ARTICLE
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The Structural Equation Modeling with Partial Least Squares: a statistical technique for Defense and International Security studies

El Modelado de Ecuaciones Estructurales con Mínimos Cuadrados Parciales: una técnica estadística para estudios de Defensa y Seguridad Internacional

Abstract: Partial least squares structural equation modeling (PLS-SEM) is a robust multivariate statistical technique that adjusts small samples and enables researchers to simply, systematically, and comprehensively answer a series of interrelated questions. This statistical technique was explicitly created to be used in the social sciences, whose studies sometimes lack large samples and new theories can be formed from the constant social changes. It achieves this by modeling the relationships between multiple dependent and independent constructs, considering different types of measures and various variables. This methodological study aims to describe the statistical technique in question, describing the assumptions of the method, its procedures, quality parameters, and limits. An analysis example illustrates the article using the SmartPLS software. In conclusion, this study brings reflection on the potential use of this statistical technique for International Security and Defense research.

Keywords: multivariate statistics; prediction; SmartPLS; constructs; structural models

Resumen: El modelo de ecuaciones estructurales de mínimos cuadrados parciales (PLS-SEM) es una sólida técnica estadística multivariada que se ajusta a muestras pequeñas y permite a los investigadores responder a una serie de preguntas interrelacionadas de manera simple, sistemática y completa. Esta técnica estadística fue creada explícitamente para ser utilizada en las ciencias sociales, donde los estudios no siempre cuentan con muestras amplias y se pueden formar nuevas teorías a partir de los constantes cambios sociales. Lo logra modelando las relaciones entre múltiples constructos dependientes e independientes, considerando diferentes tipos de medidas y diversas variables. Este ensayo metodológico tiene como objetivo presentar la técnica estadística en cuestión, describiendo los supuestos del método, sus procedimientos, parámetros de calidad y límites. Un ejemplo de análisis ilustra el artículo utilizando el software SmartPLS. En conclusión, el articulo trae una reflexión sobre el uso potencial de esta técnica estadística para la investigación en Seguridad y Defensa Internacional.

Palabras clave: estadística multivariada; predicción; SmartPLS; construcciones; modelos estructurales

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1 INTRODUCTION

Structural equation modeling (SEM) is a relatively new second-generation statistical technique that enables researchers to explain the interrelations between multiple constructs or latent variables indirectly measured by observable variables by combining factor analysis and multiple regression (HAIR *et al.*, 2014).

It differs from other analyses such as multiple regressions, multivariate analyses of variance, discriminant analyses, and other multivariate analyses by considering all dependent and independent variables at the same time, rather than focusing on the individual relations between them. This enables structural equation modeling to achieve its main objective: to expand researchers' capacity to propose and confirm new theories (HAIR; ANDERSON; BABIN, 2019).

SEM has two types: covariance-based structural equation modeling (CB-SEM) and partial least squares structural equation modeling (PLS-SEM). Based on Jöreskog's work, CB-SEM was first developed in the late 1960s and early 1970s, becoming popular by the analysis software he also created, i.e., the LISREL system (MARÔCO, 2021). CB-SEM first aims to confirm or reject theories by verifying systematic relationships between empirically measured multiple variables. CB-SEM confirms proposed theories by estimating a new covariance matrix from field data that is statistically indifferent from an original covariance matrix established in the theoretical proposition of the interrelations model. CB-SEM employs a maximum likelihood estimator (or equivalents) to estimate the relations between constructs in a covariance matrix. Although some estimators based on polychoric equations compensate for the nonparametric distribution of data, the model assumes that they adhere to a normal distribution and were collected by a minimally intervallic measurement. CB-SEM analyzes reflective models but accepts non-recursive (mutually reciprocal) and recursive (unidirectional) relations between them (HAIR *et al.*, 2014, 2019; HAIR; RINGLE; SARSTEDT, 2011; KLEM, 2006; SCHUMACKER; LOMAX, 2004).

PLS-SEM configures the recommended method if either CB-SEM assumptions are unable to be met, research aims to predict (rather than confirm) structural relationships, or formative models are predicted in theory. PLS-SEM, conceived for social science research, appeared in the late 1970s — in Wold's work (Jöreskog's advisor) above all — later receiving Lohmöller's (1989) developments. PLS-SEM uses the ordinary least squares method to estimate the relationships in the model and minimize the unexplained variance (errors) of its dependent (endogenous) variables. Its iterative algorithm separately solves measurement model blocks and estimates the path coefficients of the structural model. Due to its aim to expand the explained variance of endogenous variables, PLS-SEM is the first technique researchers consider when they wish to develop new explanations, i.e., new construct predictions to support a new theories (HAIR *et al.* 2014; HAIR; RINGLE; SARSTEDT, 2011; VINZI *et al.*, 2010).

Since the PL-SEM ordinary least squares estimator is distribution-free, data can either adhere to a normal, random or a linear distribution as the technique deals well with asymmetry and kurtosis deviations. Analyses can measure data by ratios, intervals (such as Stapel scales or semantic differentials), orders (such as Likert scales), and dichotomies (yes/no scales), the latter with some restrictions. It works with both formative and reflective measurement models, but only with recursive relationships between latent variables. As it requires neither normal distribution, large samples nor randomly collected linear data, PLS-SEM is called soft modeling — which refers neither to its quality, power nor criterion (VINZI et al., 2010).

