability; however, composite reliability and rhoA have become more favored in the PLS-SEM context due to their ability to capture the multidimensional nature of constructs. Composite reliability, for example, takes into account the actual loadings of indicators, offering a more accurate representation of internal consistency than Cronbach's alpha, which assumes equal contribution of each indicator. High reliability indicates that the indicators consistently reflect the same underlying construct, which is a necessary condition for a sound measurement model (Cepeda et al., 2024).

Convergent validity is concerned with the degree to which multiple indicators of the same construct are in agreement. In PLS-SEM, convergent validity is commonly assessed by examining the average variance extracted (AVE) and the indicator loadings. AVE measures the amount of variance captured by the construct in relation to the variance due to measurement error. A threshold of 0.50 or higher is generally considered acceptable, indicating that more than 50% of the variance is explained by the latent construct. High indicator loadings (typically above 0.70) further support convergent validity, as they imply that the indicators are strongly associated with their respective constructs (Bentler & Bonett, 1980). Together, these metrics confirm that the measurement model is capturing the intended construct with minimal error.

Discriminant validity, on the other hand, ensures that a construct is truly distinct from other constructs within the model. It tests whether concepts or measurements that are not supposed to be related are actually unrelated. Several methods are used to assess discriminant validity in PLS-SEM. The Fornell-Larcker criterion is one common approach, where the square root of the average variance extracted (AVE) for each construct should be greater than its correlations with any other construct. More recently, the Heterotrait-Monotrait (HTMT) ratio of correlations has gained prominence (Chin, Cheah, Liu, Ting, Lim, & Cham, 2020). HTMT compares the average correlations across constructs (heterotrait) with the average correlations within the same construct (monotrait), and values below established thresholds (commonly 0.85 or 0.90) suggest adequate discriminant validity. The rigorous evaluation of discriminant validity ensures that each construct captures a unique phenomenon, preventing overlap that can distort the interpretation of structural relationships.

Beyond these core concepts, other forms of validity such as nomological validity and criterion-related validity further enrich the measurement model. Nomological validity examines whether the relationships among constructs conform to established theories, providing evidence that the constructs are behaving as expected within a broader theoretical network. Criterion-related validity, on the other hand, assesses how well one measure predicts an outcome based on information from other measures, reinforcing the practical relevance of the constructs (Cheah, Roldán, Ciavolino, Ting, & Ramayah, 2020). These additional layers of validity ensure that the model not only measures construct accurately but also situates them correctly within the larger theoretical framework. Together, the rigorous assessment of reliability, convergent validity, discriminant validity, and other forms of validity forms the foundation of a robust PLS-SEM analysis. Each type of validity contributes to the overall confidence in the measurement model: reliability assures that the measures are consistent over time and across items, convergent validity confirms that the indicators adequately capture the intended construct, and discriminant validity guarantees that each construct is unique and distinct. This comprehensive approach not only enhances the internal consistency of the model but also ensures that the conclusions drawn from the analysis are both theoretically sound and practically relevant (Cho & Choi, 2019).

The significance and stability of these estimated path coefficients are assessed through rigorous statistical validation techniques, prominently the bootstrapping procedure. Bootstrapping involves repeatedly resampling the original dataset (with replacement) to generate multiple synthetic datasets, enabling researchers to determine confidence intervals and significance levels of each path coefficient. This method ensures that the resulting path estimates are not merely artifacts of a particular dataset but exhibit robustness and generalizability across potential sample variations (Hair Jr, Sarstedt, Hopkins, & Kuppelwieser, 2014). In essence, accurate model specification, precise depiction of path modeling relationships, and careful evaluation of path coefficients collectively underpin the theoretical and practical effectiveness of PLS-SEM. By clearly defining these fundamental modeling steps, researchers can robustly capture complex relational dynamics inherent in contemporary theoretical frameworks, particularly beneficial for analyzing innovative and multifaceted phenomena such as advanced artificial intelligence (AI) innovations.

3. Methodological Innovations in PLS-SEM

Partial Least Squares Structural Equation Modeling (PLS-SEM) has witnessed significant methodological innovations designed to enhance analytical rigor, improve predictive accuracy, and expand its applicability across diverse research domains. These methodological advancements, including refined approaches for assessing reliability and validity, rigorous measurement model evaluations, predictive structural modeling techniques, and sophisticated analyses such as Confirmatory Tetrad Analysis (CTA-PLS) and Importance-Performance Matrix Analysis (IPMA), have greatly increased the robustness and accuracy of PLS-SEM outcomes (Dijkstra & Henseler, 2015). Additionally, innovations such as hierarchical component modeling (higher-order constructs) facilitate the modeling of complex theoretical phenomena. Collectively, these methodological improvements empower researchers to derive more precise theoretical insights and actionable implications, particularly when addressing contemporary research challenges in business, management, and artificial intelligence.

3.1. Advanced Approaches to Reliability and Validity

Reliability and validity form foundational elements in assessing measurement quality within Partial Least Squares Structural Equation Modeling (PLS-SEM). Reliability refers to the consistency or stability of measurements, indicating whether repeated measures yield similar results under consistent conditions. Validity, on the other hand, assesses whether the measurement instrument genuinely captures what it intends to measure, ensuring accuracy in representing the theoretical constructs (Hair Jr, Sarstedt, Hopkins, & Kuppelwieser, 2014). Composite Reliability (CR) specifically measures the internal consistency reliability in reflective measurement models, offering a more robust alternative to Cronbach's alpha by considering varying indicator loadings. CR helps ensure that indicators consistently reflect the latent construct accurately. In research, the reliability of constructs indicates the consistency or repeatability of observed measurements over time. Historically, Cronbach's Alpha was predominantly employed to measure reliability. While this statistic provided an easy and intuitive approach, it was criticized for its assumption of equal indicator reliability (homogeneity). This limitation paved the way for advanced methodologies, such as Composite Reliability (CR), which provided greater precision by considering the individual indicator loadings within reflective measurement models (Fornell & Larcker, 1981). Composite Reliability reflects internal consistency by assigning varied weightings to indicators based on their respective loadings, effectively accommodating indicators' differential importance. The mathematical representation for CR is:

$$CR = \frac{(\sum \lambda_i)^2}{(\sum \lambda_i)^2 + \sum Var(\epsilon_i)}$$

In this formula, λi represents the individual indicator loadings (the correlation between each indicator and the latent variable), and $Var(\epsilon i)$ denotes the variance attributable to measurement errors. This metric robustly captures internal consistency, acknowledging the distinct contributions of each indicator rather than assuming uniform contributions, thus improving measurement accuracy and theoretical relevance (Gefen, Straub, & Boudreau, 2000).

Recognizing the limitations of traditional reliability indicators, methodological innovations have introduced rho_A as an additional and improved estimator for reliability in reflective measurement models. Rho_A enhances internal consistency reliability estimation by capturing additional information about indicator correlation patterns (Gelashvili, Martínez-Navalón, & Saura, 2021). It addresses Cronbach's alpha's limitations and complements Composite Reliability by providing a nuanced and often more precise measure of internal consistency. This has led researchers to recommend reporting rho_A alongside CR for rigorous reliability assessment.

Advancements in validity assessment have similarly progressed significantly. Traditionally, discriminant validity confirming that constructs distinctively measure separate phenomena was evaluated through the Fornell-Larcker criterion or by examining cross-loadings (Guenther, Guenther, Ringle, Zaefarian, & Cartwright, 2023). However, recent methodological critiques highlighted potential insensitivity and shortcomings of these traditional methods. To overcome these issues, scholars introduced the Heterotrait-Monotrait Ratio of Correlations (HTMT), a more stringent and theoretically robust approach. HTMT precisely measures discriminant validity by analyzing the ratio between the average correlations of indicators across different constructs (heterotrait correlations) and the average correlations of indicators within the same construct (monotrait correlations). HTMT is formally calculated as:

$$HTMT_{ij} = \frac{\bar{r}_{ij}}{\sqrt{\bar{r}_{ii} \times \bar{r}_{jj}}}$$

Here, r¯ij represents the average correlation among indicators from different constructs (heterotrait correlations), while r¯ii and r¯jj signify the average correlations among indicators within the same constructs (monotrait correlations). An HTMT value below predefined thresholds (typically 0.85 or 0.90 depending on the research context) confirms robust discriminant validity, indicating clearly distinguishable constructs. Moreover, advanced methodological standards emphasize rigorous testing of convergent validity, commonly achieved through Average Variance Extracted (AVE). AVE quantifies how well a construct captures the variance from its indicators relative to measurement errors. Formally, AVE is calculated as:

$$AVE = \frac{\sum \lambda_i^2}{n}$$

where λi denotes standardized indicator loadings, and nnn refers to the total number of indicators associated with a latent construct. AVE values greater than 0.50 imply that more than half of the indicators’ variance is accounted for by the construct, signifying strong convergent validity and confirming the indicators' theoretical appropriateness (Gye-Soo, 2016). Additionally, sophisticated reliability and validity assessments integrate sensitivity analyses to examine stability and robustness of these measures. Researchers commonly use bootstrapping and cross-validation techniques to verify the stability of reliability coefficients (such as CR and rho_A) and validity measures (e.g., HTMT and AVE) across multiple data samples. Such practices significantly increase methodological rigor, assuring confidence in research findings and the underlying theoretical frameworks. These advanced reliability and validity techniques enhance construct representation accuracy, psychometric robustness, and theoretical credibility within PLS-SEM analyses. By adopting these advanced practices, researchers ensure comprehensive measurement integrity, rigorously confirming that latent constructs are precisely captured by their indicators, thereby strengthening empirical insights and theoretical advancements in contemporary business research (Islam & Khan, 2024).

3.2. Assessment of Measurement Models

Assessment of measurement models in Partial Least Squares Structural Equation Modeling (PLS-SEM) ensures that latent constructs are properly measured by their respective observed indicators. Since latent constructs cannot be directly observed, they are operationalized using measurable indicators, making it essential to evaluate how well these indicators represent the underlying constructs (Hair, Hollingsworth, Randolph, & Chong, 2017). PLS-SEM employs two primary types of measurement models: reflective and formative models, each requiring different assessment criteria. In the case of reflective measurement models, constructs are assumed to cause variations in their indicators, necessitating an evaluation of indicator reliability, internal consistency reliability, convergent validity, and discriminant validity. In contrast, formative measurement models assume that indicators define the construct, requiring assessments such as indicator significance, variance inflation factor (VIF), and bootstrapping procedures to confirm construct validity (Hair, Ringle, & Sarstedt, 2012). Ensuring accurate assessment of measurement models is crucial for maintaining theoretical robustness, empirical validity, and meaningful interpretation of structural relationships in PLS-SEM. The subsequent sections discuss in detail the reliability and validity assessments used to verify measurement model quality in PLS-SEM.

The Figure 1 presents two contrasting approaches to measurement in structural equation modeling, focusing on the relationship between two latent constructs (ξ and η). In the common factor model (panel a), each indicator (x1, x2, x3 for ξ and x4, x5, x6 for η) is conceptualized as a reflection of its latent variable. This reflective logic assumes that changes in the underlying construct drive corresponding changes in the observed indicators. Path coefficients (λ1, λ2, ..., λ6) can be interpreted as loadings, showing how strongly each indicator responds to variations in the latent factor (Hair, Hult, Ringle, Sarstedt, Danks, & Ray, 2021). From a theoretical standpoint, this model implies that each indicator shares a common source of variance, with its own error term (e1, e2, …, e6) capturing measurement-specific noise. The correlation or structural link (ϕ) between ξ and η indicates how closely these latent factors co-vary, a relationship that can be tested for significance via bootstrapping in PLS-SEM. Reflective models are typically evaluated in terms of internal consistency (e.g., composite reliability), convergent validity (via average variance extracted), and discriminant validity (using criteria such as Fornell-Larcker or the Heterotrait-Monotrait ratio) to ensure that each construct is both accurately measured and distinct (Hair, Sarstedt, Pieper, & Ringle, 2012) .

In contrast, the composite factor model (panel b) treats each set of indicators as forming or defining its respective latent variable. Under this formative perspective, indicators are seen as causal contributors to the construct, so the direction of influence runs from the observed variables (x1, x2, x3; x4, x5, x6) to the latent factors (ξ and η). Here, path coefficients still appear, but they are interpreted more as weights than loadings, reflecting the degree to which each indicator contributes to the latent variable. While the error terms (e1, e2, …, e6) remain, they often represent unexplained variance specific to each indicator. In a PLS-SEM framework, these composites are estimated through iterative algorithms that maximize the explained variance of the constructs in the structural model (Hair, Hult, Ringle, Sarstedt, & Thiele, 2017). As before, the arrow labeled ϕ indicates the link between ξ and η, but the conceptual meaning of this correlation shifts: because the indicators define the latent constructs, overlap among them can inflate the correlation, making it crucial to examine discriminant validity carefully.

The theoretical implications of these two measurement approaches are substantial. A common factor model (reflective) aligns with theories suggesting that the latent construct is the driving force behind observable attributes, while a composite factor model (formative) fits scenarios where the construct is an aggregation of multiple causal components. PLS-SEM can accommodate both philosophies, offering flexibility that extends beyond traditional covariance-based SEM (Henseler, Dijkstra, Sarstedt, Ringle, Diamantopoulos, Straub, Ketchen, Hair, Hult, & Calantone, 2014). In reflective designs, reliability indices (such as Cronbach's alpha or composite reliability) and average variance extracted are central to confirming that the indicators genuinely reflect the latent factor. By contrast, in formative or composite designs, the focus often shifts to examining the extent to which indicators adequately form the construct, assessing whether they collectively capture the intended conceptual domain without excessive overlap or redundancy (Hair, Sarstedt, Ringle, et al., 2012).

Overall, the figure 1, two panels serve as a vivid illustration of how the specification of measurement models shapes the interpretation of latent constructs and their interrelationships. Whether adopting a reflective or formative approach, the goal remains to ensure that each construct is measured in a manner consistent with theoretical expectations and empirical realities (Hair, Sarstedt, & Ringle, 2019). Reflective models place emphasis on the internal consistency and convergent validity of indicators, whereas formative models highlight the causal contribution of indicators and the need to confirm that each composite is uniquely defined. Both approaches require careful scrutiny of discriminant validity, especially when multiple latent constructs might share common indicators or conceptual overlap. In PLS-SEM, these models can be tested through various diagnostic tools such as bootstrapping, blindfolding, and multi-group analysis to confirm their robustness, ultimately contributing to more accurate, theory-driven insights into complex phenomena (Hair, Howard, & Nitzl, 2019).

Transitioning from a one-factor model to a two-factor model is a natural evolution in assessing measurement quality in PLS-SEM. In a one-factor model, all observed indicators load onto a single latent variable, treating the construct as a unified, unidimensional entity. This approach establishes a baseline by allowing for the evaluation of internal consistency using metrics like composite reliability and convergent validity, which is typically assessed via the average variance extracted (AVE). If the indicators all load strongly on the latent variable and the reliability and validity measures are satisfactory, the one-factor structure may be considered adequate for a construct that is theoretically unidimensional (Hair, Howard, & Nitzl, 2019). However, sometimes the data or theory suggests more complexity, and the one-factor model may reveal issues such as low indicator loadings or a lower-than-expected AVE, indicating that a single latent dimension might not be capturing all aspects of the construct.

When such complexities become apparent or when theoretical arguments support multiple dimensions, it makes sense to shift to a two-factor model. By dividing the indicators into two distinct latent variables, the two-factor approach allows for a more refined assessment of measurement quality particularly discriminant validity (Hair, Matthews, Matthews, & Sarstedt, 2017). In this setup, each group of indicators is expected to reflect a different underlying dimension of the overall concept. The two-factor model not only tests whether the indicators within each group exhibit strong convergent validity but also whether the two latent variables are distinct from one another (Hair, Ringle, Gudergan, Fischer, Nitzl, & Menictas, 2018). In practical terms, this means checking that the inter-factor correlation isn't so high that it suggests redundancy between the factors, often using criteria like the Fornell-Larcker criterion or the Heterotrait-Monotrait (HTMT) ratio.

This shift from a one-factor to a two-factor model brings additional layers to both reliability and validity assessment. Under the one-factor specification, reliability is evaluated by looking at the overall consistency of all indicators together and ensuring that the latent variable captures most of the shared variance (Hair & Alamer, 2022). When moving to a two-factor model, each latent construct is assessed separately for internal consistency and convergent validity, while also examining discriminant validity ensuring that the two constructs do not overlap excessively. In other words, the one-factor model provides a simple, unified view of measurement quality, but the two-factor model offers a more nuanced perspective that can uncover hidden dimensions within the data (Henseler & Sarstedt, 2012).

In a more conversational sense, you might think of the one-factor model as your starting point a “big picture” view of a concept. If everything seems to fit together well, that’s great. But if you notice that some pieces of the puzzle don’t seem to belong together or if theory suggests that the concept should have distinct parts, the two-factor model lets you break it down into two separate but related components (Henseler & Chin, 2010). This helps ensure that each component is measured accurately and that they are indeed capturing different aspects of the overall phenomenon. Essentially, this progression deepens the validity assessment, making sure that your measurement model is both reliable and conceptually clear. Ultimately, transitioning from a one-factor to a two-factor model not only refines the measurement process but also provides richer insights into the underlying structure of the data. This approach helps to confirm whether a construct is truly unidimensional or if it comprises multiple dimensions that need to be modeled separately for a more accurate and meaningful analysis (Hair, Risher, Sarstedt, & Ringle, 2019).