2 CAN PLS-SEM BE USEFUL IN DEFENSE AND INTERNATIONAL SECURITY STUDIES?

International security and defense studies deal with political decisions to balance international power and maintain peace.

Individuals make these decisions in complex scenarios with many variables in their elaboration since they are, above all, human decisions. Thus, understanding them requires considering the multiplicity of their causal factors. Qualitative approaches describing these phenomena and evaluating their dimensions can primarily identify and understand them. PLS-SEM offers a complementary analytical step since it can predict the effects of the considered variables with empirical data. Qualitative research can evaluate relations between variables, whereas quantitative research, the extent to which variables can predict each other and if this occurs at random. Thus, researchers can predict changes in scenarios, conditions, and attitudes since decisions (endogenous variables) always depend on their context.

We found some research in the area that used this multivariate statistical technique to investigate international security and defense issues, such as logistics chain (KOUVELIS; MUNSON, 2004; RAHIMI SHEIKH; SHARIFI; SHAHRIARI, 2017), diplomacy (AKBARIYE; VAZIFEDOUST; SALEH ARDESTANI, 2018), human trafficking (RUDOLPH; SCHNEIDER, 2013), voting behavior (CWALINA; FALKOWSKI; NEWMAN, 2010), patriotism and nationalism (KARASAWA, 2002), and global strategies (BOUQUET; BIRKINSHAW, 2011), indicating that the area has accepted this technique. However, SEM seems to be less explored than other methodological alternatives.

This study aims to describe this type of structural equation modeling (PLS-SEM) to military science, defense, and international security researchers. Thus, it offers its premises, procedures, and quality parameters. We systematized this information from classic and up-to-date books and articles we cite throughout. We organized this information to conceptualize its constituent elements, describe its estimation phases (including parameter adjustment), and show criticisms to it. To better depict the technique, we describe an example of an analysis made in SmartPLS.

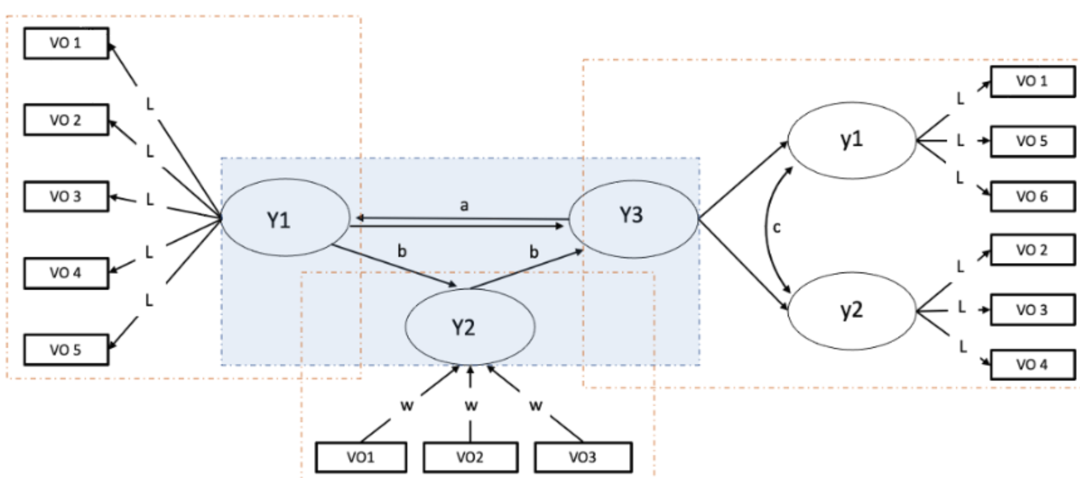
3 THE STATISTICAL TECHNIQUE IN QUESTION: PLS-SEM ELEMENTS

PLS-SEM operates by estimating interrelations between latent variables (constructs). Latent variables (e.g., safety perception) are hypothetical, i.e., unable to be directly measured. However, researchers can infer them by selected indicators, such as safety perception index items, which the PLS-SEM calls observable variables. Graphs can represent PLS-SEM models, conventionally expressing latent variables by ellipses and observed variables by rectangles (Figure 1).

The relationships established between the variables determine which the model deems dependent and independent. SEM calls independent variables exogenous and dependent variables, endogenous. Exogenous variables predict other variables/constructs in the theoretical model. It determines them outside it without specifying their causes. Endogenous variables results from at least one prediction relationship. Researchers can distinguish which exogenous variables predict each endogenous variable by relying on theory and/or their own previous experiences (HAIR; ANDERSON; BABIN, 2019; HERSHBERGER; MARCOULIDES; PARRAMORE, 2003; KLEM, 2006).

We should also mention that SEM actually consists of a structural model and a measurement model (Figure 1).

Figure 1 – Example of a structural measurement model



Source: Prepared by the authors, 2022.

The three orange hatched areas above highlight outer models. They deal with the relationships between observable and latent variables. They can contain first-order latent variables (such as Y1), which explain all observable variables in a single dimension. They may also contain second-order latent variables (Y3), which explain first-order latent variables (y1 and y2), directly connecting to observable variables and representing partial theoretical abstractions to form upper constructs (Y3) (HAIR *et al.*, 2014; VINZI *et al.*, 2010).

In this model we define its measurement theory for each latent variable, i.e., whether the latent variable will be evaluated in a reflexive or formative way. Graphically, the arrows go from latent variables to observable variables in the reflective measurement model (Y1, y1, and y2). In this type of model, constructs affect indicators, i.e., based on theoretical definitions, researchers seek elements for observation. Each latent variable affects observable variables differently and can be measured by factor outer loadings (λ). Observable variables tend to be correlated with each other, configuring more palpable manifestations of latent variables. For example, international defense capacity manifests itself as diplomatic skill, trade relation quality, power balance roles, and geopolitical importance.

On formative measurement models, observable variables are characteristic of latent variables. Each observable variable composes a portion of the construct, represented by outer weights (ω). A small change in one of them alters the construct, e.g., combat capacity consists of the amount of armored, trained men; mass destruction weapons; fighter aircrafts; and available ammunition. In the graphical representation above (Figure 1), arrows come out of indicators (equivalent to observable variables in formative models) to manifest variables or domains (equivalent to latent variables in formative models; Y2) (BECKER; KLEIN; WETZELS, 2012; HAIR *et al*., 2014, 2019; VINZI *et al*., 2010).

Structural (or inner) models predict the relations between the studied constructs (the blue area in Figure 1). In structural models, researchers define how variables relate to each other. Their structural coefficients (β) describe the strength and direction of this relation. Graphically, relations are established from left to right. The left margin of the image refers to exogenous variables (Y1) — which only emit arrows —, whereas its right margin refers to endogenous variables (Y3) — which receive path arrows —, and some that receive and emit arrows — also called endogenous (Y2) — but that may also include moderating variables depending on the approach (HAIR; RINGLE; SARSTEDT, 2011; VINZI *et al*., 2010).

Arrows indicate the type of relation between latent and observable variables. The unidirectional arrows (b) in Figure 1 indicate a recursive relation between them, whereas bidirectional arrows (a) indicate a non-recursive relation between variables, i.e., a mutual and reciprocal relation. Curved bidirectional lines (c) represent the correlation between the latent variables in the model (GARVER; MENTZER, 1999; HAIR; ANDERSON; BABIN, 2019; HERSHBERGER; MARCOULIDES; PARRAMORE, 2003).

During the definition of structural models, researchers delimit their theoretical propositions and propose to answer questions such as: how can we explain the studied factor relations? What influences them significantly? What would be a valid prediction? These questions should find support in the research theoretical framework – even if it is yet to be fully defined. We should mention that all mathematical analysis on data with this statistical method will be in vain in the absence of theoretical support. We must keep this assumption in mind.

4 THE PLS-SEM ESTIMATION PROCESS

More current approaches propose that the decision process to estimate PLS-SEM takes place in six stages (HAIR; ANDERSON; BABIN, 2019) divided into three phases: (i) research preparation; (ii) model analysis and adjustment; and (iii) the further exploration of results.

Today, several alternatives to process data and perform PLS-SEM analyses with the aid of software are available (e.g., SmartPLS; MPlus; PLS-Graph, and the R PLS package). Some formulas in this section aim to facilitate readers' understanding of the concept. In short, researchers must choose their measurements, determine their predictions, collect data, program the software, interpret their results for structural measurement models, and further explore their data, reflecting the six stages we will describe next, except for software (programming), whose choice remains at researchers' discretion.

4.1 Phase 1: research preparation

The first stage deals with defining research objectives and selecting model constructs. As for objectives, PLS-SEM is the ideal multivariate statistical method when researchers wish to investigate multiple relations in constructs for cases in which the underlying theory is yet vague, i.e., in the absence of clear predictive relations, when researchers want to create a new theoretical perspective from the empirical evidence stemming from evaluating possibly related constructs; or when research problems deal with "how," "why," and "when" questions as PLS-SEM basically accepts all measurement levels (HAIR; ANDERSON; BABIN, 2019).

Then, researchers should choose the proper evaluation instruments to generate data. Measurement instruments with reflective models are evaluated for their quality based on their validity and reliability metric evidence. Those based on formative models have their quality evaluated by their factor weights and collinearity between their indicators. Keeping this in mind is of special relevance at this stage. After all, researchers can only test prediction hypotheses between constructs (the ultimate goal of PLS-SEM) if the way to measure them offers reliable data and properly evaluates the investigated construct.

The validity evidence of a measure indicates what is being measured (construct representation) and what inferences can be made from it (score interpretation) (URBINA, 2004). They must be considered in the application context. Thus, validity evidence, rather than belonging to the instrument, appropriates the measure in a given country for a certain population (HURTZ; BANDEIRA; TRENTINI, 2015).

Classically, up to 31 types of validity can be distinguished (PASQUALI, 2007), of which we highlight construct validity, which aims to experimentally show that the instrument indeed measures what it aims to measure (BROWN, 2000). Construct validity have three subtypes: discriminant validity (evidence of distinct factors in the constitution of the construct), convergent validity (evidence that the selected variables represent well each unifactorial construct factor), and nomological validity (evidence of association between constructs, observable variables, and constructs and observable variables) (NUNNALLY; BERNSTEIN, 1994; PASQUALI, 2007; URBINA, 2004). Construct validity can be verified by different statistical tests, but minimally, the definition of the factorial structure (how items are organized into factors and how factors are identified) is defined by what is necessary to consider as primary evidence of construct validity (MARÔCO, 2021).