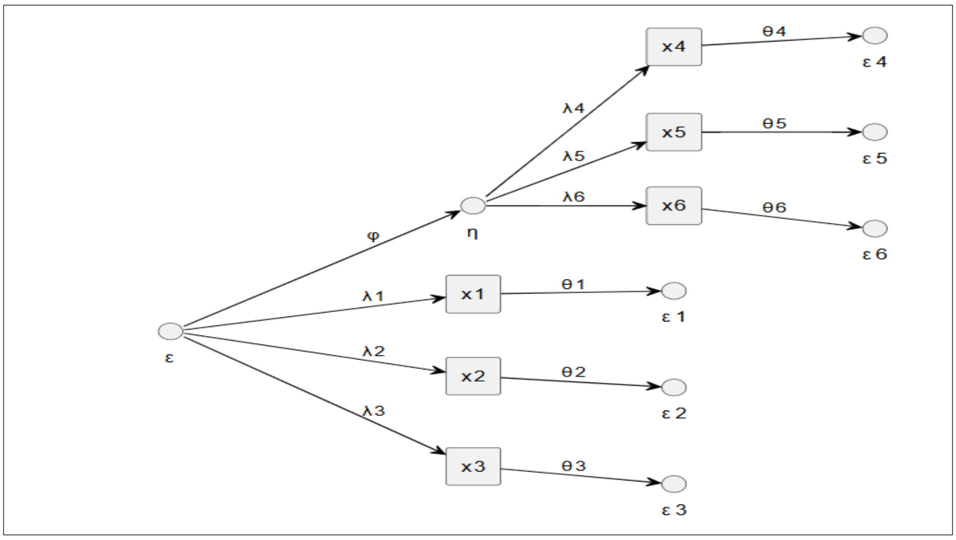

Figure 1 Common factor model of PLS SEM

3.2.1. Assessment of Reflective Measurement Models

Reflective measurement models assume that indicators are manifestations of the underlying latent construct, meaning that changes in the latent construct should induce proportional changes in all associated indicators. Because these indicators are theoretically interchangeable, their reliability and validity must be rigorously evaluated. The assessment of reflective measurement models in PLS-SEM involves the following key criteria:

Indicator Reliability: Factor Loadings and Standardized Loadings

In reflective measurement models, indicator reliability refers to the degree to which an observed indicator accurately represents the corresponding latent construct. High indicator loadings indicate that an indicator is strongly associated with the latent variable it measures, reducing measurement error. Typically, factor loadings above 0.708 are considered acceptable, as they indicate that the indicator explains at least 50% of its variance through the construct it is associated with (Hult, Hair, Proksch, Sarstedt, Pinkwart, & Ringle, 2018). If loadings are below this threshold, researchers must investigate potential measurement weaknesses, reconsider construct definition, or remove low-loading indicators.

Mathematically, factor loadings (λ) represent the relationship strength between a latent variable (ξ) and its corresponding observed indicator (x_i):

$$x_i = \lambda_i \xi + \delta_i$$

where:

Xi represents the observed indicator,
λi represents the factor loading (standardized regression coefficient),
ξ is the latent construct,
δi represents the measurement error.

High factor loadings (λi) indicate strong relationships between indicators and latent variables, thereby minimizing measurement errors. Indicators with weak loadings introduce unreliable variance, which can distort results and weaken construct validity. Researchers must either remove weak indicators or employ specification techniques such as modifying the measurement model to improve indicator strength (Haji-Othman & Yusuff, 2022).

Internal Consistency Reliability: Composite Reliability (CR)

Reliability is a key measurement property in PLS-SEM, ensuring that all indicators assigned to a construct consistently reflect its theoretical meaning. While Cronbach's Alpha has traditionally been used to measure reliability, it assumes equal factor loadings among indicators, which may not hold true in PLS-SEM models. Composite Reliability (CR) overcomes this limitation by accounting for individual indicator contributions based on their factor loadings, providing a more precise measure of internal consistency (Henseler, Hubona, & Ray, 2016).

CR is computed using the following formula:

$$CR = \frac{(\sum \lambda_i)^2}{(\sum \lambda_i)^2 + \sum Var(\epsilon_i)}$$

where:

λi represents the factor loadings of the indicators,
Var(ϵi) refers to the variance of measurement errors.

A CR value above 0.70 is typically considered acceptable, ensuring that indicators reliably measure the construct. Lower values suggest inconsistency, implying that some indicators may not adequately capture the construct. Higher values, closer to 0.90, indicate strong reliability but may also suggest redundancy among indicators, potentially leading to multicollinearity issues. Researchers must balance high reliability with parsimony, ensuring that constructs retain theoretical validity without excessive redundancy (Henseler, Ringle, & Sarstedt, 2015).

Convergent Validity: Average Variance Extracted (AVE)

Convergent validity assesses whether a latent construct meaningfully explains the variance among its indicators, ensuring that all indicators capture the same theoretical concept. The Average Variance Extracted (AVE) quantifies the proportion of variance that a construct accounts for relative to measurement error. A construct demonstrates strong convergent validity if AVE is 0.50 or higher, meaning that at least 50% of the indicator variance is explained by the latent construct (Khan, Sarstedt, Shiau, Hair, Ringle, & Fritze, 2019).

Mathematically, AVE is calculated as:

$$AVE = \frac{\sum \lambda_i^2}{n}$$

where:

λi represents the standardized loadings of the indicators,
n is the total number of indicators.

If AVE falls below 0.50, this indicates low construct validity, suggesting that indicators may not be capturing a unified latent concept. Researchers can address weak AVE values by either removing low-loading indicators or revising the construct definition to improve theoretical clarity. In cases where a construct is conceptually well-defined but exhibits low AVE, researchers may also consider modifying or respecifying indicators to enhance construct representation (Ketchen, 2013).

Discriminant Validity: Heterotrait-Monotrait (HTMT) Ratio

Discriminant validity is crucial in PLS-SEM, ensuring that each construct is empirically distinct and not measuring overlapping theoretical concepts. If constructs are highly correlated, it becomes difficult to distinguish between them, leading to issues in model interpretation and construct validity (Leguina, 2015). Traditionally, discriminant validity was assessed using Fornell-Larcker criterion, but recent advancements emphasize the Heterotrait-Monotrait (HTMT) ratio, which provides a more robust measure of construct distinctiveness.

The HTMT ratio is computed as:

$$HTMT_{ij} = \frac{\bar{r}_{ij}}{\sqrt{\bar{r}_{ii} \times \bar{r}_{jj}}}$$

where:

r¯ij represents the average correlation between indicators of different constructs (heterotrait correlations),
r¯ii and r¯jj denote the average correlations within the same construct (monotrait correlations).

A construct achieves discriminant validity if HTMT < 0.90, confirming that it is theoretically distinct from other constructs. If HTMT values exceed 0.90, it suggests high construct overlap, requiring researchers to reconsider theoretical distinctions, refine construct definitions, or merge highly similar constructs to prevent redundancy.

Theoretical and Practical Implications of Measurement Model Assessment

A rigorous assessment of measurement models in PLS-SEM ensures that theoretical constructs are empirically valid, reliable, and distinct. Failure to properly assess indicator reliability, internal consistency, convergent validity, and discriminant validity can lead to misinterpretation of relationships, biased parameter estimates, and flawed theoretical conclusions. Proper validation techniques, such as HTMT for discriminant validity, bootstrapping for formative model significance, and VIF for collinearity checks, enhance measurement precision and empirical robustness (Rönkkö, McIntosh, Antonakis, & Edwards, 2016). From a practical perspective, businesses, policymakers, and academics leverage PLS-SEM models to analyze consumer perceptions, organizational behavior, and AI-driven decision-making systems. Ensuring accurate measurement models allows for meaningful theoretical contributions and strategic business insights, reinforcing the importance of thorough assessment methodologies. Thus, PLS-SEM measurement model assessment is not merely a statistical step, it is an essential methodological process that underpins the validity and reliability of research conclusions, enabling researchers to derive robust and generalizable insights (Rigdon, Ringle, & Sarstedt, 2010).

3.2.2. Assessment of Formative Measurement Models in PLS-SEM

Formative measurement models play a fundamentally different role in Partial Least Squares Structural Equation Modeling (PLS-SEM) compared to reflective models. While reflective measurement models assume that latent constructs cause their indicators, formative models assume that indicators collectively define or shape the construct (Ravand & Baghaei, 2016). In this framework, indicators are not interchangeable, meaning that removing one can significantly alter the construct's meaning. As a result, the assessment of formative measurement models is not based on internal consistency reliability measures such as Cronbach's Alpha or Composite Reliability (CR). Instead, formative model assessment focuses on indicator relevance, multicollinearity diagnostics, and contribution significance to ensure theoretical precision and empirical validity (Monecke & Leisch, 2012). Since formative indicators define the construct rather than reflect it, their evaluation requires distinct techniques such as bootstrapping to test significance, Variance Inflation Factor (VIF) to check multicollinearity, and outer weights analysis to assess individual contribution strength. The following sections provide a detailed theoretical and technical explanation of each aspect of formative measurement model assessment.

Indicator Relevance: Significance of Indicator Weights

In formative measurement models, the contribution of each indicator to the latent variable is assessed using indicator weights rather than factor loadings. Unlike reflective indicators, which are expected to highly correlate due to their common underlying construct, formative indicators represent different aspects of the construct and may not correlate at all (Nitzl, Roldán, & Cepeda, 2017). Therefore, assessing indicator relevance is critical to confirm that each indicator contributes significantly to the formation of the construct. The primary technique used to test indicator significance is bootstrapping, a non-parametric resampling method that generates confidence intervals and standard errors for indicator weights. Bootstrapping involves drawing random samples from the original dataset with replacement and recalculating model parameters across multiple iterations (Richter, Hauff, Ringle, & Gudergan, 2022). The results help determine whether an indicator's weight is significantly different from zero. If an indicator's bootstrap confidence interval includes zero, it suggests that the indicator does not contribute meaningfully to defining the construct, and its inclusion should be reconsidered. In such cases, three possible actions can be taken:

- **Retaining the indicator** if theoretical justification supports its inclusion.
- **Removing the indicator** if its contribution is negligible and lacks theoretical importance.
- **Re-specifying the model** by adjusting the set of indicators to ensure a more robust formative construct.

Mathematically, indicator significance is assessed using t-values and p-values from the bootstrapping results. An indicator weight (wi) is considered significant if its t-value exceeds 1.96 (for a 95% confidence level) or 2.58 (for a 99% confidence level).

$$t_i = \frac{w_i}{SE(w_i)}$$

where:

Wi = estimated outer weight of the indicator
SE(wi)= standard error of the indicator weight
If the p-value associated with the t-statistic is below 0.05, the indicator weight is deemed significant, confirming that the indicator meaningfully contributes to forming the latent construct.

Multicollinearity: Variance Inflation Factor (VIF)

One of the major concerns in formative measurement models is multicollinearity, which occurs when two or more indicators are highly correlated. Since formative indicators define the construct, high correlations among them can lead to redundant information, distorting the estimation of indicator weights and making it difficult to determine the unique contribution of each indicator (Ringle, Sarstedt, & Straub, 2012).

To detect multicollinearity, Variance Inflation Factor (VIF) is used, which quantifies how much an indicator's variance is inflated due to its correlation with other indicators in the model. The VIF for an indicator i is calculated as:

$$VIF_i = \frac{1}{1 - R_i^2}$$

where:

Ri^2= the proportion of variance in indicator i that is explained by the other indicators in the model.

A VIF value below 5 suggests acceptable levels of multicollinearity, ensuring that each indicator provides unique information. If VIF exceeds 5, it indicates that an indicator shares too much variance with other indicators, reducing the reliability of weight estimates. In such cases, the following adjustments can be made:

Removing the highly correlated indicators to reduce redundancy.

Merging indicators into a single composite variable if they measure highly similar aspects of the construct.

Using principal component analysis (PCA) or orthogonalization techniques to transform correlated indicators into independent components.

Maintaining low multicollinearity is essential to ensure that formative constructs retain theoretical distinctiveness and empirical robustness.

Indicator Contribution: Outer Weights and Loadings

Since formative indicators define a latent construct, their individual contributions are evaluated using outer weights, which indicate the relative importance of each indicator. Outer weights are estimated during the PLS-SEM model estimation process and provide a ranking of indicators based on their influence on the construct. Unlike reflective models, where outer loadings measure indicator reliability, formative models rely on outer weights to determine construct validity (Ringle, Sarstedt, & Schlittgen, 2013). An indicator with a higher weight contributes more significantly to defining the latent construct, whereas an indicator with a low weight has minimal influence.

Mathematically, the outer weight (wi) of an indicator is estimated through multiple regression:

$$\xi = w_1 x_1 + w_2 x_2 + \cdots + w_n x_n + \zeta$$

where:

- ξ= latent construct
- wi = outer weight of indicator xi
- xi = observed indicator
- ζ = residual error term

A high absolute outer weight indicates that an indicator is crucial for construct formation, whereas indicators with low weights may be less relevant. To further validate indicator contributions, outer loadings, which represent the correlation between each indicator and the latent construct, are also examined (Lowry & Gaskin, 2014). In some cases, indicators with low outer weights may still have high outer loadings, suggesting they are still useful in defining the construct. The following guidelines help determine indicator relevance:

- If both outer weight and loading are high, the indicator is highly relevant.
- If outer weight is low but loading is high, the indicator may still provide meaningful content to the construct.
- If both outer weight and loading are low, the indicator should be reconsidered or removed.

By ensuring that each indicator uniquely and significantly contributes to the construct, theoretical clarity and empirical accuracy are enhanced in formative PLS-SEM models.

Theoretical and Practical Implications of Formative Model Assessment

Proper assessment of formative measurement models is essential to ensure that latent constructs are accurately defined by their indicators. Unlike reflective models, where reliability and validity metrics confirm measurement accuracy, formative models require distinct evaluation techniques such as bootstrapping for significance testing, VIF for multicollinearity checks, and outer weights analysis for contribution assessment. From a theoretical perspective, a mis-specified formative model can lead to biased path estimates, incorrect theoretical conclusions, and invalid structural relationships (Liengaard, 2024). It is crucial to carefully validate indicator significance, control for multicollinearity, and assess contribution strength to ensure that the construct retains theoretical relevance and empirical robustness. From a practical perspective, businesses and policymakers employing PLS-SEM in AI-driven research, marketing analytics, or behavioral modeling must ensure that predictive models and decision frameworks rely on well-defined formative constructs. A poorly assessed formative measurement model can result in erroneous insights, misleading strategic decisions, and flawed business intelligence (McIntosh, Edwards, & Antonakis, 2014). Assessing formative measurement models in PLS-SEM requires a distinct methodological approach that focuses on indicator relevance (bootstrapping significance), multicollinearity (VIF diagnostics), and contribution strength (outer weights analysis). Thus, rigorous assessment of formative models is critical for maintaining theoretical accuracy, empirical validity, and actionable insights in PLS-SEM research.

3.3. Structural Model Assessment and Predictive Relevance in PLS-SEM

The structural model in Partial Least Squares Structural Equation Modeling (PLS-SEM) represents the relationships between latent variables, forming the foundation for testing causal hypotheses within a theoretical framework. While the measurement model assessment ensures that latent constructs are accurately measured, the structural model assessment focuses on evaluating the strength, significance, and predictive accuracy of the relationships between these constructs (Rönkkö & Evermann, 2013).

To fully understand how structural model assessment works in PLS-SEM, it is essential to define key terms:

- Endogenous variables: These are dependent latent variables that are explained by one or more predictor (independent) variables in the model. They serve as outcomes of causal relationships.
- Exogenous variables: These are independent latent variables that act as predictors but are not influenced by any other variable in the model. They provide input into the structural relationships.
- Coefficient of Determination (R^2): A measure of explained variance, indicating how well the predictor variables account for changes in an endogenous variable.
- Predictive Relevance (Q^2): Assesses the model's ability to make accurate predictions in an out-of-sample context, ensuring real-world applicability.

A comprehensive structural model evaluation involves multiple key criteria, including path coefficients, R^2, effect size (f^2), predictive relevance (Q^2), and model diagnostics. These assessments ensure that relationships between variables are statistically robust, theoretically sound, and practically relevant.

3.3.1. Path Coefficients: Evaluating Causal Relationships

Path coefficients represent the **strength and direction** of the relationships between latent variables. These coefficients function similarly to regression weights, showing the magnitude of change in the dependent variable for a **one-unit increase** in the independent variable (Ringle, Goetz, Wetzels, & Wilson, 2009).

Mathematically, a structural model can be represented as:

$$\eta_i = \sum \beta_{ij}\eta_j + \sum \gamma_{ik}\xi_k + \zeta_i$$

where:

η_i = endogenous (dependent) latent variable
η_j = other endogenous variables influencing η_i
ξ_k = exogenous (independent) latent variables
β_{ij} = structural path coefficient from η_j to η_i
γ_{ik} = structural path coefficient from ξ_k to η_i

ζi = structural model residual error

To determine statistical significance, bootstrapping is employed, which generates confidence intervals and t-values for each path coefficient. A t-value greater than 1.96 (95% confidence level) or 2.58 (99% confidence level) confirms statistical significance.

Key Interpretations:

- Strong path coefficients (>0.50 suggest substantial causal relationships.
- Moderate path coefficients (.20–0.50) indicate moderate influence between variables.
- Weak path coefficients (<0.20) imply a weak or non-significant relationship that may require model adjustments.

3.3.2. Coefficient of Determination (R^2): Measuring Explained Variance

The **coefficient of determination (R^2)** quantifies the proportion of variance in an endogenous variable that is **explained by its predictors.** It provides insight into the **model's explanatory power** and is a key indicator of model strength (Putra, 2022).

$$R^2 = 1 - \frac{\sum(Y_{\text{actual}} - Y_{\text{predicted}})^2}{\sum(Y_{\text{actual}} - Y_{\text{mean}})^2}$$

where:

- Yactual = observed values of the dependent variable
- Ypredicted = predicted values from the model
- Ymean = mean of the observed values

Interpretation of R^2 values in PLS-SEM:

- $R^2 \geq 0.75$ → Substantial explanatory power
- $0.50 \leq R^2 < 0.75$ → Moderate explanatory power
- $0.25 \leq R^2 < 0.50$ → Weak explanatory power
- R2<0.25 → Very low explanatory power

Since PLS-SEM prioritizes prediction over covariance-based model fit, R2R^2R2 alone is not sufficient to determine a model's validity, it must be complemented by effect size and predictive relevance tests.

3.3.3. Effect Size (f^2): Assessing Predictor Contributions

Effect size (f^2) measures how much an independent variable **contributes** to explaining the variance of a dependent variable. It evaluates the **practical significance** of a predictor beyond statistical significance (Rigdon, Sarstedt, & Ringle, 2017).

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

where:

- R^2 included = R^2 with the predictor variable included
- R^2 excluded = R^2 after removing the predictor variable

Interpretation of f^2 values:

- $f^2 \geq 0.35$ → Large effect
- $0.15 \leq f^2 < 0.35$ → Moderate effect
- $0.02 \leq f^2 < 0.15$ → Small effect
- $f^2 < 0.02$ → Negligible effect

3.3.4. Predictive Relevance (Q^2): Ensuring Out-of-Sample Accuracy

Predictive relevance (Q^2) measures how well a model predicts unseen data, ensuring that the model retains real-world applicability.

$$Q^2 = 1 - \frac{\sum (Y_{\text{actual}} - Y_{\text{predicted}})^2}{\sum Y_{\text{actual}}^2}$$

where:

$Q^2 > 0$ → The model has predictive relevance.

$Q^2 \leq 0$ → The model lacks predictive power, suggesting a need for refinements.

Blindfolding, a cross-validation technique, systematically omits portions of data, predicts those values, and evaluates the prediction accuracy.

Interpretation of Q^2 values:

- $Q^2 > 0.35$ → Strong predictive relevance
- $0.15 \leq Q^2 < 0.35$ → Moderate predictive relevance
- $0.02 \leq Q^2 < 0.15$ → Weak predictive relevance

Ensuring high predictive relevance strengthens confidence in the model's ability to make real-world predictions, making it particularly valuable for AI-driven applications, business forecasting, and decision analytics.

3.3.5. Model Fit Diagnostics in PLS-SEM

Unlike covariance-based SEM, which relies on absolute model fit indices, PLS-SEM focuses on predictive accuracy rather than fit measures. However, diagnostics such as Standardized Root Mean Square Residual (SRMR), Normed Fit Index (NFI), and exact model fit tests (d_ULS, d_G) can be used for additional validation (Nitzl, Roldán, & Cepeda, 2016).

- SRMR (<0.08) suggests a good model fit.
- NFI (closer to 1) indicates better model efficiency.
- d_ULS and d_G provide advanced assessments for consistency.

Though PLS-SEM does not require absolute fit measures, these diagnostics help verify model robustness. A comprehensive structural model assessment in PLS-SEM involves evaluating path coefficients, explained variance (R^2), effect sizes (f^2), predictive relevance (Q^2), and diagnostic checks (Richter, Sinkovics, Ringle, & Schlägel, 2016). These assessments ensure that the relationships between variables are both statistically sound and practically useful.

3.4. Confirmatory Tetrad Analysis (CTA-PLS)

Confirmatory Tetrad Analysis (CTA) is a statistical procedure originally developed to test the null hypothesis that certain combinations of covariances (known as tetrads) are equal to zero. In the context of PLS-SEM, CTA-PLS is used as a diagnostic tool to assess the nature of the measurement model specifically, to determine whether indicators should be modeled reflectively or formatively. Under a reflective measurement specification, the covariance structure among the indicators is such that specific tetrad differences are expected to be zero (Ringle, Sarstedt, Mitchell, & Gudergan, 2018). Conversely, a formative model typically does not impose this zero-tetrad restriction.

- **Mathematical Formulation:** Consider a latent variable measured by four indicators, Y1, Y2, Y3 and Y4. The tetrad difference is defined as:

$$\delta_{(i,j;k,l)} = \mathrm{Cov}(Y_i, Y_j) \times \mathrm{Cov}(Y_k, Y_l) - \mathrm{Cov}(Y_i, Y_k) \times \mathrm{Cov}(Y_j, Y_l)$$

Under a reflective model, theory predicts that $\delta(i,j;k,l)=0$ for all valid combinations of i,j,k, and l. In practice, significance tests (often employing bootstrapping) are used to determine whether these tetrad differences are statistically indistinguishable from zero (Rasoolimanesh, Ringle, Sarstedt, & Olya, 2021). A significant deviation may indicate that the model is mis-specified (i.e., the indicators may be better conceptualized as forming a composite rather than reflecting a latent variable).

Practical Implications: Model Specification: CTA-PLS provides a formal statistical test to validate the assumption of reflective measurement. If tetrad differences are nonzero, researchers may need to reconsider the measurement model and possibly re-specify indicators as formative (Richter, Cepeda, Roldán, & Ringle, 2016). Complementary Assessment: While CTA-PLS is powerful, it is often used in conjunction with other assessments (e.g., cross-loadings or the HTMT ratio) to ensure that the chosen specification robustly captures the underlying construct.

3.5. Importance-Performance Matrix Analysis (IPMA)

Importance-Performance Matrix Analysis (IPMA) extends the basic outcomes of PLS-SEM by incorporating an additional layer of managerial insight. While the primary PLS path model focuses on the structural relationships between constructs (i.e., the "importance" derived from total effects), IPMA overlays a "performance" dimension that reflects the average latent variable scores. This dual focus allows researchers to prioritize areas for improvement (Ringle, Sarstedt, Sinkovics, & Sinkovics, 2023).

Methodological Steps and Equations - Importance (Total Effects): The importance of a predictor construct is typically derived from its total effect on a target construct. If β_{ij} denotes the path coefficient from construct i to construct j, the overall importance I_i of construct I on the target Y can be defined as:

$$I_i = \sum_j \beta_{ij} \quad \text{(including both direct and indirect effects)}$$

- **Performance:** Performance is assessed by the average latent variable score (usually normalized to a scale from 0 to 100). Let $\bar{L}_I$ represent the average score of constructs i:

$$P_i = \bar{L}_i$$

Matrix Construction: The results are then plotted on a two-dimensional matrix with importance on one axis and performance on the other. This visualization enables the identification of constructs that are critical (high importance) yet underperforming (low performance) and hence should be the focus of managerial intervention.

Practical Application and Considerations: Prioritization: IPMA facilitates decision-making by highlighting constructs that not only influence outcomes but also have room for improvement. Sensitivity Analysis: Researchers must account for potential scale differences across constructs, ensuring that performance scores are interpretable and comparable (Roldán & Sánchez-Franco, 2012). Integration with PLS-SEM: The combination of structural path coefficients and latent scores strengthens the explanatory power of the PLS-SEM results, providing both theoretical and practical insights.

3.6. Higher-Order Constructs and Hierarchical Component Models

Higher-order constructs (HOCs) allow researchers to model multidimensional concepts that are not fully captured by a single latent variable (Sarstedt, Hair, Nitzl, Ringle, & Howard, 2020). Hierarchical Component Models (HCMs) are particularly useful when the construct of interest is composed of several related but distinct dimensions (first-order constructs). Modeling HOCs improves the parsimony of the structural model and helps to reduce multicollinearity among constructs.

3.6.1. Common Approaches to Modeling HOCs

- **Repeated Indicators Approach:** In this method, the indicators of all first-order constructs are assigned to the higher-order construct. If F1, F2,...., Fm represent the first-order constructs with their corresponding indicator sets {Y1k},{Y2k},...,{Ymk}, then the higher-order construct H is measured by the union of these indicators. The weights for each indicator are estimated using the PLS algorithm, effectively aggregating the information across dimensions (Shiau, Sarstedt, & Hair, 2019).

$$H = f(Y_{11}, Y_{12}, \ldots, Y_{mk})$$

- **Two-Stage Approach:** In the first stage, the scores of the first-order constructs are estimated using PLS-SEM. In the second stage, these latent variable scores are used as manifest variables to estimate the higher-order construct. Mathematically, this can be represented as:

$$H = \sum_{i=1}^{m} w_i F_i$$

where wi are the weights that reflect the contribution of each first-order construct Fi to the higher-order construct H.

- **Hybrid Approaches:** studies may integrate elements from both the repeated indicators and two-stage approaches. For example, certain indicators might be directly assigned to the higher-order construct, while others are mediated through first-order constructs (Sarstedt, Hair, Pick, Liengaard, Radomir, & Ringle, 2022).

3.6.2. Measurement Considerations and Equations

- **Reflective vs. Formative Specification:** The choice between reflective and formative measurement for HOCs depends on the theoretical conceptualization. In reflective HOCs, changes in the higher-order construct are assumed to reflect in all lower-order dimensions (Schermelleh-Engel, Werner, Klein, & Moosbrugger, 2010). In formative HOCs, the first-order constructs are viewed as causal indicators that collectively form the higher-order construct.
- **Reliability and Validity Testing:** It is crucial to assess the reliability (e.g., composite reliability, Cronbach's alpha) and validity (e.g., convergent and discriminant validity) of both first-order and higher-order constructs (Sarstedt, Hair, & Ringle, 2022). For instance, the composite reliability CR_H for a reflective HOC may be computed using the weights wi and the reliability scores CR_{Fi} of the first-order constructs:

$$CR_H = \sqrt{\sum_{i=1}^{m} w_i^2 \times CR_{F_i}^2}$$

- **Practical Implications**: **Model Complexity and Parsimony:** Incorporating HOCs can simplify the structural model by reducing the number of direct relationships. However, the estimation strategy must be carefully chosen to ensure that the multidimensionality is properly captured.
- **Theoretical Rigor:** The use of HOCs should be grounded in theory, ensuring that the aggregation of first-order constructs is conceptually justified.
- **Software Implementation:** Modern PLS-SEM software packages (e.g., SmartPLS, SEMinR) provide specific routines to handle higher-order constructs, making it easier to implement the repeated indicators, two-stage, or hybrid approaches. In summary, the advanced techniques discussed CTA-PLS, IPMA, and modeling of HOCs serve distinct but complementary roles in enhancing PLS-SEM analyses. CTA-PLS provides a formal test for the measurement model's specification, ensuring that reflective indicators behave as theoretically expected. IPMA augments the explanatory power of the model by integrating managerial relevance through the dual lenses of importance and performance (Sarstedt & Moisescu, 2023). Finally, higher-order constructs enable the modeling of complex, multidimensional phenomena, balancing model parsimony with theoretical depth.

Table 2 R^2, Q^2, and f^2 value ranges to determine the model fitness

Value Range	R2 Interpretation (Chin, 1998; Hair et al., 2011/2017)	Q2 Interpretation (Hair et al., 2019)	f2 Interpretation (Cohen, 1988)
0.00 – 0.19	Very weak or weak	< 0 indicates no predictive Power	< 0.02 = no effect
0.20 – 0.33	Weak	(no specific benchmark)	0.02 – 0.15 = small effect
0.34 – 0.50	Moderate	~0.02 = small predictive Relevance	0.15 – 0.35 = medium effect
0.51 – 0.67	Moderate to substantial	~0.15 = medium predictive Relevance	> 0.35 = large effect
≥ 0.67	Substantial	~0.35 = strong predictive Relevance	> 0.35 = large effect
≥ 0.75	Substantial (sometimes used as a higher threshold)	(no specific benchmark)	> 0.35 = large effect

Note: These value ranges serve as general guidelines in PLS-SEM. However, it's essential to apply these guidelines thoughtfully and consider the specific context of your research.

A simple Path model

Exogenous and endogenous constructs are central concepts in structural equation modeling, including PLS-SEM. In essence, exogenous constructs act as independent variables in the model and are not predicted by other latent variables, while endogenous constructs function as dependent variables and are explained by one or more exogenous constructs (Sarstedt, Richter, Hauff, & Ringle, 2024). In the attached figure, each exogenous latent variable (Y_1, Y_2, Y_3) is measured with either formative or reflective indicators, meaning that some indicators are viewed as causing the latent variable (formative) while others reflect the latent variable (reflective). These exogenous constructs, located on the left side of the diagram, connect to the endogenous constructs (Y_4, Y_5) in the center and right side, which themselves are measured reflectively. The arrows within the middle (inner) portion of the diagram show the hypothesized paths among these latent variables, indicating how Y_1, Y_2, and Y_3 may each influence Y_4 and Y_5. In PLS-SEM, the iterative algorithm estimates both the outer measurement models (defining how indicators relate to each latent variable) and the inner structural model (capturing the relationships among latent variables). This allows for the flexible handling of data that may be non-normal or limited in sample size (Sarstedt & Cheah, 2019). Formative indicators in the exogenous constructs require careful evaluation of weights and potential multicollinearity, while reflective indicators in both exogenous and endogenous constructs are assessed using traditional reliability and validity metrics such as composite reliability, average variance extracted (AVE), and discriminant validity checks (for example, via the Heterotrait-Monotrait ratio). By accommodating different measurement approaches—formative on the left for certain exogenous variables and reflective on the right for endogenous variables—this figure illustrates a hybrid model that captures the complexity of real-world phenomena (Rönkkö, McIntosh, & Antonakis, 2015). Ultimately, the paths in the center of the figure denote how each exogenous latent variable is posited to explain variance in the endogenous constructs, and the final estimated path coefficients and significance levels can be tested via bootstrapping. Through this setup, researchers can investigate a wide range of theoretical relationships, ensuring that the constructs are accurately measured while simultaneously modeling the causal connections that drive outcomes of interest.

The below figure 2 presents a detailed path model in PLS-SEM that illustrates a hybrid measurement approach, incorporating both exogenous and endogenous constructs, each measured using either formative or reflective indicators. On the left side of the diagram, the exogenous constructs labeled Y_1, Y_2, and Y_3 are depicted with a combination of formative and reflective items (Sarstedt & Liu, 2023). In this setup, certain indicators (for example, "Item 1 (formative)" and "Item 2 (formative)" for Y_1) are shown with arrows directed from the indicators to the construct, indicating that these indicators serve as causal inputs that form the latent variable. In contrast, other indicators (such as "Item 3 (reflective)") are represented with arrows going from the construct to the indicator, implying that the latent variable is assumed to cause the observed scores on these measures. This mixed approach underlines the flexibility of PLS-SEM in handling multidimensional constructs, where different theoretical dimensions may require distinct measurement modes (Sharma, Liengaard, Hair, Sarstedt, & Ringle, 2022).

At the center of the Figure 2, the inner (structural) model is presented, showcasing the hypothesized causal relationships among the latent constructs. The diagram illustrates direct paths from the exogenous constructs (Y_1, Y_2, and Y_3) to the endogenous constructs (Y_4 and Y_5). The directionality of these arrows conveys the presumed causation—for instance, an arrow from Y_1 to Y_5 suggests that variations in Y_1 are expected to explain changes in Y_5. Moreover, the presence of multiple exogenous and endogenous constructs highlights the model's complexity and the potential for mediation, where an exogenous variable might influence an endogenous construct directly and indirectly through another latent variable. This central portion of the model is critical for testing theoretical hypotheses regarding how different factors interact to affect outcomes within the system.

On the right side of the Figure, the endogenous constructs Y_4 and Y_5 are shown with reflective indicators exclusively. In these reflective models, arrows extend from the latent constructs to the indicators, signaling that any changes in the latent variable are manifested in the observed measures. This arrangement reinforces the expectation that indicators measuring an endogenous construct will co-vary, thereby supporting assessments of internal consistency, composite reliability, and convergent validity through metrics such as average variance extracted (AVE). The clear differentiation between the formative measurement style of some exogenous constructs and the reflective measurement style of the endogenous constructs underscores the versatility of PLS-SEM in accommodating different types of measurement approaches within a single model (Tenenhaus, Vinzi, Chatelin, & Lauro, 2004).

The implications for PLS-SEM analysis are significant. Because PLS-SEM is a variance-based approach, it is capable of handling both formative models (as seen in parts of the exogenous constructs) and reflective models (as seen in the endogenous constructs) within the same analysis. The iterative estimation process used by PLS-SEM computes latent variable scores, updates indicator weights or loadings, and estimates path coefficients in the structural model, accommodating non-normal data distributions and smaller sample sizes more flexibly than covariance-based SEM approaches (Wetzels, Odekerken-Schröder, & Van Oppen, 2009). Furthermore, mixing formative and reflective indicators can raise important issues regarding discriminant validity; thus, techniques such as the Fornell-Larcker criterion or the Heterotrait-Monotrait (HTMT) ratio are essential for verifying that each latent construct is distinct from the others.