Reliability, on the other hand, refers to evidence that the instrument consistently performs measurements without errors (i.e., score fluctuations are irrelevant to what is being measured) (COZBY, 2001; URBINA, 2004). The scales researchers must choose in this first stage must show evidence of previous validity and reliability.

In formative models, researchers should check the hypothesis of evidence of no multicollinearity (correlations between indicators) and whether indicator factor weights (w) are relative or absolutely significant for measures (HAIR *et al.*, 2017; ROBERTS; THATCHER, 2009).

The second stage is the study design, which defines the sample size to be collected and missing data treatment. Sample size estimation must aim to preserve the statistical power of the method — i.e., the ability of tests to identify correct answers — which must be at least 80% (COHEN, 1992). This calculation should also consider model complexity — the number of latent variables, observable variables, and estimated causal relations — and sample heterogeneity (HAIR; ANDERSON; BABIN, 2019; VINZI *et al.*, 2010).

Sample size estimation has some available options. One of the first rules for setting the minimum required sample size was called the 10×-rule (BARCLAY; HIGGINS; THOMPSON, 1995), which determines that the number of indicators of the largest formative model or the largest number of arrows (paths) directed to a given construct in the model be multiplied by 10. This rule has received serious criticism (KOCK, 2018; KOCK; NADAYA, 2018) and is currently deemed as poorly (if at all) adequate (KOCK, 2018; KOCK; NADAYA, 2018). Alternatively, recommendations suggest that minimum sample sizes be estimated by software such as G*Power[1] (using its calculations to test regressions) or alternative methods, such as the inverse square root (which uses the inverse square root of a sample size to estimate standard errors) and the gamma-exponential method (which corrects the gamma and exponential smoothing function applied to a previous method) (KOCK; NADAYA, 2018). Other rules that consider significance levels and explained variables can also estimate sample size (COHEN, 1992). Researchers should keep in mind that the more heterogeneous their population, the greater the required sample size to properly evaluate the idiosyncrasies of the evaluated manifestations (HAIR; RINGLE; SARSTEDT, 2011; HAIR *et al.*, 2012; HAIR; ANDERSON; BABIN, 2019; VINZI *et al.*, 2010).

Researchers should carefully consider missing data as PLS-SEM is quite sensitive to them. Listwise deletion configures the most judicious way to do so, i.e., excluding subjects (be it

1 Free software, available at: http://www.psycho.uni-duesseldorf.de/abteilungen/aap/gpower3/. It has the advantage of considering effect sizes and sampling power to estimate sample numbers.

States or individuals) for which researchers' databases lack information of some variable. As listwise deletion potentially shrinks databases, it may often be far from ideal — despite being the most judicious choice. After data collection, researchers must also evaluate missing data patterns to evaluate if they have systematically failed to answer some observable variable. If so, they should consider measurement biases (HAIR; ANDERSON; BABIN, 2019).

In the third stage, researchers more clearly define which hypothesis they will test in their research. This process begins with researchers' theoretical propositions based on the relations between the studied constructs — the first definition of the structural model. This stage has three critical elements: (i) researchers should know the investigated topic to determine which variables are endogenous and exogenous; (ii) they should indicate the dependencies and predictive or causal relations in the literature among latent variables; and finally, (iii) they should employ the measurement instruments they chose in the first research stage with the pertinent metric quality evidence (whether formative or reflective) for the data they collected in the country in which they are to conduct their study.

Researchers define their structural theory and prediction paths at this point in analysis planning. A literature review on their study constructs with evidence on their sample will support these decisions as will researchers or their colleagues' previous studies (HAIR; ANDERSON; BABIN, 2019; VINZI *et al*., 2010). Researchers must constitute a theoretical background to support their predictions.

Researchers should go to the field after deciding that PLS-SEM statistical analysis meets their objectives and choosing what measures, sample, and theoretical assumption they will use to collect data. The following stages already consider that researchers have collected data and are now testing the metric fit of their instruments to their sample and exploring the significance of the proposed causal relations.

4.2 Phase 2: analysis and adjustments to measurement and structural models

The fourth stage consists of evaluating measurement models. This process changes if the chosen assessment instruments are reflective or formative. Reflective instruments require researchers to evaluate the evidence of validity and reliability of their sample measurements. Researchers must first observe the factor loadings of their observable variables, which should ideally equal or exceed 0.71, indicating about 50% of the variation in latent variables. Close values are to be tolerated as long as they compromise neither reliability nor validity, but it is highly recommended to eliminate those below 0.40. Researchers can eliminate some observable variables from their measurement models to improve the quality of their measurements, a common procedure. When they eliminate all observable variables with very low factor loadings (< 0.40), they must continue to refine their measurements — including further exclusions — considering their impact on the measurement reliability and validity (HAIR *et al*., 2009, 2014, 2019).

The evaluated PLS-SEM reliability refers to internal consistency, i.e., the internal coherence of the indicators in relation to latent variables. PLS-SEM evaluates construct reliability by the "degree to which the indicators of a latent construct are internally consistent with each other" (HAIR *et al*., 2009, p. 467). The following formula estimates construct reliability:

$$\text{construct reliability} = \frac{\left(\sum_{i=1}^{n} \lambda_1\right)^2}{\left(\sum_{i=1}^{n} \lambda_1\right)^2 + \left(\sum_{i=1}^{n} e_i\right)}$$

in which ∑ refers to summation; λ_i, the standardized factor loading of observable variables of a latent variable; and *i*, the measurement error of each item of the latent variable, estimated as 1 (observable variable reliability).