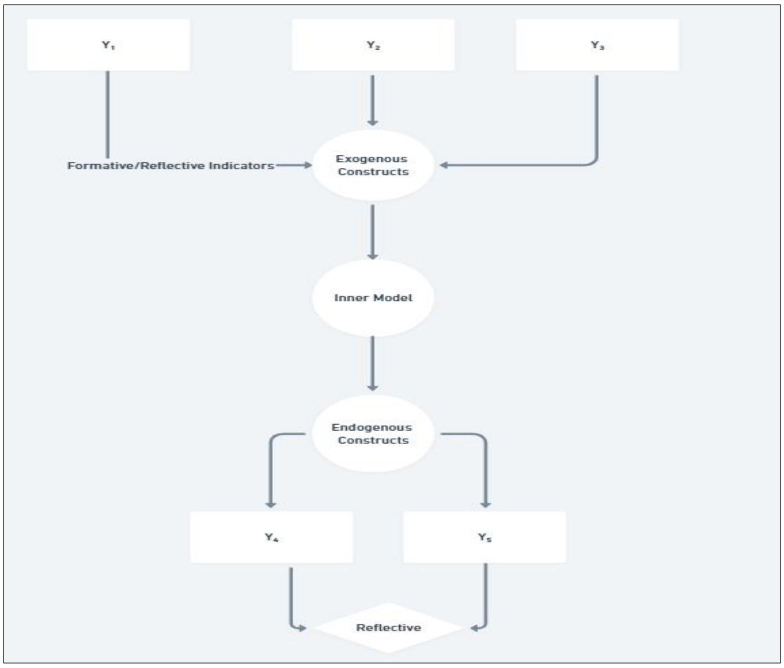

Figure 2 A simple path model Logic

In summary, the figure 2 illustrates a simple yet comprehensive path model that effectively combines both formative and reflective measurement within the same framework. The exogenous constructs on the left are measured by a mix of indicator types, the inner model in the center captures the structural relationships between these constructs and the endogenous outcomes, and the reflective indicators on the right ensure that the outcomes are measured with high internal consistency. This design not only demonstrates the theoretical underpinnings of different measurement approaches in PLS-SEM but also highlights practical considerations for ensuring reliability, validity, and discriminant validity within complex causal models. The model's structure serves as a robust example of how PLS-SEM can be used to capture the multidimensional nature of constructs while providing a clear roadmap for parameter estimation and hypothesis testing.

4. Critical Techniques and Algorithms in PLS-SEM

In this section, a comprehensive exploration of the advanced computational methods underpinning PLS-SEM is presented. The discussion begins with an in-depth look at the PLS algorithm, detailing its iterative approach, underlying mathematical framework, and how it maximizes explained variance in complex latent constructs. Next, the focus shifts to bootstrapping, a nonparametric resampling technique that provides robust inferential statistics by estimating standard errors, confidence intervals, and t-statistics without relying on normality assumptions. Finally, the blindfolding procedure is introduced as a vital cross-validation technique to assess a model's predictive relevance through the Q^2 statistic (Sarstedt, Hair, Cheah, Becker, & Ringle, 2019). Together, these methods offer a rigorous and integrated framework that not only ensures the accurate estimation of model parameters but also validates their stability and predictive power. This synthesis of techniques forms the backbone of PLS-SEM, enabling both theoretical depth and practical applicability in diverse empirical settings.

4.1. PLS Algorithm: Computation and Application

The PLS algorithm is designed to maximize the explained variance of endogenous latent constructs. It achieves this by estimating latent variable scores as linear combinations of observed indicators while simultaneously estimating the relationships among latent constructs (Sharma, Shmueli, Sarstedt, Danks, & Ray, 2018).

Initialization - Step: Assign initial weights to each indicator (e.g., equal weights or values derived from principal component analysis).

Outer Model (Measurement Model) Estimation - Step: For each latent variable ηj, compute its score as:

$$\eta_j = \sum_{i=1}^{p_j} w_{ij}\, x_{ij}$$

where xij is the ith indicator for latent construct j and wij is its weight.

Inner Model (Structural Model) Estimation - Step: Model the structural relationships among constructs as:

$$\eta_k = \sum_{j \in \text{Predictors}} \beta_{kj}\, \eta_j + \zeta_k$$

where βkj is the path coefficient from predictor ηj to the endogenous construct ηk and ζk is the error term.

- Weight Updating and Iteration - Step: Update the weights by regressing the indicators on the latent scores from the inner model. Iterate until convergence, when the changes in weights become negligible.
- Final Estimation - Step: After convergence, use the final latent variable scores, outer loadings, and inner model coefficients for subsequent reliability, validity, and predictive assessments.
- Key Advantages - Flexibility with Data Distributions: The PLS algorithm does not require multivariate normality, making it robust when applied to datasets with skewed or non-normal distributions. This flexibility is especially useful in real-world applications where data often deviate from ideal statistical assumptions. Focus on Prediction: PLS is designed to maximize the explained variance in endogenous constructs. This prediction-oriented approach is ideal for exploratory analysis or when the primary goal is forecasting rather than confirming an already established theory (Sarstedt, Ringle, & Hair, 2017). Handling Complex Models: The algorithm efficiently accommodates models with reflective, formative, and higher-order constructs, even with relatively small sample sizes. Its iterative nature allows modeling of complex relationships without the stringent requirements seen in covariance-based SEM.

- Practical Considerations - Initialization Sensitivity: The starting weights assigned to indicators can influence convergence. Conducting sensitivity analyses with different initialization schemes can help ensure that the final model is robust. Monitoring Convergence - Setting appropriate stopping criteria (e.g., when changes in weights fall below a pre-set threshold) is crucial to ensure that the iterative process has truly converged to a stable solution. Software Implementation Widely used software tools such as SmartPLS or SEMinR streamline the implementation of the PLS algorithm (Wang, Cheah, Wong, & Ramayah, 2023). However, it is important to be mindful of default settings and parameter choices to avoid misinterpretation of the results.

4.2. Bootstrapping in PLS-SEM

Bootstrapping is a resampling method that provides nonparametric estimates of standard errors, confidence intervals, and t-statistics, thereby strengthening the inferential power of PLS-SEM estimates without relying on the normality assumption.

- Resampling- Step: Generate B bootstrap samples (typically between 500 and 5,000) by sampling with replacement from the original dataset.
- Model Re-Estimation - Step: Re-estimate the entire PLS model for each bootstrap sample to obtain a distribution of parameter estimates.
- Calculation of Standard Errors - Step: For a parameter β^, compute the standard error as:

$$SE(\hat{\beta}) = \sqrt{\frac{1}{B-1}\sum_{b=1}^{B}\left(\hat{\beta}^{(b)} - \overline{\hat{\beta}}\right)^2}$$

Hypothesis Testing - Step: Compute t-statistics by:

$$t = \frac{\hat{\beta}}{SE(\hat{\beta})}$$

- Outcome: Confidence intervals are typically derived using percentile-based or bias-corrected methods.
- Key Advantages - Nonparametric Inference: Bootstrapping generates robust standard errors, confidence intervals, and t-statistics without relying on the normality assumption. This is highly suitable for PLS-SEM when data may not follow a normal distribution. Model Stability Assessment: By repeatedly re-estimating the model on resampled datasets, bootstrapping offers insights into the stability and reliability of the parameter estimates, enhancing confidence in the reported results (Venturini & Mehmetoglu, 2019).
- Practical Considerations - Computational Intensity: The resampling process can be computationally demanding, particularly with large or complex models that require many bootstrap replications. Adequate computational resources and appropriate replication numbers must be planned. Number of Replications: Choosing the right number of bootstrap samples (commonly between 500 and 5,000) is critical. Too few replications may yield imprecise estimates, while too many can extend computation time unnecessarily. Method of Interval Estimation: The selection between percentile-based and bias-corrected intervals can affect the interpretation of results. It is important to choose the method that best aligns with the data characteristics and research objectives (Schuberth, Rademaker, & Henseler, 2022).

4.3. Blindfolding Procedure and Predictive Power

Blindfolding is used to assess a model's predictive relevance by systematically omitting parts of the data and predicting the omitted values. This process leads to the calculation of the Q^2 statistic.

- **Omission Distance Definition - Step:** Set an omission distance D (e.g., every 7th observation) to guide the systematic omission process.
- **Data Omission and Prediction - Step:** Omit a data point, re-estimate the model using the remaining data, and predict the omitted value.
- **Calculation of Q^2 - Step:** Compute the Q^2 statistic as:

$$Q^2 = 1 - \frac{\sum_{i=1}^{N}(y_i - \hat{y}_i)^2}{\sum_{i=1}^{N}(y_i - \bar{y})^2}$$

where yi is the observed value, y^i is the predicted value, and y¯ is the mean of the observed values. A Q^2 value above zero indicates that the model has predictive relevance.

Key Advantages Assessment of Predictive Relevance: Blindfolding systematically omits data points and predicts the omitted values to calculate the Q^2 statistic. This process directly tests whether the model can accurately predict unseen data, serving as a crucial check against overfitting. Cross-Validation: As an internal validation technique, blindfolding ensures that the model's predictive performance is not limited to the training data but generalizes well to new observations (Sukhov, Friman, & Olsson, 2023).

Practical Considerations Selection of Omission Distance: The choice of omission distance (e.g., every 7th observation) is key. An inappropriate omission distance may lead to biased predictions or underrepresent the model's variability, thereby distorting the Q^2 assessment. Sample Size Requirements: A sufficiently large dataset is required for blindfolding to yield stable and meaningful results. Small samples may compromise the reliability of the cross-validation process (Shmueli, Sarstedt, Hair, Cheah, Ting, Vaithilingam, & Ringle, 2019). Interpretation of Q^2: Although heuristic thresholds exist (e.g., 0.02 for small, 0.15 for medium, and 0.35 for large predictive relevance), these values must be interpreted within the specific context. The absolute value of Q^2 is only one indicator of predictive relevance.

4.4. Synthesis and Theoretical Integration

The integration of the PLS algorithm, bootstrapping, and blindfolding creates a robust framework for PLS-SEM, where each technique plays a complementary role:

Unified Estimation and Validation: The PLS algorithm provides a flexible and prediction-focused method for estimating complex models. Bootstrapping adds a layer of statistical rigor by offering nonparametric inferential statistics, while blindfolding ensures that the model's predictive power is thoroughly evaluated through cross-validation (Sarstedt, Hair, & Ringle, 2022).

Theoretical Coherence: Together, these techniques form a coherent framework where theoretical constructs are accurately measured and validated. This integration ensures that the model not only fits the sample data well but also generalizes to new data, reinforcing both reliability and practical applicability (Rönkkö & Evermann, 2013).

Enhanced Decision-Making: The combination of these methods provides a clear roadmap for model validation. It enhances confidence in the conclusions drawn from the model and supports informed decision-making based on both explanatory and predictive insights (Venturini & Mehmetoglu, 2019).

Contextual Adaptation: The application of these techniques must always be contextualized within the specifics of the domain. It is advisable to adjust thresholds, select appropriate parameters, and interpret results in light of particular data characteristics and theoretical frameworks (Sarstedt & Liu, 2023).

5. Addressing Measurement Challenges in PLS-SEM

Measurement challenges are a key concern in PLS-SEM, as they can significantly affect the validity and reliability of the findings. This section discusses three critical areas: evaluating discriminant validity using the HTMT criterion, conceptualizing and assessing higher-order constructs, and dealing with common method bias.

5.1. Evaluating Discriminant Validity (HTMT Criterion)

Discriminant validity ensures that each construct in the model is empirically distinct from every other construct. Traditional approaches, such as the Fornell-Larcker criterion and examining cross-loadings, have been widely used. However, the Heterotrait-Monotrait (HTMT) ratio offers a more robust and reliable alternative for assessing discriminant validity in PLS-SEM (Sarstedt, Ringle, & Hair, 2017).

Definition and Calculation: The HTMT ratio compares the average correlations of indicators across different constructs (heterotrait correlations) to the average correlations of indicators within the same construct (monotrait correlations).

A commonly accepted guideline is that HTMT values should be below 0.85 or 0.90, depending on how conceptually similar the constructs are. Values exceeding these thresholds may signal insufficient discriminant validity. To further strengthen the assessment, HTMT bootstrapping can be employed to determine whether the HTMT value is statistically below the chosen critical threshold (Cho et al., 2022).

The following equation illustrates how HTMT is computed for two constructs a and b:

$$\mathrm{HTMT}_{ab} = \frac{\mathrm{mean}(|r_{ij}|;\ i \in a,\ j \in b)}{\sqrt{\mathrm{mean}(|r_{ii'}|;\ i, i' \in a) \times \mathrm{mean}(|r_{jj'}|;\ j, j' \in b)}}$$

where rij represents the correlation between indicator i of construct a and indicator j of construct b. The numerator captures the heterotrait (i.e., inter-construct) correlations, while the denominator captures the monotrait (i.e., intra-construct) correlations for each construct separately.

Practical Application: Applying the HTMT criterion provides a clearer view of whether constructs overlap excessively. If the HTMT values remain below the established threshold (e.g., 0.85), it can be concluded that the constructs in question are sufficiently distinct. When HTMT bootstrapping indicates that the ratio does not exceed the threshold at a chosen confidence level (e.g., 95%), there is further evidence supporting discriminant validity (Becker et al., 2023).

5.2. Higher-Order Constructs: Conceptualization and Assessment

Reflective-Reflective HOC: A reflective-reflective higher-order construct (HOC) is one in which both the higher-level construct and each of its lower-order components (LOCs) are measured reflectively. In other words, changes in the latent trait at each level are assumed to be manifested by changes in the observed indicators. The key assumption here is that the indicators are highly interchangeable, and each set of indicators captures essentially the same underlying dimension (Cho & Choi, 2019). For instance, a higher-order concept such as “service quality” may be divided into sub-dimensions like “tangibles,” “responsiveness,” and “empathy,” each of which is measured reflectively. If “service quality” itself is also specified reflectively, it implies that variations in the overall construct are reflected in each sub-dimension, and variations in each sub-dimension are similarly reflected in their respective indicators. The reflective-reflective approach is relatively straightforward to implement but requires strong theoretical support to justify that both the LOCs and the HOC reflect an underlying common factor at their respective levels (Durdyev et al., 2018).

Reflective-Formative HOC: In a reflective-formative HOC, the higher-order construct is measured with a reflective model, while each lower-order component is measured formatively. This implies that the overall HOC is conceptualized as an underlying factor that manifests in the form of various dimensions. However, each dimension (the LOC) is seen as a composite of formative indicators, where changes in the indicators cause changes in the dimension itself (Becker et al., 2023). For example, suppose the overall latent trait is “brand equity” measured reflectively at the higher level, but each sub-dimension (e.g., brand awareness, brand associations, and perceived quality) is captured by a formative set of indicators. In this scenario, each LOC is formed by its indicators, yet changes in the higher-order brand equity construct are believed to reflect in all LOCs collectively. This approach is particularly useful when the dimensions are seen as distinct facets that combine to form a broader latent trait, but each facet is influenced by multiple causal indicators (Carrión, Nitzl, & Roldán, 2017).

Formative-Reflective HOC: A formative-reflective HOC takes the opposite stance compared to the reflective-formative model. The higher-order construct is specified formatively, meaning that the various LOCs collectively cause or form the overarching concept. Each LOC, however, is measured with reflective indicators, assuming that changes in the LOC manifest in changes across its indicators (Dijkstra & Henseler, 2015). This structure is suitable for situations in which the overall HOC is considered an aggregate of multiple reflective sub-dimensions. For instance, consider a concept like “work engagement” measured formatively at the higher level, with sub-dimensions such as “vigor,” “dedication,” and “absorption,” each measured reflectively. If the sub-dimensions are combined to form the overall construct, then a change in any sub-dimension (e.g., dedication) can alter the overall level of work engagement. However, each sub-dimension itself is captured through a set of reflective items that represent its underlying latent nature.

Formative-Formative HOC: In the formative-formative HOC, both the higher-order construct and the LOCs are measured formatively. This implies that each sub-dimension is formed by its respective indicators, and these sub-dimensions together form the overarching construct. Such a specification is common when the construct is truly composite in nature (Becker et al., 2023). For example, consider an overarching concept like “socioeconomic status,” which might be formed by sub-dimensions such as income, education, and occupation. Each of these sub-dimensions could itself be composed of multiple formative indicators (e.g., different income brackets, highest degree obtained, occupational prestige). Changes in one sub-dimension (e.g., income) can substantially alter the overall construct, but each sub-dimension is similarly formed by multiple indicators. This approach demands a clear theoretical rationale for why the overall concept is considered an aggregate of multiple formative sub-dimensions and why each dimension is also best modeled formatively (Cheah, Amaro, & Roldán, 2022).

5.3. Common Method Bias and Remedies

Common method bias (CMB) refers to the systematic variance in observed measures attributable to the measurement method rather than to the constructs themselves. This bias can inflate or deflate observed relationships and, if unaddressed, may compromise the validity of conclusions drawn from PLS-SEM models. Below is a detailed exploration of the nature of CMB, its detection, and possible remedies. The discussion is organized into multiple paragraphs to ensure comprehensive coverage (Durdyev et al., 2018).

Definition and Scope: Common method bias arises primarily when the same measurement method (e.g., a single survey instrument) is used to collect data on multiple constructs. If respondents apply a consistent but unintended response style (such as always agreeing with statements or responding in a socially desirable manner), the resulting data can exhibit correlations driven by method artifacts rather than true relationships. Such bias is particularly relevant in fields like behavioral research, marketing, or organizational studies, where self-reported surveys are common (Henseler & Sarstedt, 2012).

Causes of CMB: Several factors can give rise to common method bias. One prominent cause is "common rater effects," in which a single respondent provides data on both the predictor and outcome variables. This situation can lead to spurious correlations if the respondent's mood, fatigue, or desire to provide socially acceptable answers systematically influences responses. Another cause is the presence of "item characteristic effects," where poorly worded items or ambiguous scales create consistent patterns of responses that do not truly reflect the underlying constructs (Hair & Alamer, 2022).

Impact on Research Findings: The presence of CMB can severely distort path coefficients in PLS-SEM, either by artificially inflating them (leading to Type I errors) or masking true effects (Type II errors). This distortion is especially problematic when the theoretical relationships among constructs are subtle or newly proposed, as inflated correlations can misleadingly support hypotheses that are not actually valid. Conversely, genuine effects might be obscured if the bias works in the opposite direction (Islam & Khan, 2024).

Procedural Remedies During Study Design: One of the most effective strategies to mitigate CMB is to address it at the study design phase. For instance, implementing temporal separation of measurements (collecting data on predictors and outcomes at different times) can reduce the likelihood that respondents carry over consistent biases in a single sitting (Hair, Matthews, Matthews, & Sarstedt, 2017). Using different response formats, such as alternating Likert scales with semantic differentials, may disrupt the tendency to respond uniformly. Additionally, carefully wording questions to minimize ambiguity or social desirability cues can lessen the risk that participants respond in a patterned, biased manner (Henseler & Chin, 2010).

Marker Variable Technique: In some cases, a marker variable that is theoretically unrelated to the primary constructs is included in the survey. By examining correlations between the marker variable and other constructs, it becomes possible to gauge the extent of method bias. If correlations with the marker variable are unexpectedly high, it may suggest that a consistent method-related factor is at play across the dataset (Rigdon, Ringle, & Sarstedt, 2010).

Harman's Single-Factor Test: A widely referenced but sometimes criticized method for detecting CMB is Harman's single-factor test. Here, all items from the model are subjected to an exploratory factor analysis to see if one factor accounts for the majority of variance. While easy to implement, this test has been criticized for its lack of sensitivity and its inability to precisely isolate the effect of a single measurement method (Putra, 2022).

Common Latent Factor Approach: Another statistical approach involves introducing a common latent factor into the structural equation model. This latent factor is linked to all the indicators, capturing the variance that is potentially attributable to the measurement method. By comparing model fit or path estimates before and after including the common latent factor, it becomes possible to estimate how much of the variance in indicators is explained by method bias (Rigdon, Ringle, & Sarstedt, 2010).

Partial Correlation Procedures: In partial correlation approaches, the variance explained by the suspected bias (e.g., from a marker variable or common factor) is partial out from the correlations among the primary constructs. This procedure adjusts the path coefficients, thereby offering a clearer view of the true relationships. However, it also requires a sound theoretical basis for selecting the marker variable or the common factor (Lowry & Gaskin, 2014).

Balancing Practicality and Rigor: While statistical techniques are valuable, the best line of defense against CMB often lies in well-considered procedural designs. In many real-world scenarios, implementing time separation or multiple measurement methods may be challenging. Therefore, balancing feasibility with methodological rigor is essential. Even partial implementation of procedural remedies such as randomizing item order or using varied scale endpoints can reduce CMB to a manageable level (Nitzl, Roldán, & Cepeda, 2017).

Importance for Validity and Generalizability: Addressing CMB is not merely a technical concern but a cornerstone of valid inference. When CMB is ignored, relationships among constructs may appear stronger or weaker than they truly are, leading to flawed theoretical conclusions or misguided managerial implications. By proactively detecting and mitigating CMB, it becomes possible to present more trustworthy findings, thereby enhancing both the internal and external validity of the research (Rönkkö & Evermann, 2013).

Concluding Remarks on CMB: Ultimately, common method bias represents a serious but manageable threat to the integrity of findings in PLS-SEM. A multifaceted strategy combining thoughtful study design, robust measurement procedures, and thorough statistical checks offers the best means to mitigate this bias. When these efforts are integrated, they ensure that any observed relationships are genuinely reflective of the constructs under investigation, rather than artifacts of the measurement method. This heightened reliability is particularly vital when the goal is to advance theoretical understanding or inform evidence-based practice (Liengaard, 2024).

Each type of higher-order construct offers a unique way of modeling complex, multidimensional phenomena. Choosing among reflective-reflective, reflective-formative, formative-reflective, or formative-formative specifications should be driven by clear theoretical justification and empirical plausibility. Meanwhile, addressing common method bias through both procedural and statistical remedies is essential to preserve the integrity of these measurement models. Together, these considerations enable PLS-SEM to provide accurate, credible insights into the structural relationships among latent constructs (Rönkkö, McIntosh, & Antonakis, 2015).

6. Guidelines for implementing PLS-SEM

The Figure illustrates a broad workflow for carrying out a PLS-SEM analysis, beginning with early considerations and moving through measurement model checks, structural model evaluation, and, finally, robustness checks. This layout demonstrates how PLS-SEM can adapt to different data characteristics, measurement setups, and research objectives. At the outset, it is crucial to verify key elements like sample size, distributional assumptions, and whether secondary data can be used effectively (Henseler & Chin, 2010). Even though PLS-SEM is more tolerant of smaller samples and non-normal distributions than covariance-based SEM, having enough observations remains important for stable parameter estimates and sufficient statistical power. It is also essential to confirm that any secondary data align with the study's theoretical underpinnings (Rigdon, Sarstedt, & Ringle, 2017). Moreover, since PLS-SEM focuses on predictive power rather than a single, overarching fit metric, the notion of "goodness-of-fit" differs from what is commonly used in covariance-based SEM approaches.

The next phase focuses on the measurement model, which may incorporate both reflective and formative indicators. When indicators are reflective, they are seen as manifestations of the underlying latent construct, meaning they should correlate highly with each other and all be driven by the same concept (Hair, Sarstedt, Pieper, & Ringle, 2012). Reliability in these cases is checked through metrics such as Cronbach's alpha or composite reliability, and convergent validity is often measured via the average variance extracted (AVE). Discriminant validity is tested using methods like the Fornell-Larcker criterion or the Heterotrait-Monotrait ratio to confirm that each latent variable is indeed distinct (Liengaard, 2024). For formative constructs, the indicators are considered causes of the latent variable, so the emphasis shifts to the significance of indicator weights, variance inflation factors (VIF) to watch for multicollinearity, and possibly a redundancy check if a reflective benchmark exists. This dual capacity to handle reflective and formative indicators highlights PLS-SEM's adaptability to diverse measurement scenarios.

Once the measurement model is confirmed, attention turns to the structural model, where the hypothesized relationships among latent variables come into play. Researchers often begin by examining R^2 values for the endogenous constructs, revealing how much variance is explained by the exogenous constructs. Another central concern is predictive relevance, evaluated through Q^2 statistics from blindfolding or more recent techniques like

PLSpredict, which assesses predictive performance at both the indicator and construct levels (Henseler, Hubona, & Ray, 2016). Significance testing of path coefficients typically uses bootstrapping to generate t-values and confidence intervals, ensuring that the hypothesized links are robust. If multiple structural configurations are possible, comparing them through changes in R^2, Q^2, or predictive metrics can indicate which specification aligns best with both theoretical and empirical evidence (Hair, Matthews, Matthews, & Sarstedt, 2017).

The final stage involves various robustness checks that enhance confidence in the results. Confirmatory Tetrad Analysis (CTA-PLS) helps determine whether a measurement model is accurately specified as reflective or formative by examining sets of tetrad differences. Endogeneity poses another challenge if an exogenous construct correlates with the error term, potentially biasing path estimates (Henseler & Chin, 2010). Solutions might include instrumental variables or Gaussian copulas to address endogeneity within the PLS-SEM framework. Meanwhile, sample heterogeneity where different subgroups may behave differently can be explored using methods such as finite mixture PLS (FIMIX-PLS), which segments the data to see whether certain relationships hold across all subpopulations or only within specific clusters (Fordellone & Vichi, 2020). These steps collectively ensure that findings are not artifacts of an ill-fitting model or unaccounted-for sample characteristics.

The Figure 3 shows how these stages fit together into a coherent sequence for a thorough PLS-SEM analysis. Researchers start by determining whether the data meet fundamental requirements, then move on to confirm that the constructs are measured properly, whether reflective or formative before assessing the structural paths that link the constructs. Predictive and explanatory power are scrutinized through R^2, Q^2, and bootstrapped path estimates, culminating in robustness checks like CTA-PLS and analyses for endogeneity or heterogeneity (Cepeda et al., 2024). By following this systematic approach, the method balances theoretical rigor with practical considerations, ultimately allowing for reliable insights into how latent variables interact in complex models.

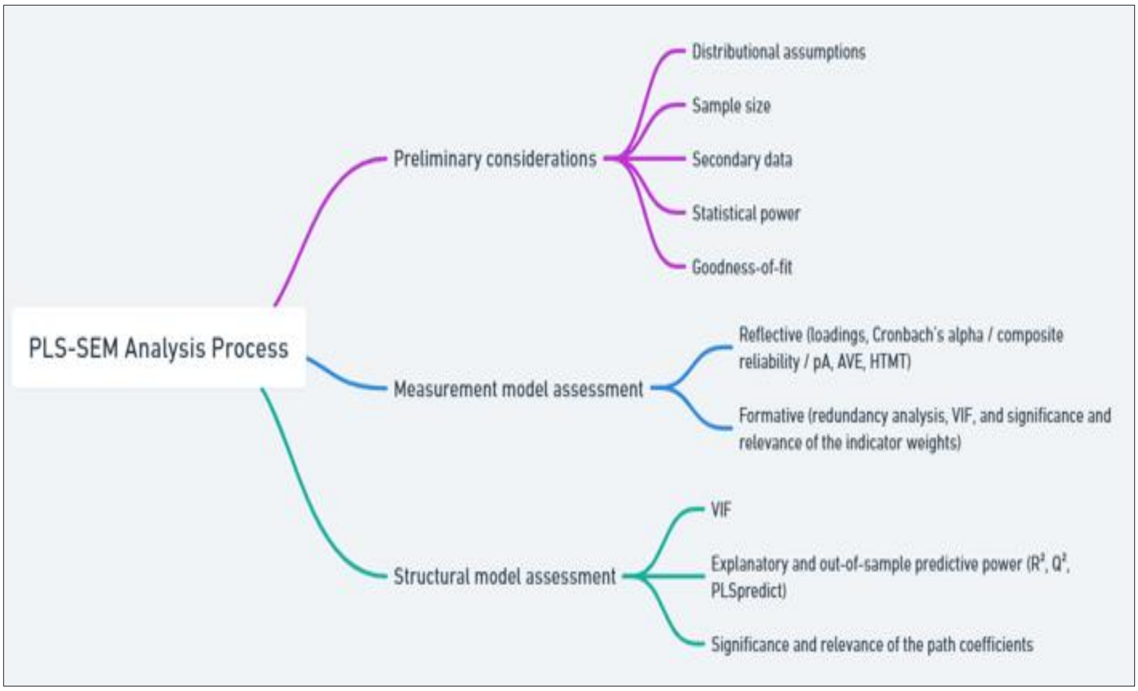

Figure 3 Stages in the PLS SEM analysis

Table 3 Rule of Thumb for a PLS SEM analysis

Criterion / Category	Recommendations / Rules of Thumb
Data Characteristics	**General Description of the Sample**: Aim for enough observations to achieve adequate statistical power.
	Distribution of the Sample: PLS-SEM handles non-normal data, but check for outliers and skewness.
	Use of Holdout Sample: If possible, split data for model training and validation.
	Data Type: Metric or quasi-metric (ordinal) scales are suitable. Nominal variables require specialized procedures.
Scale of Measurement	Works well with metric and quasi-metric data. Ordinal data can be used if appropriately coded. Nominal data should be treated carefully, often requiring specific techniques.
Model Characteristics	**Complexity**: Handles models with multiple constructs and structural paths.
	Relationships Among Constructs: Accommodates formative and reflective constructs, plus higher-order constructs.
	Model Setup: Emphasizes prediction and explained variance instead of a global fit index.
Preliminary Considerations	**Sample Size**: Ensure the number of observations is sufficient for the model's complexity. One guideline is to have at least ten times the largest number of formative indicators or structural paths.
	Statistical Power: Conduct a power analysis when possible.
	Secondary Data: Confirm alignment between the original data purpose and the current theoretical framework.
	Distributional Assumptions: Non-normal data is generally acceptable; watch for extreme skew or kurtosis.
	Goodness-of-Fit: Traditional fit measures (like RMSEA) are not directly applied; focus on predictive capability.
Measurement Model: Reflective	**Indicator Reliability**: Indicator loadings typically above 0.70, though slightly lower can be acceptable in exploratory work.
	Internal Consistency: Cronbach's alpha above 0.70 and composite reliability above 0.70 indicate adequate reliability.
	Convergent Validity: Average Variance Extracted (AVE) of 0.50 or higher.
	Discriminant Validity: Fornell-Larcker criterion or Heterotrait-Monotrait (HTMT) ratio, usually below 0.85–0.90.
Measurement Model: Formative	**Indicator Relevance**: Report weights and check their significance.
	Multicollinearity: Variance Inflation Factor (VIF) should be 3.0–5.0 or lower. High VIF suggests redundancy among indicators.
	Redundancy Analysis: If a reflective benchmark is available, correlate the formative construct with that benchmark to assess convergent validity.
	Significance: Non-significant weights may indicate limited contribution, though theory often guides retention or removal.
Cross Loadings	Each indicator should load highest on its designated latent variable. If an item has similarly high loadings on multiple constructs, discriminant validity could be compromised.
Structural Model Evaluation	**R^2**: Interpretation depends on the research domain (e.g., 0.75, 0.50, 0.25 can be labeled substantial, moderate, or weak).
	f^2 (Effect Size): Thresholds of 0.02, 0.15, 0.35 for small, medium, and large effects.
	Significance of Paths: Use bootstrapping (5,000–10,000 subsamples) for t-values and confidence intervals.
	Predictive Relevance (Q^2): Values above 0 indicate predictive relevance.
	PLSpredict: Assess item-level and construct-level errors to evaluate out-of-sample predictive performance.
Model Comparisons	Check R^2, Q^2, and predictive metrics across different structural specifications. When investigating group differences, use multi-group analysis to see if path coefficients vary by subgroup.
Additional Analyses	**Mediation**: Identify if an exogenous variable influences an endogenous variable indirectly via a mediator.
	Moderation: Include interaction terms to test whether a third variable alters the relationship between two constructs.
	Higher-Order Constructs: Use repeated indicators or two-stage approaches for multidimensional concepts.
	Robustness Checks: Confirmatory Tetrad Analysis (CTA-PLS), endogeneity controls, finite mixture PLS for heterogeneity, and so on.
Outliers and Unobserved Heterogeneity	**Outliers**: Check for extreme data points that may skew the results.
	Heterogeneity: Consider finite mixture PLS or segmentation methods to see if subpopulations behave differently, possibly revealing unique structural paths.
Reporting Guidelines	Explain why formative or reflective measures were chosen. Provide reliability and validity metrics for each construct. Report structural paths, R^2, Q^2, and significance levels. Note any robustness checks (CTA-PLS, endogeneity, heterogeneity). Discuss limitations and align results with theoretical expectations.

7. Applications of PLS-SEM Across Business Domains

PLS-SEM has emerged as a versatile analytical tool, perfectly suited for investigating the complex relationships that define modern business phenomena. Its flexibility to handle reflective, formative, and higher-order constructs even when dealing with small sample sizes or non-normal data makes it an ideal choice across a wide range of business settings. Moreover, specialized PLS approaches, such as consistent PLS (PLSc) or multi-group PLS analysis, can be tailored to the unique requirements of each domain (Cho & Choi, 2019). Below is an integrated discussion on how PLS-SEM is applied across various business areas, how variables are analyzed, and the overall impact on each domain.

7.1. Marketing and Consumer Behavior

In marketing and consumer behavior, PLS-SEM is widely used to explore intricate relationships among latent constructs such as brand equity, customer satisfaction, perceived quality, and purchase intention. The method typically employs the basic PLS algorithm, which is well suited when constructs are measured with multiple reflective indicators (Fong & Law, 2013). However, when modeling composite constructs like customer experience, which may involve dimensions such as service quality, brand image, and price perception - a formative or mixed measurement model may be adopted. In some cases, consistent PLS (PLSc) is chosen to adjust for bias in formative indicators. Variable Analysis and Impact: Variables in this domain are analyzed by estimating path coefficients, outer loadings, and reliability metrics such as composite reliability and average variance extracted (AVE). Advanced techniques like importance-performance matrix analysis (IPMA) are often used to determine which factors most significantly impact key outcomes like loyalty or satisfaction (Gefen, Straub, & Boudreau, 2000). The insights derived from these analyses help pinpoint the primary drivers of consumer behavior, allowing for more targeted marketing strategies, optimal resource allocation, and improved customer engagement. As a result, companies can refine product positioning, fine-tune advertising campaigns, and ultimately enhance overall marketing effectiveness.

7.2. Organizational Behavior and HR Management

Within organizational behavior and HR management, PLS-SEM is employed to investigate constructs like job satisfaction, employee engagement, leadership effectiveness, and organizational commitment. Here, reflective measurement models are common, particularly for constructs such as employee satisfaction and commitment (Danks, Sharma, & Sarstedt, 2020). When dealing with multidimensional constructs like leadership style, which may encompass both transformational and transactional dimensions higher-order constructs are integrated using either the repeated indicators or two-stage approach. Multi-group PLS-SEM can further be applied to compare outcomes across various departments or demographic segments. Variable Analysis and Impact: In these studies, relationships among variables are assessed via path coefficients, and the internal consistency of constructs is evaluated through composite reliability, convergent, and discriminant validity (Gefen, Straub, & Boudreau, 2000). Moderating factors such as organizational culture or work environment are often included to capture their effect on employee outcomes. The practical impact of PLS-SEM in HR management is significant; by quantifying the influence of leadership, training programs, and performance management systems, the approach aids in designing evidence-based HR interventions. This leads to better work environments, increased employee morale, and enhanced overall organizational performance.

7.3. Innovation and Entrepreneurship

Innovation and entrepreneurship are domains characterized by rapid change and high uncertainty, making flexible and predictive modeling essential. PLS-SEM is particularly beneficial in these fields, as it supports exploratory model development where constructs such as innovation capability, risk-taking, and opportunity recognition may not be fully established. In these dynamic environments, a mix of reflective and formative measurement models is common, and the focus on prediction allows for effective modeling of evolving constructs (Benitez et al., 2019). Variable Analysis and Impact: In this area, variables are analyzed by examining the relationships among constructs like absorptive capacity, technological innovation, and market orientation. Techniques such as bootstrapping are used to assess the reliability of estimates, while blindfolding tests the model's predictive power. Multi-group analysis might be employed to compare early-stage startups with more established firms. The insights gained from these analyses help in identifying the critical drivers of innovation, guiding strategic decisions related to resource allocation, competitive positioning, and process improvement. Such insights empower entrepreneurs and managers to navigate challenges and seize emerging opportunities, ultimately driving sustainable growth (Cho & Choi, 2019).