Moreover, researchers can evaluate internal consistency with other tests and add reliability evidence to their measurements. The Cronbach's alpha test is the classic test to generate this evidence, producing a Cronbach's alpha coefficient (α) from the correlations between observable variables. However, this indicator has been widely questioned as an adequate measure for non-interval scales or an accurate representation of the internal consistency of measurements (SIJTSMA, 2009). Some still advocate its use, and the test tends to be maintained since it can interpret accumulated evidence (TAVAKOL; DENNICK, 2011). Researchers can employ other tests to correct the deviations the Cronbach's alpha test may have for non-interval scales, such as the ordinal alpha test, omega, and the greatest lower bound test (PETERS, 2014). All reliability tests we mentioned recommend values above 0.70, tolerating those above 0.60 (HAIR; ANDERSON; BABIN, 2019).

Researchers should then evaluate construct validity, generating evidence of convergent and discriminant validity. A measurement error variance below the captured variance constitutes convergent validity, indicating the extent to which observable variables converge in the construct. This is established with the help of the average variance extracted (AVE) by the formula:

$$\text{Average variance extracted} = \frac{\sum_{i=1}^{n} \lambda_j^2}{n}$$

in which ∑ refers to summation;. λ_i, the standardized factor loading of the observable variables in the latent variable, and *n*, the number of items in each factor. Values above 0.50 are considered adequate (HAIR *et al*., 2014, 2019).

Discriminant validity, in turn, points to the extent to which a latent variable differs from another. It can be evaluated by cross-correlations analysis, the Fornell-Larcker criterion, and the heterotrait-monotraitrat ratio of correlations (HTMT) test. Regarding cross-factor loading analysis, factor loading indicators in the assigned construct should exceed all loads of other constructs (HAIR; RINGLE; SARSTEDT, 2011).

The Fornell-Larcker criterion (FORNELL; LARCKER, 1981) compares the square root of the AVE with construct correlation. The logic underpinning this indicator is that latent variables should better explain the variance of their own indicators rather than that of other latent variables. Therefore, the square root of the AVE of each construct must exceed the correlations with other latent constructs (HAIR *et al*., 2014).

The HTMT test is the most recent alternative to investigate discriminant validity. Henseler, Ringle, and Sarstedt (2015) showed its superior performance in comparison to the two aforementioned alternatives by studying the Monte Carlo simulation and recommending its use. HTMT values close to 1 indicate a lack of discriminant validity. Some authors suggest a 0.85 (KLINE, 2015) and even 0.90 limit (TEO; SRIVASTAVA; JIANG, 2008). For Henseler, Ringle, and Sarstedt (2015), values must reside between -1 and 1 to evince discriminant validity. Lower values elicit more important evidence of discriminant validity.

Adjusting measurement instruments to meet reliability and validity criteria mainly involves eliminating items with very low loadings (< 0.40) and deciding to eliminate or maintain items those between 0.40 and 0.70. Researchers may maintain items that showed no negative impact on validity and reliability indicators with factor loadings between 0.69 and 0.41 to better preserve the content validity of their measurements (HAIR; ANDERSON; BABIN, 2019).

However, in the presence of instruments with formative measurement models, researchers should be aware that evaluating the quality of the measurement model containing these instruments involves other parameters since those described so far are largely based on correlations between observable variables. Thus, as indicators are expected to be independent or, at most, weakly correlated in formative models, the aforementioned measures to evince validity and reliability should be avoided in this case (ROBERTS; THATCHER, 2009). Analyses should focus on determining (i) unwanted correlations between two or more indicators — collinearity; and (ii) the indicator factor weights (w) (HAIR *et al*, 2017).

A correlation between two indicators creates collinearity — which is problematic in this model as it assumes that each indicator contributes independently to the construct (if more indicators are involved, this situation is called multicollinearity). Collinearity (or multicollinearity) increases standard errors and decreases the ability of regressions to correctly estimate factor weights — both in their value and in their significance. This is particularly concerning for small samples, in which standard errors are usually large (HAIR *et al*., 2014).

Researchers can check for multicollinearity by estimating tolerance (TOL). TOL evaluates how much the variance of an indicator remained unexplained by other indicators in the same latent (or preferably, manifest) variable. TOL is estimated as follows:

$$\text{TOL} = R_{x1}^2$$

in which R_{x1}^2 refers to the v*ariance proportion of* x_1 associated with other indicators. Each indicator in the model has a TOL value which must be estimated. A measure related to TOL is the variance inflation factor (VIF), which can be estimated as:

$$\text{VIF} = {}^{1}/_{TOL}$$

These two collinearity measures can analyze retention criteria in instruments, although only reporting the VIF has become the most common practice. Values < 5 are deemed acceptable and < 3.3, preferable (HAIR *et al*., 2017; DIAMATOPOULOS; SIGUAW, 2006). For indicators exceeding these values, researchers should consider eliminating them from their model since other indicators explain a large portion of their variance. However, they must have some certainty that this exclusion will fail to affect the constitution of the manifest variable (BIDO *et al*., 2010; LATAN, RAMLI, 2013).