7.4. Supply Chain Management

In supply chain management, PLS-SEM is employed to model the intricate relationships among constructs such as supply chain integration, operational efficiency, and performance outcomes. The method is valuable for quantifying the impact of process improvements and collaborative practices on overall supply chain effectiveness, enabling organizations to identify bottlenecks and optimize processes (Gelashvili, Martínez-Navalón, & Saura, 2021). Variable Analysis and Impact: Variables are typically analyzed by estimating path coefficients, outer loadings, and reliability metrics such as composite reliability and average variance extracted (AVE). These analyses support strategic decisions aimed at streamlining operations, reducing costs, and enhancing efficiency across the supply chain, ultimately driving improved performance outcomes.

7.5. Strategic Management and Operations

In the field of strategic management and operations, PLS-SEM is used to model constructs such as strategic alignment, resource-based capabilities, and organizational performance. The method facilitates the understanding of competitive dynamics and operational efficiencies by capturing the complex interrelationships between strategic initiatives and performance metrics (Cho et al., 2022). Variable Analysis and Impact: The analysis involves estimating the effects of various strategic factors through path coefficients and evaluating model fit using reliability and validity metrics. This comprehensive approach enables organizations to assess how different strategic initiatives interact to drive success, informing decisions related to competitive positioning and long-term planning (Hair & Alamer, 2022).

7.6. Financial Services

Within financial services, PLS-SEM is instrumental in analyzing constructs such as customer trust, perceived risk, and service quality. The method helps reveal the nuanced interplay between these variables and their influence on customer loyalty and overall market performance, which is crucial for maintaining competitive advantage in a dynamic industry. Variable Analysis and Impact: Variables are analyzed through the estimation of structural paths, outer loadings, and consistency metrics (Lowry & Gaskin, 2014). Insights gained from these analyses support the development of strategies that enhance service delivery, improve customer satisfaction, and ultimately boost financial performance, contributing to a stronger market position.

Across these diverse business domains, PLS-SEM offers a unifying framework that combines theoretical robustness with practical applicability. The method's flexibility in handling complex, multidimensional constructs and its robustness in the face of non-normal data and limited sample sizes make it an ideal tool for a wide range of applications (Henseler & Chin, 2010). Whether forecasting consumer behavior, optimizing HR practices, driving innovation, streamlining supply chain operations, informing strategic management decisions, or enhancing financial services, PLS-SEM provides reliable insights that support informed decision-making and strategic planning.

By integrating reflective, formative, and higher-order constructs with specialized methods like PLSc and multi-group analysis, PLS-SEM bridges the gap between theory and practice. Its predictive orientation ensures that findings are not only statistically sound but also practically relevant, allowing businesses to adapt and thrive in competitive environments (Hair, Ringle, & Sarstedt, 2012) . The comprehensive nature of PLS-SEM ensures that it captures the complexity of modern business phenomena, delivering actionable insights that enhance both theoretical understanding and real-world performance.

8. Reporting Standards and Best Practices

Effective reporting in PLS-SEM is crucial to ensure that findings are communicated with clarity, transparency, and accuracy. This section outlines best practices for reporting, common pitfalls to avoid, and advanced visualization techniques that enhance the presentation of results.

8.1. Guidelines for Clear and Effective Reporting

Clear and effective reporting in PLS-SEM begins with a comprehensive description of the entire research model, which encompasses both the measurement and structural models. Start by clearly defining the theoretical framework and providing a detailed model specification that outlines the constructs under investigation, whether reflective, formative, or higher-order, and explains the rationale behind their selection and the nature of their interrelationships (Ketchen, 2013). It is crucial to provide complete data characteristics by specifying the sample size, data collection methods, and any issues concerning data quality, such as missing values or non-normality, as this transparency allows readers to assess the robustness of the analysis. The measurement model should be reported in depth, including all key metrics related to construct reliability and validity, such as outer loadings, composite reliability, average variance extracted (AVE), and the Heterotrait-Monotrait (HTMT) ratio for discriminant validity, ensuring that the scales used are both consistent and valid. Equally important is the presentation of the structural model results, which involves reporting the estimated path coefficients, significance levels obtained via bootstrapping (including t-statistics and confidence intervals), and the explained variance (R^2) for each endogenous construct, thereby lending additional rigor to the findings (Liengaard, 2024). Furthermore, a clear description of the methodological details is essential; this includes specifying the exact PLS-SEM approach used, be it basic PLS, consistent PLS, or multi-group analysis, as well as the number of bootstrap replications and the settings and criteria applied for procedures like bootstrapping and blindfolding, all of which are vital for reproducibility (Hair & Alamer, 2022). Finally, contextual interpretation ties the analysis together by discussing how the results align with or challenge the existing theoretical framework, outlining practical implications, and suggesting potential avenues for further research. This holistic approach serves as a working guide for anyone employing PLS-SEM, ensuring that all aspects of the analysis are reported with clarity, precision, and transparency.

8.2. Common Mistakes and How to Avoid Them

Even with advanced analytical tools like PLS-SEM, clear and transparent reporting is crucial for ensuring that findings are understood and replicable. However, several common reporting mistakes can compromise the clarity and utility of the results. Below is a detailed explanation of these potential pitfalls, including the technical and theoretical aspects associated with each.

- **Insufficient Model Description:** One common error is the failure to provide a comprehensive description of the overall model encompassing both the measurement model (which defines how latent constructs are measured by observed indicators) and the structural model (which describes the relationships among latent constructs). From a technical perspective, omitting a full model specification leaves the theoretical foundations ambiguous, as key details such as construct operationalization and hypothesized linkages remain unclear (Richter, Cepeda, Roldán, & Ringle, 2016). Detailed diagrams (path models) and narrative explanations are essential. These should include clear representations of the measurement model (showing reflective or formative specifications, outer loadings, and error terms) as well as the structural model (with path coefficients, error variances, and potential moderating effects). Such a thorough description supports the interpretability and reproducibility of the analysis (Sarstedt & Moisescu, 2023).
- **Omitting Data Characteristics:** Another frequent mistake is the neglect of data characteristics. Reporting sample size, response rates, and any anomalies such as outliers, missing values, or non-normal distributions is critical. Technically, these aspects inform the reader about the quality and representativeness of the data, which can have profound implications for the reliability and validity of the PLS-SEM results (Ringle, Sarstedt, & Schlittgen, 2013). For instance, non-normality might be addressed by PLS-SEM's nonparametric approach, but without explicit mention of data distribution, the robustness of findings remains uncertain. Documenting these characteristics allows for a critical evaluation of the statistical power and potential biases in the analysis.
- **Overlooking Model Diagnostics:** A rigorous PLS-SEM report should include comprehensive model diagnostics. Key diagnostic measures such as outer loadings, cross-loadings, composite reliability, average variance extracted (AVE), and fit indices (like R^2 and Q^2) are central to assessing the quality of both the measurement and structural models (Monecke & Leisch, 2012). Neglecting these diagnostics can obscure issues like multicollinearity, low indicator reliability, or poor discriminant validity. From a theoretical standpoint, these diagnostics underpin the construct validity of the model ensuring that latent variables are measured consistently and accurately reflect the intended theoretical concepts (Rigdon, Ringle, & Sarstedt, 2010).
- **Misinterpretation of Bootstrapping Results:** Bootstrapping is a cornerstone of inferential statistics in PLS-SEM, providing nonparametric estimates of standard errors, confidence intervals, and t-statistics. A common mistake is to rely solely on point estimates without discussing the accompanying confidence intervals or the stability of these estimates across bootstrap samples (Sarstedt & Liu, 2023). Technically, the bootstrap distribution offers critical insight into the variability and precision of parameter estimates. Failing to interpret these intervals can lead to overconfidence in the results and an underestimation of model uncertainty. Discussing bootstrap outcomes in detail helps to verify the robustness of the estimates and ensures a more nuanced understanding of the model's reliability (Gye-Soo, 2016).
- **Neglecting Visual Representations:** Relying solely on text to report complex relationships in PLS-SEM can make the findings difficult to interpret. Advanced visual representations such as path diagrams, heatmaps of correlation matrices, and importance-performance matrix analyses can greatly enhance the reader’s comprehension of the model (Henseler, Ringle, & Sarstedt, 2015). Technically, visuals provide an immediate, intuitive grasp of relationships among constructs and the overall model fit, which might be obscured in a dense textual description. Incorporating figures and tables ensures that key results are accessible, supports cross-validation of the text, and aids in communicating complex statistical findings effectively.
- **Overcomplicating the Presentation:** While detailed reporting is essential, overcomplicating the presentation with excessive technical jargon can alienate non-specialist audiences. A balance must be struck between technical precision and clarity. The report should be written in a manner that explains technical terms where necessary and integrates complex statistical results with accessible language. This ensures that the insights are broadly understandable while still maintaining the depth required for rigorous academic or practical evaluation (Hair, Hult, Ringle, Sarstedt, Danks, & Ray, 2021).
- **Lack of Transparency in Methodological Choices:** Ambiguity in reporting the specific methodological choices such as the type of PLS-SEM approach used (basic, consistent, or multi-group), the number of bootstrap replications, or the criteria for procedures like blindfolding can lead to uncertainty about the replicability and validity of the results (Henseler & Sarstedt, 2012). From a technical perspective, every parameter and setting

in a PLS-SEM analysis has the potential to influence the outcomes. Clear justification and explanation of these choices are essential to validate the results and allow others to replicate the study accurately.

- **Failing to Report Negative Findings:** Selective reporting, where unexpected or non-significant results are omitted, introduces bias and undermines the integrity of the analysis. From a theoretical standpoint, negative findings are crucial, they contribute to the understanding of the phenomenon under study and may offer insights into model limitations or areas needing further exploration. Comprehensive reporting, including all findings with their respective confidence intervals and t-statistics, enhances the overall credibility and transparency of the analysis (Fong & Law, 2013).
- **Poor Organization of Content:** A disorganized report that intermingles methodological details with results and interpretations can lead to confusion. A clear, logical structure separating methodology, results, and discussion is essential for conveying the narrative of the analysis. This structured approach not only makes the report more readable but also ensures that each aspect of the analysis is given due attention, facilitating a more systematic evaluation of the research (Lowry & Gaskin, 2014).
- **Inadequate Integration of Theory and Practice:** Finally, reporting results without linking them back to the broader theoretical framework or discussing practical implications weakens the overall impact of the study. The report should always connect the empirical findings with theoretical constructs and real-world applications (Ringle, Goetz, Wetzels, & Wilson, 2009). This integration is vital for demonstrating how the statistical results inform and refine existing theories, and for highlighting how they can guide strategic decision-making in practice. By thoroughly discussing these connections, the report becomes a comprehensive guide that is both academically rigorous and practically relevant.

Each of these points forms a critical part of a working guide for anyone using PLS-SEM. Addressing these common mistakes with detailed attention to both technical and theoretical aspects not only improve the clarity and reproducibility of the analysis but also ensures that the findings can be reliably used to inform practical decisions and further theoretical developments (Ringle, Sarstedt, & Straub, 2012).

8.3. Advanced Visualization Techniques

Advanced visualization techniques play a critical role in the effective communication of complex PLS SEM results. They transform dense numerical output into accessible, intuitive representations that clarify relationships among constructs and provide strategic insights. By leveraging these techniques, the intricate dynamics of measurement and structural models become more comprehensible, aiding in both the interpretation and dissemination of findings (Richter, Sinkovics, Ringle, & Schlägel, 2016).

Path diagrams form the cornerstone of PLS SEM visualization. These diagrams are carefully designed to illustrate both the measurement model, which shows how latent variables are measured by observed indicators, and the structural model, which displays the hypothesized relationships among latent variables. Each diagram should include clear labels for latent constructs, observed variables, path coefficients, and significance levels (often derived from bootstrapping). Tools such as SmartPLS and R packages like SEMinR facilitate the creation of high-quality path diagrams that are both technically accurate and aesthetically appealing. From a theoretical standpoint, these diagrams provide a visual summary of the conceptual framework, allowing users to quickly grasp the interdependencies and causal paths in the model (Nitzl, Roldán, & Cepeda, 2017).

Importance Performance Matrix Analysis (IPMA) is another advanced visualization technique that integrates both the importance of constructs (measured by total effects) and their performance (as indicated by latent scores) into a single matrix. This visualization helps identify which constructs are critical in driving outcomes and which ones require improvement (Ringle, Sarstedt, Mitchell, & Gudergan, 2018). The matrix is typically color coded and plotted along two axes, one representing importance and the other representing performance, so that areas with high importance but low performance can be easily identified. The technical strength of IPMA lies in its ability to quantify and visually prioritize factors for managerial intervention, directly linking statistical findings to actionable strategic decisions.

Bootstrapping distribution plots provide further insights into the stability and variability of parameter estimates. By representing the distribution of bootstrap estimates through histograms or density plots, these visualizations reveal the spread, skewness, and potential bias in the parameter estimates. This graphical representation is crucial because it complements numerical bootstrap statistics, such as standard errors and confidence intervals, with an intuitive understanding of the estimate distribution. These plots help validate the robustness of the model and ensure that the estimates are not unduly influenced by sample specific peculiarities (Nitzl, Roldán, & Cepeda, 2017).

Heatmaps for correlation matrices are particularly useful when assessing discriminant validity using measures like the HTMT ratio. These heatmaps visually display the strength of correlations between different constructs by using a color gradient, which makes it easier to spot problematic areas where constructs may not be sufficiently distinct. The theoretical rationale behind this approach is that if constructs are truly distinct, the inter construct correlations should be noticeably lower than the intra construct correlations. By providing a visual summary, heatmaps serve as an effective diagnostic tool that supports and complements traditional statistical tests (Islam & Khan, 2024).

Visualizations in multi group analyses are designed to compare structural relationships across different groups or sub samples. Overlaying path diagrams or employing bar charts for each group allows for a clear comparative analysis. This method highlights significant differences in path coefficients or latent variable means between groups, offering insights into how various factors may operate differently in distinct contexts. Such visual comparisons are particularly useful for understanding the moderating effects of demographic or situational variables, thereby enhancing the theoretical generalizability of the model (Nitzl, Roldán, & Cepeda, 2016).

Interactive dashboards represent the next frontier in data visualization for PLS SEM. They enable stakeholders to dynamically explore multiple facets of the model, such as drilling down into specific constructs or filtering data by sub groups. These dashboards integrate several types of visualizations, such as path diagrams, IPMA matrices, and bootstrap plots, into a unified interface (Ringle, Sarstedt, & Straub, 2012). The interactive nature of these tools encourages users to engage with the data actively, fostering a deeper understanding of the complex relationships within the model. From a technical perspective, interactive dashboards often leverage modern programming environments and visualization libraries, ensuring that the data can be updated in real time as new information becomes available.

Consistency and clarity in visual outputs are essential to maintain interpretability. All figures should adhere to a uniform style, using legible fonts, consistent color schemes, and clear legends. Each visual should be accompanied by concise explanations that highlight the key insights, ensuring that even those less familiar with advanced statistical methods can understand the findings (McIntosh, Edwards, & Antonakis, 2014). This consistency not only enhances the professional appearance of the report but also minimizes potential misinterpretation of the data.

Customizable reports further enhance the usability of visualizations. Software tools now offer options to tailor the complexity and level of detail in visual outputs based on the intended audience, whether academic, managerial, or technical (Islam & Khan, 2024). This customization allows the presentation of results to be both comprehensive and accessible, ensuring that the insights are communicated in a manner that best suits the audience needs.

Color coding and annotations are additional techniques that significantly boost the interpretability of complex diagrams and matrices. By differentiating various constructs and relationships through strategic use of color and explicit annotations, the visuals become more intuitive. These enhancements draw attention to critical findings and make it easier for stakeholders to quickly identify patterns, trends, and potential issues within the model (Sarstedt, Richter, Hauff, & Ringle, 2024).

Finally, integrating text and visuals seamlessly is crucial. Each figure should be referenced within the narrative, with clear explanations of how the visual supports the overall findings and contributes to the understanding of the model. This integration ensures that the report is not just a collection of disjointed images and paragraphs but a coherent document that tells a complete story about the analysis.

In synthesis, advanced visualization techniques in PLS SEM create a robust reporting framework that bridges the gap between complex statistical analysis and practical decision making. Detailed path diagrams, IPMA matrices, bootstrap distribution plots, heatmaps, multi group visuals, interactive dashboards, and other tools not only enhance the clarity and accessibility of the results but also provide critical insights that drive strategic actions. By ensuring consistency, customization, and clear integration with the written narrative, these visualization methods enable the effective communication of sophisticated analytical outcomes, thereby increasing both the theoretical rigor and practical relevance of the research.

9. Software Tools and Computational Resources

SmartPLS is widely recognized for its intuitive graphical user interface, which enables users to build, estimate, and visualize PLS-SEM models through a point-and-click environment. This ease of use is particularly beneficial when constructing complex measurement models, including reflective, formative, and higher-order constructs. Under the hood, SmartPLS implements iterative algorithms to compute latent variable scores, update weights, and assess model fit through bootstrapping and blindfolding procedures, all while accommodating non-normal data distributions (Venturini & Mehmetoglu, 2019). In contrast, SEMinR is an R package that offers extensive flexibility for users who prefer a coding environment. It allows for seamless integration with other R packages, thereby supporting advanced statistical analyses, custom visualizations, and reproducible research workflows. SEMinR's programmatic approach enables fine-tuning of every aspect of the PLS-SEM process, from indicator weighting to the configuration of bootstrap replications. Meanwhile, cSEM focuses on composite-based SEM and emphasizes methodological rigor through consistency corrections and advanced diagnostics. Its design caters to both academic and applied settings where ensuring the validity of composite measures is paramount. Together, these tools illustrate the spectrum of software options available for PLS-SEM, each with unique strengths that address different user needs and technical requirements (Sarstedt, Hair, & Ringle, 2022).