The factorial weight of indicators (ω) evaluate the contribution of each indicator to the manifest variable. It derives from the multiple regression of manifest variable (dependent variable) and indicators (independent variables) scores. Ω is standardized so it can be compared with others from the same manifest variable, enabling researchers to assess its relative importance in the formation of constructs (HAIR *et al*., 2014). To be important, ω must be significant and preferably (though not necessarily) > 0.50. When ω is insignificant but has a high factor loading (λ) (> 0.50), the indicator should be interpreted as absolutely important (i.e., the information it gives is important, but it fails to consider other indicators). In this situation, the indicator would usually be kept in the formative model but when indicators have non-significant ω and $\lambda < 0.50$, researchers must decide whether to retain or exclude them by examining their theoretical relevance and the overlap of potential content with other indicators in the same construct (HAIR *et al*., 2014).

The fifth stage begins when researchers can examine their structural model after ensuring validity, reliability, and/or collinearity, and the value and significance of the factorial weights of measurement model indicators. The first step of the fifth stage is to evaluate the collinearity between exogenous constructs (predictors). The variance inflation factor (VIF) is calculated for each latent predictor variable and, as a rule, higher VIF values indicate collinearity. Researchers can also infer collinearity by a bivariate correlation test between latent predictor variables, seeking correlations lower than 0.50 to indicate absence of collinearity. In such a case, researchers may create a second-order factor for the construct in question to deal with this problem without losing variables in their model (HAIR; ANDERSON; BABIN, 2019).

Next, researchers can deal with actual prediction relations (the structural model). The coefficient of determination (R^2) ranges from 0 to 1 and higher values indicate greater ability to explain structural models and thus better predict endogenous variables. In general, values equal to 0.25; 0.50, and 0.75 indicate weak, moderate, and substantial effects, respectively. However, in the social sciences, the 0.02; 0.13, and 0.26 limit values are recommended to interpret variables as weak, moderate, and substantial, respectively (COHEN, 1988; HAIR *et al*., 2014).

Effect size (f^2) represents the change to the coefficient of determination by omitting an exogenous variable from the model, and may be interpreted as how useful each construct is to adjust the model. Values equal to 0.02; 0.15, and 0.35 are considered as small, medium, and large effects of an exogenous latent variable and values below 0.02 indicate no effect (i.e., no predictive capacity) (HAIR *et al*., 2014; 2019).

The next step is evaluating the predictive power of the model (Q^2; Stone-Geisser indicator). As a rule, its value is obtained by blindfolding, considering the cross-redundancy approach available in most PLS-SEM analysis software. Values equal to or above zero for each endogenous construct of the model indicate an acceptable predictive accuracy of the model, and higher values indicate greater predictive accuracy (HAIR *et al*., 2014, 2019; VINZI *et al*., 2010).

Finally, researchers should evaluate the size and significance of predictive relations by structural coefficients (graphically represented by arrows in the model and which conceptually explain prediction relations). Structural coefficients must be significant — if $p < 0.05$, $t > 1.96$, and confidence intervals without zeroes. Values greater than these additionally indicate collinearity in the model (Table 1). Structural coefficient values must be interpreted in the light of theory to assess their importance, whereas their mathematical interpretation should follow the betas (β) of simple or ordinary linear regressions. Values that can be considered acceptable depend on model complexity and research context (HAIR; ANDERSON; BABIN, 2019; RINGLE; SILVA; BIDO, 2014).

Table 1 — Summary of Smart PLS adjustments

INDICATOR	PURPOSE	REFERENCE VALUES/CRITERIA	REFERENCES
VIF	Multicollinearity evaluation.	VIF < 5 VIF < 3.3 (stricter)	HAIR *et al*. (2017)
AVE	Convergent validity evaluation.	AVE 0.50	HENSELER; RINGLE; SINKOVICS (2009)
HTMT	Discriminant validity evaluation.	HTMT < 0.85	HAIR *et al*. (2019)
Composite reliability	Model reliability evaluation.	CC 0.70	HAIR *et al*. (2017)
Student's t-test	Correlation and regression significance evaluation.	t > 1.96	HAIR *et al*. (2017)
Pearson's coefficient of determination (R^2)	Evaluation of the variance portion of endogenous variables, explained by the structural model.	For the social and behavioral sciences, an R^2 = 2% is classified as a small effect, an R^2 = 13%, as medium effect, and an R^2 = 26%, as a large effect.	COHEN (1988)
Cohen's indicator (f^2)	Evaluation of how much each construct is useful to adjust models.	Values of 0.02, 0.15, and 0.35 are considered small, medium, and large, respectively.	HAIR *et al*. (2017)
Stone-Geisser indicator (Q^2)	Evaluation of the accuracy of adjusted models.	$Q^2 > 0$	HAIR *et al*. (2017)
Structural coefficient (β)	Causal relation evaluation.	Interpretation of values in the light of theory.	HAIR *et al*. (2017)

Source: Ringo, Silva, and Bido (2014); Hair *et al*. (2017, 2019)

4.3 Phase 3: Further exploration of results

In the sixth stage of the PLS-SEM estimation process, researchers can do additional analyses to better explain, specify, or even interpret their model. We highlight two possible analyses: the investigation of sample heterogeneity and the presence of mediating or moderating variables.

Multigroup analysis can evaluate differences between sample subgroups formed from categorical variables (e.g., continent, government system, etc.). This is called observed heterogeneity. The subsamples by which heterogeneity is to be investigated must meet power and sampling significance criteria (i.e., they must exceed the calculated minimum, considering the studied model). The structural coefficients for each sample will be estimated and the variation between them analyzed. No variation ($p > 0.05$) will suggest the absence of sample heterogeneity. The approach to these analyses is called PLS-MGA (PLS — multigroup analysis) and is built into the most common software.

Researchers can also evaluate unobserved heterogeneity — groups differ by a characteristic researchers failed to observe. It can be approached by the probability of sample participants belonging to segments (subsamples) and by differences in segment structural coefficients. Researchers must predict the number of possible segments from the ratio between their total sample and the minimum required sample. The number of segments will be the smallest integer value closest to this ratio. The finite mixture partial least squares (FIMIX) configures a specific method to estimate structural model heterogeneity. Another approach is prediction-oriented segmentation (PLS-POS), which also observes heterogeneity in structural and measurement models but with the advantage that it does so for models with formative and reflective variables and generates information about explained variance (R^2) by forming homogeneous groups, reassigning observations (if it improves the quality criteria of the models), and working with specific distance measures for formative variables. Hair *et al* (2017) recommend that these two methods be used together, starting with FIMIX and segment analysis. Failure to reject the existence of heterogeneity in structural models suggests continuing analyses with the PLS-POS. A third option is response-based procedure for detecting unit segments (REBUL-PLS), which analyzes heterogeneity in structural and measurement models with reflective variables, observing model and latent variable residuals (HAIR *et al.*, 2017, 2019).

In cases in which a variable both predicts an exogenous variable and is explained by an endogenous variable (Y2 in Figure 1), researchers should investigate whether that variable mediates or moderates the prediction of exogenous variables over endogenous variables. Moderating variables contaminate the predictive relations between independent and dependent variable and must then be controlled as it affects the strength and direction of the prediction (for example, between the need to deter an enemy and actually doing so, this outcome can be moderated by confidence in combat ability). Mediating variables, in turn, explain the relation process between two variables, i.e., an intermediary between independent and dependent variables (for example, sleep quality can affect combat performance as a function of cognitive alertness). Knowing whether the variable has a mediating or moderating effect enables the evaluation of the total effects between constructs, more completely evaluating predictions (HAIR *et al*., 2017, 2019).

5 LIMITATIONS AND CRITICISMS

Although the PLS-SEM can deal with data of different measurement levels; data that fail to adhere to normal distribution; relatively small samples; and relatively poor theoretical support — thus contributing to the maturation of the investigated theory —, the method has received criticisms.

First, this structural model forbids non-recursive relations (reciprocal influence between variables). If researchers' theoretical prediction or previous evidence indicates that considering this relation is important to the model, researchers should consider using CB-SEM, rather than PLS-SEM (HAIR *et al*., 2014, 2017, 2019; VINZI *et al*, 2010).

Secondly, it is stated that the PLS-SEM estimates are inefficient and potentially biased when compared with CB-SEM measurements (e.g., MARCOULIDES; SAUNDERS, 2006; MCINTOSH; EDWARD; ANTONAKIS, 2014; RÖNKKÖ, 2014; RÖNKKÖ; EVERMAN, 2013). The central argument supporting these criticisms is that PLS-SEM estimates are inconsistent because they are aggregated from observed variables and include measurement errors. This bias tends to manifest itself in slightly higher estimates for factor loadings and lower path coefficient estimates.

In response, researchers working with PLS-SEM argue that it has been shown that its estimates will approach true parameter values when they increase the number of indicators per construct and sample size (VINZI *et al*., 2010). For those who compare PLS-SEM and CB-SEM, it has been shown that the mathematical differences between the estimates are irrelevant, with PLS-SEM being as good a choice as CB-SEM to treat reflective models and superior to the latter, to treat formative models (SARSTEDT *et al*., 2016).

6 APPLIED EXAMPLE

To exemplify the application of this statistical technique to a database, we chose to use the SmartPLS software. It is intuitive, simple to use, and has free licenses for students[2]. Books, articles, and videos support users and offer technical clarifications about it. Our example used the fourth version of SmartPLS, released in August 2022.