9.1. Criteria for Selecting Appropriate Software

Selecting the most appropriate PLS-SEM software involves multiple criteria that bridge both usability and advanced analytical capabilities. First, usability is critical; the chosen software should align with the user's technical proficiency and preferred workflow. For those who favor visual interfaces, SmartPLS offers a user-friendly environment, while more technically inclined users might prefer the coding flexibility of SEMinR or cSEM. Functionality is another key consideration (Sukhov, Friman, & Olsson, 2023). The software must support a range of model specifications, including reflective, formative, and higher-order constructs, and provide robust tools for procedures such as bootstrapping, blindfolding, and multi-group analyses. Compatibility with large datasets and integration with other statistical or data management tools are also important factors, ensuring that the software can handle the computational demands of modern research. Cost and accessibility further influence the decision; open-source platforms like SEMinR and cSEM may offer greater flexibility and community-driven improvements compared to proprietary solutions. Lastly, strong support through comprehensive documentation, active user communities, and regular updates are essential for both troubleshooting and keeping pace with the latest methodological advancements (Venturini & Mehmetoglu, 2019).

9.2. Emerging Computational Trends in SEM

Emerging computational trends in SEM are rapidly transforming the way models are estimated, validated, and interpreted. One significant trend is the integration of machine learning techniques with traditional SEM approaches, which enhances automated model selection, prediction accuracy, and even real-time updating of models. This convergence allows for more adaptive models that can learn from new data streams, increasing both the precision and practical utility of SEM analyses. Another trend is the adoption of cloud-based computing and parallel processing techniques, which dramatically reduce the time required for complex computations such as bootstrapping and multi-group analysis (Sarstedt & Moisescu, 2023). This shift enables the analysis of large-scale datasets and models with numerous parameters that were previously computationally prohibitive. Furthermore, the growing emphasis on reproducibility and open science has led to the development of more transparent, customizable software platforms. These platforms facilitate collaborative projects and ensure that analyses can be easily replicated and verified by others. Collectively, these trends are not only expanding the computational capabilities of SEM software but are also making advanced analytical techniques more accessible and practical for a wide range of applications, ultimately bridging the gap between cutting-edge research and real-world decision making. Each of these sections is integral to understanding how to effectively select and utilize software tools for PLS-SEM while also staying current with technological advancements that enhance both theoretical rigor and practical application in complex research environments (Sarstedt & Liu, 2023).

10. Ethical and Methodological Considerations

Ethical standards in PLS-SEM research are essential to ensure that every phase of the study is conducted with integrity and fairness. At its core, these standards require that all stages from conceptualizing the model to interpreting the data adhere to principles of honesty and accuracy. This means that the theoretical framework must be well-founded, the data collection methods must be rigorous, and the reporting of results must be unbiased. A transparent presentation of both significant and non-significant findings not only builds trust among peers but also helps advance collective knowledge. Such openness enables others to critically assess, replicate, or extend the work, reinforcing the reliability of the conclusions drawn from the analysis (Sarstedt, Ringle, & Hair, 2017).

Data Privacy and Security: Data privacy and security are critical in any research involving sensitive or personal information, and PLS-SEM is no exception. Researchers must treat all data whether gathered from surveys, experiments, or secondary sources with strict care, ensuring compliance with privacy regulations such as GDPR or HIPAA. This involves using secure storage solutions, encrypting data during transfer, and implementing robust access controls so that only authorized individuals can handle the data (Rönkkö, McIntosh, Antonakis, & Edwards, 2016). Additionally, anonymizing data by removing personally identifiable information and aggregating details into broader categories significantly reduces the risk of re-identification. Before any data are shared or made public, it is important to obtain informed consent and, where necessary, the appropriate ethical approvals from review boards. These measures protect individual privacy and uphold the ethical integrity of the research process (Monecke & Leisch, 2012).

Transparency and Reproducibility: Transparency and reproducibility form the backbone of robust scientific research. In PLS-SEM studies, this means meticulously documenting every step of the process, including data collection methods, model specification, estimation procedures, and even the specific settings used such as the number of bootstrap replications or the omission distance in blindfolding (Ketchen, 2013). Detailed reporting allows others to understand exactly how the analysis was conducted and to reproduce the results using the same data and methods. Sharing datasets, computer code, and comprehensive procedural notes via open-access platforms further enhances reproducibility. By ensuring that every aspect of the analysis is transparent, the research community can identify and correct potential errors, thereby refining the overall methodological approach and bolstering confidence in the findings (Rigdon, Ringle, & Sarstedt, 2010).

Governance Frameworks in PLS-SEM Research: A robust governance framework is crucial for managing both ethical and methodological aspects of PLS-SEM research. Such frameworks establish clear protocols for data handling, model estimation, and the reporting of results, ensuring that every stage of the research is subject to systematic oversight. These frameworks typically include standard operating procedures (SOPs) for managing data, a code of conduct for team members, and mechanisms for regular audits or peer reviews. Governance frameworks ensure that research activities adhere to both internal policies and external regulatory requirements, maintaining consistency across studies and fostering a culture of accountability (Ringle, Sarstedt, Sinkovics, & Sinkovics, 2023). This structured oversight not only safeguards the integrity of individual studies but also contributes to the long-term credibility of research within the field.

Ethical AI Frameworks for SEM: As artificial intelligence becomes more intertwined with structural equation modeling, ethical AI frameworks have emerged to address new challenges. These frameworks guide the responsible integration of machine learning techniques into SEM, ensuring that the algorithms used do not introduce or amplify biases (Nitzl, Roldán, & Cepeda, 2017). They emphasize transparency in automated decision-making processes and require that the AI components are both explainable and aligned with principles of fairness and accountability. Technically, this may involve bias mitigation strategies, regular audits of algorithm performance, and detailed documentation on how AI methods interact with SEM procedures. The goal is to harness the power of AI to enhance model specification, data preprocessing, and interpretation, while maintaining the ethical integrity of the research process.

Sustainability Considerations in PLS-SEM Research: Sustainability in PLS-SEM research addresses broader environmental, social, and economic impacts. On the environmental front, researchers are increasingly adopting practices that minimize the carbon footprint associated with computational analyses. This includes using energy-efficient hardware, optimizing code for better performance, or leveraging cloud-based services that emphasize sustainable operations. Social sustainability involves ensuring that research practices promote ethical data use and equitable collaboration, contributing positively to society by supporting transparent and inclusive research practices (Henseler, Ringle, & Sarstedt, 2015). Economically, sustainable research practices encourage the efficient use of resources, ensuring that funding and time are allocated wisely and that data and findings are responsibly shared. By embedding sustainability into every stage of the research lifecycle, studies not only advance theoretical and methodological understanding but also align with broader societal goals of environmental stewardship, social responsibility, and economic efficiency.

11. Advanced Statistical Techniques Integrated with PLS-SEM

Advanced statistical techniques expand the capabilities of PLS-SEM by allowing researchers to explore complex relationships that go beyond simple direct effects. These techniques enhance the understanding of how variables interact in real-world settings, adding nuance to both theoretical models and practical applications.

Moderation and Mediation Analysis: Moderation and mediation are central to understanding the intricate mechanisms underlying observed relationships. Moderation analysis in PLS-SEM investigates how the strength or direction of a relationship between two constructs changes when a third variable is introduced. In this context, the moderator can either amplify or diminish the effect of the independent variable on the dependent variable (Lowry & Gaskin, 2014). Technically, this is often implemented by creating interaction terms between the independent variable and the moderator and testing the significance of these terms through bootstrapping. Mediation analysis, on the other hand, focuses on the process through which an independent variable affects a dependent variable indirectly through one or more mediators. It decomposes total effects into direct and indirect effects, helping to reveal the pathways through which causal influences operate. Together, moderation and mediation analyses enable a more detailed exploration of underlying processes, revealing not only whether relationships exist but also how and under what conditions they occur (Ringle, Sarstedt, Sinkovics, & Sinkovics, 2023).

Multi-Group Analysis (MGA) in PLS-SEM: Multi-group analysis (MGA) in PLS-SEM is used to compare the structural relationships among latent constructs across different groups, such as demographic segments, organizational units, or different contexts. This technique is particularly valuable when there is theoretical or empirical evidence to suggest that relationships may differ between subpopulations. MGA involves estimating the model for each group separately and then statistically testing whether the path coefficients differ significantly between groups (Hair Jr, Sarstedt, Hopkins, & Kuppelwieser, 2014). This process often utilizes permutation tests or parametric approaches to evaluate group differences. From a technical perspective, MGA helps in ensuring that the findings are robust and generalizable, revealing whether the proposed theoretical model holds consistently across diverse settings or if there are significant group-specific variations that need to be addressed (Gye-Soo, 2016).

Nonlinear and Interaction Effects: Real-world relationships are rarely purely linear, and incorporating nonlinear and interaction effects in PLS-SEM allows for a more realistic representation of complex phenomena. Nonlinear effects capture curvilinear relationships between constructs, indicating that the effect of one variable on another might change at different levels of the predictor (Fong & Law, 2013). This is often modeled by including squared or higher-order terms in the analysis. Interaction effects, meanwhile, involve the combined influence of two or more variables on an outcome, where the effect of one independent variable depends on the level of another. In PLS-SEM, interaction terms are created by multiplying the indicators of the interacting constructs and are then included in the model to test for significant effects. These approaches require careful interpretation, as significant nonlinear or interaction effects can suggest threshold effects, saturation points, or synergy between variables insights that are crucial for both theory development and practical decision-making (Danks, Sharma, & Sarstedt, 2020).

12. Data Governance and Quality Assurance

Ensuring that data is trustworthy, accurate, and appropriately managed is essential for drawing reliable conclusions in PLS-SEM research. This section outlines the ethical and methodological strategies used to guarantee data quality, manage data accuracy, and identify as well as mitigate common method bias. The following discussion provides a detailed technical and theoretical explanation of these aspects.

Ensuring Data Quality in PLS-SEM Studies: Ensuring data quality is the foundation of any robust analysis. In PLS-SEM studies, the quality of the data directly influences the reliability of the measurement model and the validity of the structural relationships. Data quality begins with the design phase, where it is crucial to develop clear, unambiguous survey items or data collection instruments that accurately capture the constructs of interest (Becker et al., 2023). During this phase, careful attention is paid to the operational definitions of constructs, ensuring that the items are theoretically grounded and relevant. Technically, data quality assurance involves rigorous pre-testing of the measurement instruments, such as pilot testing and cognitive interviews, to confirm that respondents interpret the questions as intended. Once data collection is underway, procedures such as double data entry, automated checks for missing or inconsistent values, and statistical tests for outliers and skewness are implemented (Carrión, Nitzl, & Roldán, 2017). These steps help identify any anomalies that could bias the estimation process. Moreover, the use of statistical techniques like confirmatory factor analysis can provide additional evidence that the data reliably reflect the latent constructs. This multi-layered approach to data quality ensures that subsequent analyses in PLS-SEM are built on a solid, error-minimized foundation.

Managing Data Quality and Accuracy: Managing data quality goes beyond initial data collection; it requires continuous monitoring and maintenance throughout the analysis. At this stage, accuracy is managed through systematic data cleaning and validation processes. Techniques such as imputation for missing values, outlier detection, and sensitivity analysis are employed to ensure that the data do not contain errors that could distort the results (Danks, Sharma, & Sarstedt, 2020). For instance, when dealing with missing data, multiple imputation methods may be used to replace missing values in a way that preserves the underlying data structure, rather than simply deleting incomplete cases, which can lead to reduced statistical power and biased estimates. From a technical standpoint, managing data quality also involves the use of software tools that facilitate the detection and correction of errors. Automated scripts in programming environments like R or Python can perform consistency checks and flag unusual patterns, ensuring that data integrity is maintained. Additionally, maintaining detailed logs of data transformations and cleaning procedures is critical for both transparency and reproducibility (Dijkstra & Henseler, 2015). These logs serve as documentation that can be reviewed and audited, helping to confirm that the data management process has been conducted with due diligence and that the final dataset is both accurate and robust for analysis in PLS-SEM.

Common Method Bias: Identification and Remedies: Common method bias (CMB) is a potential threat in PLS-SEM research that occurs when variance is attributed not to the constructs being measured, but to the measurement method itself. This bias can lead to inflated or deflated correlations among constructs, potentially distorting the interpretation of the structural model. The identification of CMB starts with a theoretical consideration of the data collection method, if a single source or method (such as a self-reported questionnaire) is used for all measures, the risk of common method variance is heightened. Technically, several diagnostic techniques are available to detect CMB (Cheah, Amaro, & Roldán, 2022). One widely used approach is Harman's single-factor test, where an exploratory factor analysis is conducted on all items; if a single factor emerges that accounts for the majority of the variance, it suggests that common method bias may be present. More sophisticated methods include the use of a common latent factor, which involves adding a factor to the model that is linked to all indicators to capture the shared variance due to the measurement method. The Heterotrait-Monotrait (HTMT) ratio of correlations can also provide insight into whether constructs are being artificially inflated by common method effects (Benitez et al., 2019).

Once identified, there are several remedies to mitigate the impact of common method bias. Procedural remedies include designing the study to minimize bias from the outset—this might involve collecting data at different points in time, using multiple sources for data collection, and ensuring that items are worded in a clear, non-leading manner (Cho & Choi, 2019). Statistical remedies can also be applied during the analysis phase. For example, incorporating a marker variable; an unrelated construct expected to be free from substantive relationships with the primary constructs can help control for method bias. Additionally, partial correlation techniques can adjust for the variance explained by common method effects, thereby providing a clearer picture of the true relationships among the constructs.

13. Human-AI Collaboration in PLS-SEM Analysis

Augmented Intelligence and Decision Making: In the realm of PLS-SEM, augmented intelligence represents the fusion of human expertise with advanced computational tools to enhance decision making. This collaboration allows practitioners to leverage the strengths of both human judgment and algorithmic precision. On the technical side, machine learning models and automated data processing pipelines can rapidly handle large datasets, perform complex estimations, and generate key metrics such as path coefficients, loadings, and predictive statistics (Carrión, Nitzl, & Roldán, 2017). However, the human element remains essential: researchers must interpret these outputs in the context of established theories, validate assumptions, and make nuanced decisions about model refinement. Augmented intelligence in this setting means that while AI can identify patterns and suggest optimal model configurations, the ultimate decision about model structure, variable inclusion, and theoretical interpretation rests with the human analyst. This synergy enhances decision making by reducing computational overhead and potential bias in routine calculations while ensuring that theoretical insights and domain expertise guide the final analysis (Durdyev et al., 2018).

Collaborative AI Tools for Research Teams: Collaborative AI tools have become increasingly important in facilitating teamwork during PLS-SEM analysis. Modern platforms allow multiple users to work on the same project simultaneously, sharing data, code, and model outputs in real time. Technically, these tools integrate version control systems and cloud-based computing, ensuring that changes are tracked and that the latest models and data are always accessible to the team (Cho et al., 2022). For instance, platforms that support collaborative coding in R or Python enable research teams to jointly develop and refine their SEM models, conduct bootstrapping, and generate advanced visualizations without duplicating efforts or losing consistency. Moreover, these tools often include features for annotating and commenting on specific parts of the analysis, which can be invaluable for discussing complex methodological decisions. In practice, the use of collaborative AI tools not only accelerates the research process but also enhances the quality of the analysis by bringing diverse perspectives and expertise to bear on challenging problems (Cepeda et al., 2024).

Explainable AI (XAI) Integration with PLS-SEM: The integration of Explainable AI (XAI) into PLS-SEM represents a significant step towards making complex statistical models more interpretable and transparent. XAI techniques focus on elucidating how and why an algorithm reaches a particular decision or output, providing clear explanations that can be understood by humans. Within PLS-SEM, this might involve generating detailed reports that break down the contributions of each indicator to a latent construct, or visualizing the influence of individual data points on overall model estimates (Hair, Howard, & Nitzl, 2019). Technically, XAI methods can help demystify the inner workings of bootstrapping algorithms, interaction effects, or complex mediation and moderation processes, thereby increasing confidence in the model's findings. This level of transparency is crucial, especially when models are used to inform high-stakes decisions in business or policy-making. By integrating XAI frameworks, PLS-SEM analyses can bridge the gap between advanced statistical modeling and practical interpretability, ensuring that stakeholders not only receive accurate results but also understand the underlying rationale, which in turn supports better-informed decision making (Henseler & Chin, 2010).

14. Rule-Based Models: Explicit Human-Readable Decision Logic

AI-Enabled Real-Time Decision Support Systems: The convergence of artificial intelligence (AI) with real-time decision support systems is transforming how organizations leverage PLS-SEM in dynamic environments. This integration allows for immediate analysis of complex, multidimensional data, enabling predictive analytics and risk assessment to be conducted on the fly. By incorporating real-time data streams and AI algorithms, decision-makers gain the ability to monitor and respond to evolving trends, making informed choices almost instantaneously (Hair, Howard, & Nitzl, 2019). The following sections detail the technical and theoretical underpinnings of real-time decision-making, predictive risk assessment, and the seamless integration of real-time data with PLS-SEM.

Real-Time Decision-Making and Predictive Analytics: Real-time decision-making in a PLS-SEM framework involves using AI-enabled tools to process and analyze incoming data continuously. Predictive analytics models are developed to forecast outcomes based on current trends and historical data (Hair & Alamer, 2022). Technically, this involves setting up automated pipelines that ingest data from multiple sources such as sensors, transaction systems, or social media feeds and feeding it into PLS-SEM models that are recalibrated in near real time. The integration of machine learning algorithms allows for continuous updating of model parameters, ensuring that the estimates reflect the most current state of the environment. The theoretical foundation rests on the assumption that even in rapidly changing conditions, underlying relationships among latent constructs remain stable enough to allow for reliable forecasting (Haji-Othman & Yusuff, 2022). This enables decision support systems to provide actionable insights and trigger timely interventions, ultimately improving responsiveness and strategic agility.

Predictive Risk Assessment and Decision Support: Predictive risk assessment in real-time decision support systems utilizes the dynamic capabilities of PLS-SEM combined with AI to evaluate potential risks as they emerge. In practice, this means continuously monitoring key risk indicators and evaluating how they interact with one another to impact overall system performance. From a technical perspective, models are constructed to quantify risk by estimating the probability and impact of adverse events through metrics such as risk scores or predictive error measures (Hair, Matthews, Matthews, & Sarstedt, 2017). Advanced techniques, such as bootstrapping and blindfolding, are applied in real time to assess the stability and predictive accuracy of these risk metrics. The theoretical framework here emphasizes the importance of early warning systems if risk factors are detected or if unexpected shifts in latent variables occur, the system can alert decision-makers to potential issues before they escalate. This proactive approach not only mitigates potential losses but also supports strategic planning by allowing organizations to adjust their risk management strategies promptly.

Integration of Real-Time Data with PLS-SEM: Integrating real-time data with PLS-SEM involves establishing robust data pipelines and leveraging cloud-based or distributed computing resources to ensure that models are updated continuously (Henseler & Chin, 2010). On the technical side, this requires linking PLS-SEM software with live databases or data streams, often through APIs or middleware that automatically fetches and pre-processes data for analysis. Real-time dashboards are then employed to visualize key metrics such as path coefficients, R^2, Q^2, and risk indicators, allowing stakeholders to observe changes as they happen. The theoretical rationale is that real-time integration enhances the responsiveness of the model by ensuring that all estimates are based on the most current data available, thereby reducing lag and improving the predictive accuracy of the model (Hair, Sarstedt, & Ringle, 2019). This dynamic updating is particularly critical in fast-paced environments, where delays in data processing can lead to outdated insights and missed opportunities for intervention.

15. PLS-SEM Analysis of AI Product Innovations

PLS-SEM offers a powerful framework to examine how various AI product innovations work by modeling the complex relationships among latent constructs underlying user experience, technological performance, and business outcomes. In the realm of recommender systems like those used by Netflix, Spotify, or Amazon, PLS-SEM can be employed to explore how variables such as algorithmic accuracy, user satisfaction, perceived personalization, and purchase intention interact. By modeling these latent variables, it becomes possible to assess both the predictive and explanatory power of recommender systems. The approach allows for the estimation of path coefficients that show the impact of algorithm performance on user engagement, while also accounting for the multidimensionality of factors such as content relevance and recommendation transparency (Henseler, Ringle, & Sarstedt, 2015).

When it comes to voice assistants such as Alexa, Google Assistant, and Siri, PLS-SEM helps elucidate the interplay between technological innovation and user adoption. Variables like speech recognition accuracy, ease of use, perceived reliability, and trust can be modeled as latent constructs that drive user acceptance and continued usage (Hair, Sarstedt, Pieper, & Ringle, 2012). Here, the emphasis is not only on verifying the consistency and validity of measurement scales for these constructs but also on testing how changes in system performance or design features might moderate user satisfaction and loyalty. This detailed analysis offers insights into which features are most influential, guiding product enhancements and strategic decision-making (Gye-Soo, 2016).

Autonomous vehicles, or self-driving cars, represent another frontier where PLS-SEM can offer significant insights. In this context, the latent constructs might include system safety, driving performance, user trust, and overall satisfaction with autonomous technology (Henseler & Sarstedt, 2012). PLS-SEM can model how improvements in sensor accuracy and algorithm reliability translate into enhanced safety perceptions and higher trust levels among users. By simultaneously evaluating multiple interrelated factors, this approach aids in understanding the trade-offs between technological capabilities and user acceptance, thus helping to shape policy and design guidelines for autonomous systems.

In the area of AI-powered healthcare diagnostics, PLS-SEM is particularly valuable in unpacking the complex relationships between diagnostic accuracy, ease of use, trust in technology, and patient outcomes. Latent variables such as diagnostic precision, clinician acceptance, and perceived reliability can be modeled to assess how technological advancements in AI translate into improved healthcare delivery (Hair, Ringle, Gudergan, Fischer, Nitzl, & Menictas, 2018). This method allows for the exploration of mediating factors, such as user confidence and operational efficiency, which may influence the overall impact of these innovations on patient care. The ability to rigorously test these relationships ensures that healthcare providers can make evidence-based decisions regarding the adoption of AI diagnostic tools.

Similarly, AI-enhanced educational platforms benefit from the use of PLS-SEM to examine the multifaceted effects of technology on learning outcomes. Constructs such as student engagement, personalized learning, platform usability, and academic performance can be integrated into a structural model (Hair, Sarstedt, Pieper, & Ringle, 2012). By analyzing how these factors interact, it is possible to assess not only the direct impact of AI on learning but also how mediators like adaptive feedback or digital resource accessibility influence educational success. This detailed approach supports the development of platforms that are both effective and user-friendly, ultimately contributing to better educational experiences (Haji-Othman & Yusuff, 2022).

Fraud detection systems are another critical area where PLS-SEM proves its worth. In financial and transactional environments, latent constructs such as anomaly detection accuracy, system responsiveness, user trust, and operational efficiency can be modeled to understand the effectiveness of AI-based fraud detection tools (Gelashvili, Martínez-Navalón, & Saura, 2021). By examining the relationships between these factors, organizations can evaluate how well these systems predict and mitigate fraudulent activities. The structural analysis in PLS-SEM provides a nuanced understanding of which elements drive system performance and where improvements can lead to more robust fraud prevention strategies (Ketchen, 2013).

Finally, AI-powered marketing tools are increasingly integral to modern business strategies. PLS-SEM can be used to model key constructs such as targeting accuracy, customer engagement, campaign effectiveness, and ROI. The analysis helps to identify which aspects of AI-driven marketing contribute most to improved performance, whether through enhanced personalization, better segmentation, or more efficient budget allocation (Hair, Matthews, Matthews, & Sarstedt, 2017). By revealing the strength and significance of these relationships, the method enables companies to fine-tune their marketing strategies in a data-driven manner, ensuring that technological investments yield tangible business benefits.

16. AI-Enabled Risk Management and Decision Analytics

Advances in artificial intelligence are revolutionizing risk management and decision analytics by enabling real-time, data-driven insights. In the context of PLS-SEM, these innovations facilitate the development of predictive models and robust analytical frameworks that help businesses anticipate risks, manage uncertainties, and evaluate potential failure modes (Ravand & Baghaei, 2016). By integrating AI techniques with traditional statistical approaches, organizations can make better-informed decisions even in volatile environments. The following sections provide detailed explanations of predictive risk assessment models, strategies for managing business uncertainties, and the application of Failure Mode and Effect Analysis (FMEA) within a PLS-SEM framework.

- **Predictive Risk Assessment Models:** Predictive risk assessment models use historical and real-time data to forecast potential risks and their impacts on business operations. In a PLS-SEM context, these models are constructed by first identifying latent constructs that represent key risk dimensions, such as operational risk, financial risk, and reputational risk (Rigdon, Sarstedt, & Ringle, 2017). Each of these constructs is measured by multiple observed indicators, and the structural model is then used to examine how these risk factors interact and contribute to adverse outcomes. Technically, the strength of the relationships among these constructs is evaluated through path coefficients, and the explanatory power is assessed via R^2 values. Moreover, bootstrapping techniques provide confidence intervals for the risk predictions, enhancing the robustness of the model. The theoretical underpinning of predictive risk assessment lies in the idea that, by understanding the complex interdependencies among risk factors, organizations can identify early warning signals and implement proactive measures (Ringle, Sarstedt, & Straub, 2012). This approach enables decision-makers to prioritize risks based on their potential impact and likelihood, thereby improving resource allocation and crisis preparedness.

- **Managing Business Uncertainties with PLS-SEM:** Business environments are inherently uncertain, and managing these uncertainties requires a flexible, multi-dimensional approach. PLS-SEM offers a valuable framework for modeling uncertainty by allowing for the simultaneous analysis of multiple latent variables that represent various sources of unpredictability, such as market volatility, supply chain disruptions, and technological changes (Ringle, Goetz, Wetzels, & Wilson, 2009). The methodology's focus on predictive analytics, through the use of Q^2 statistics and PLSpredict procedures, helps quantify how well the model can forecast outcomes under different scenarios. From a technical standpoint, PLS-SEM is particularly suited for such applications because it is robust to non-normal data and small sample sizes, conditions that often prevail in rapidly changing business contexts. The structural model can incorporate mediators and moderators to capture complex interactions and contextual effects, ensuring that the analysis reflects the dynamic nature of business uncertainties (Putra, 2022). This comprehensive approach provides decision-makers with nuanced insights, enabling them to adjust strategies in real time and mitigate potential adverse impacts effectively.
- **Failure Mode and Effect Analysis (FMEA) with PLS-SEM:** Failure Mode and Effect Analysis (FMEA) is a systematic method used to identify and evaluate potential failures in a system, process, or product. When integrated with PLS-SEM, FMEA can be enhanced by quantitatively modeling the relationships between failure modes, their causes, and their impacts on overall system performance. In this integrated approach, latent constructs may represent critical dimensions such as failure probability, severity of impact, and detectability. Observed indicators are used to measure these dimensions, and the structural model estimates the interplay among them (Roldán & Sánchez-Franco, 2012). By doing so, organizations can calculate risk priority numbers (RPNs) for different failure modes based on the estimated path coefficients and explained variances. Technically, the use of PLS-SEM in FMEA allows for a more refined and data-driven assessment compared to traditional FMEA methods. Bootstrapping provides statistical validation for the estimated relationships, while advanced metrics like Q^2 ensure that the model has predictive relevance. This methodological integration not only supports a more precise identification of critical failure points but also guides the development of targeted mitigation strategies, ultimately enhancing system resilience and operational efficiency.

17. Limitations and Critical Reflections

Common Methodological Limitations: While PLS-SEM is a powerful and flexible tool for modeling complex relationships among latent variables, it is not without its methodological challenges. One major limitation is its inherent focus on maximizing explained variance rather than on model fit. Unlike covariance-based SEM, which offers a range of global fit indices, PLS-SEM relies heavily on predictive metrics like R^2 and Q^2. This focus can sometimes result in models that prioritize predictive accuracy at the expense of theoretical rigor, potentially leading to overfitting in situations where the sample size is limited or the model is overly complex. Additionally, the iterative algorithm used in PLS-SEM can be sensitive to initial parameter settings, which means that the final estimates might vary if the starting values or convergence criteria are not carefully chosen. This sensitivity underscores the need for rigorous diagnostic testing, such as bootstrapping, to assess the stability and reliability of the estimates (Rigdon, Ringle, & Sarstedt, 2010). Furthermore, when dealing with formative measurement models, issues such as multicollinearity among indicators and the proper specification of indicator weights can introduce additional complexity. If not addressed properly, these issues may distort the interpretation of the latent constructs, thereby limiting the model's overall validity.

Misuse and Misinterpretations: Another significant concern is the potential misuse or misinterpretation of PLS-SEM results. One common pitfall is the incorrect application of reflective validity criteria to formative models. Because formative and reflective models operate under different theoretical assumptions, applying the same standards can lead to erroneous conclusions about construct validity. For example, a low indicator loading in a formative model should not be automatically interpreted as poor reliability, since in formative measurement the emphasis is on the weights rather than the loadings. Similarly, relying solely on R^2 as an indicator of model quality without considering the context or the predictive relevance (Q^2) can result in overconfidence in the findings (Monecke & Leisch, 2012). There is also the risk of misinterpreting the structural path coefficients; even if these coefficients are statistically significant, their practical significance may be minimal if the effect sizes are small. Such misinterpretations can lead to misguided decisions if the theoretical framework or the operational context is not carefully taken into account. Moreover, the lack of standardized reporting in PLS-SEM often means that critical details about data preparation, parameter settings, and diagnostic tests are omitted, making it difficult for readers to fully assess the robustness of the analysis. This lack of transparency can lead to a cascade of misuses, where subsequent studies rely on flawed models, further propagating errors across the literature.

18. Future Trends and Methodological Developments

The integration of PLS-SEM with machine learning and AI is rapidly reshaping the landscape of structural equation modeling. Researchers are increasingly exploring hybrid approaches that combine the strengths of PLS-SEM such as its ability to handle complex, multidimensional constructs and small sample sizes with advanced machine learning algorithms that offer automated feature selection, non-linear modeling, and real-time data processing. This convergence allows for dynamic model adjustments and enhanced predictive accuracy, as AI tools can continuously learn from incoming data while PLS-SEM maintains a solid theoretical framework. In practice, such integration paves the way for more adaptive decision support systems and the creation of models that are both empirically robust and theoretically grounded. Innovative methodological directions in PLS-SEM are emerging as researchers seek to extend its capabilities beyond traditional applications (Roldán & Sánchez-Franco, 2012). New techniques are being developed to address limitations related to model specification, measurement error, and latent variable interactions. For instance, the refinement of bootstrapping procedures, the incorporation of advanced multigroup analyses, and the development of hybrid models that seamlessly combine formative and reflective measurements are all pushing the boundaries of what PLS-SEM can achieve. These methodological innovations not only improve the precision of parameter estimates but also enhance the overall interpretability of complex models, ensuring that theoretical insights are translated into practical outcomes. Looking further ahead, the potential integration of quantum computing with PLS-SEM represents a bold frontier in computational statistics. Quantum computing promises to dramatically speed up complex calculations and optimize large-scale data analyses that are currently challenging with classical computing methods. Although still in the early stages, research into quantum algorithms for optimization and simulation suggests that future PLS-SEM analyses could leverage quantum computing to handle massive datasets and extremely intricate models more efficiently. This technological leap could open up entirely new possibilities for predictive analytics and real-time decision support, ultimately transforming how theoretical models are estimated and validated in business research.

19. Practical Recommendations

When applying PLS-SEM, a structured, step-by-step approach can greatly enhance both the efficiency and reliability of the analysis. A comprehensive checklist might begin with clearly defining the research objectives and theoretical framework, followed by rigorous data collection and preparation. Next, carefully specify the measurement model, choosing between reflective and formative constructs based on the conceptual underpinnings of the study. Proceed to estimate the structural model, ensuring that key diagnostic metrics such as R^2, Q^2, and path coefficients are properly evaluated through bootstrapping and blindfolding procedures. Finally, incorporate robustness checks and validate the findings through multi-group analyses or other segmentation methods (Ravand & Baghaei, 2016). This systematic approach ensures that each aspect of the analysis is addressed and documented, reducing the risk of oversight and enhancing the overall quality of the research. Addressing reviewer feedback effectively is crucial for refining and strengthening a PLS-SEM study. It is recommended to carefully document every methodological decision, justify the chosen model specifications, and provide detailed diagnostic outputs. When reviewers raise concerns about model fit, measurement validity, or data quality, it is beneficial to include additional sensitivity analyses or robustness checks to demonstrate the stability of the findings. Transparency in reporting is key explaining any changes made in response to feedback and linking these modifications back to the theoretical framework can help convince reviewers of the study's rigor. Engaging in open dialogue with reviewers, if possible, further contributes to a more comprehensive revision process and ultimately enhances the credibility of the work.

In any complex analysis, challenges are inevitable. Common issues in PLS-SEM include inadequate sample sizes, convergence problems, multicollinearity among formative indicators, and potential misinterpretations of bootstrapping or blindfolding results. To mitigate these challenges, it is essential to perform preliminary power analyses, conduct thorough data cleaning, and systematically test for outliers and measurement anomalies. Establishing clear criteria for model convergence and ensuring that the appropriate statistical tests are applied for reliability, convergent, and discriminant validity will further safeguard against common pitfalls. Proactively addressing these issues during the planning phase, and documenting them meticulously in the report, creates a more robust analytical process and improves overall research outcomes.

20. Conclusion

In summary, the methodological contributions of PLS-SEM are significant, particularly when integrated with advanced statistical and computational techniques. Its flexibility in handling both reflective and formative models, along with its capacity for predictive analytics, makes it a powerful tool for examining complex relationships in business research. By incorporating innovative methods such as machine learning integration, robust multi-group analyses, and even emerging quantum computing technologies, PLS-SEM is poised to address increasingly sophisticated research questions. The implications for business research are profound. PLS-SEM not only enhances theoretical understanding by providing a nuanced analysis of latent constructs and their interrelationships but also offers practical insights that can guide strategic decision-making. Whether it is forecasting consumer behavior, optimizing organizational processes, or managing risks in uncertain environments, the application of PLS-SEM yields actionable intelligence that bridges the gap between theory and practice. Looking to the future, there are many promising avenues for further research. Areas for exploration include the continued integration of AI and machine learning techniques with PLS-SEM, the development of more robust methods for handling non-linear and interaction effects, and the potential for leveraging quantum computing to process large-scale and complex datasets. These advances are expected to drive both methodological and practical innovations, contributing to a more dynamic and responsive research environment. As the field evolves, maintaining transparency, rigor, and ethical standards will remain paramount, ensuring that PLS-SEM continues to provide reliable and impactful insights into the complexities of modern business phenomena.

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