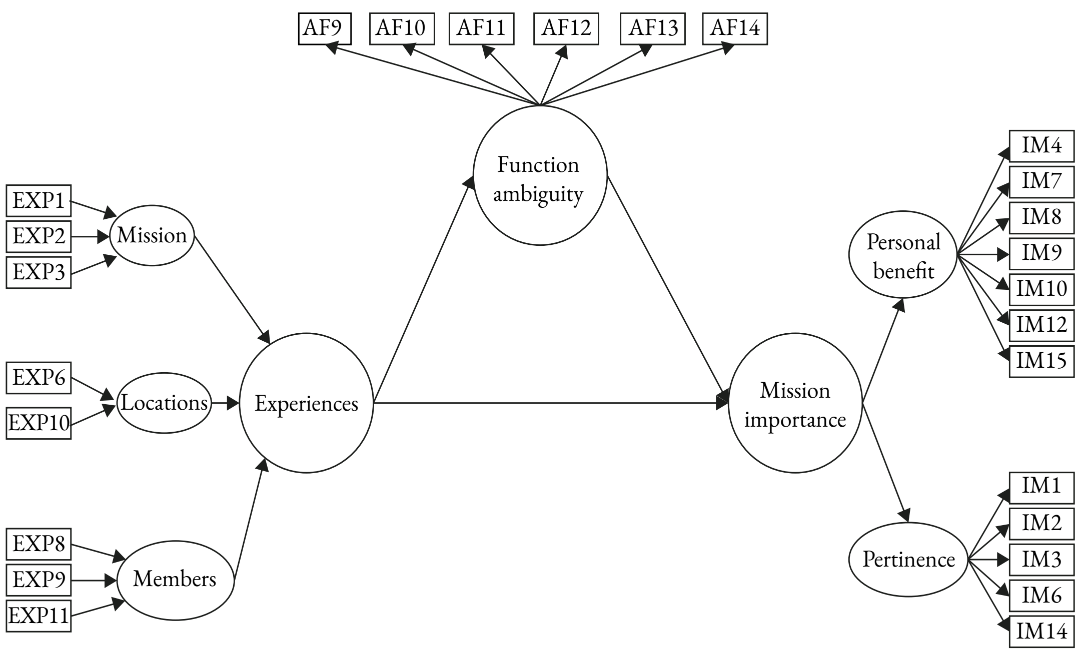
We tested a hypothetical model in which the experiences of military personnel on the ground predict their evaluation of the importance of a mission, which may or may not be mediated by function ambiguity. This model was theoretically conceived from evidence that borders the theme, gathered by a systematic review of the literature — a greater discussion about the

2 https://www.smartpls.com/

theoretical bases of this model used for example lies outside the scope of this study but can be found in Neves (2022).

A formative model operationalizes the first exogenous variable, ground experience. A reflective model operationalized the second exogenous variable and the endogenous variable. Both ground experience and the importance of a mission constitute second-order latent variables, i.e., composed of other latent variables (mission, locations, and members; personnel, and pertinence, respectively). A metric study previously analyzed all these measures, pointing out which observable variables should be retained for each latent variable in a sample similar to our database (NEVES, 2022). We find a direct prediction between ground experience and the importance of a mission and a prediction that function ambiguity may mediate this. Ellipses represent latent variables; rectangles, observable variables; and arrows, prediction paths (Figure 2).

Figure 2 — Hypothetical theoretical model for the applied example



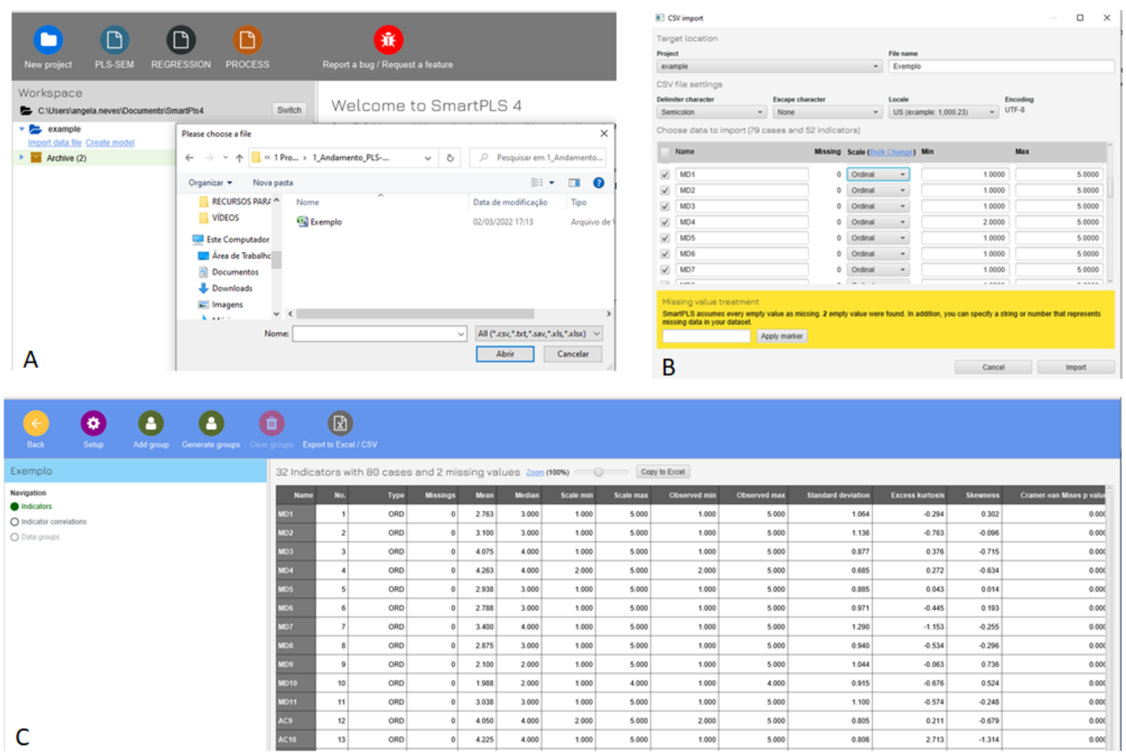
Source: Elaborated by the authors, 2022.

We estimated the minimum sample size to test this model on G*Power, according to Bido *et al* (2014). Thus, two exogenous variables (ground experience and function ambiguity) predict the endogenous variable (importance of a mission), and considering a 0.15 effect size, 80% power, and a 0.05 alpha, the suggested minimum sample size is 68 participants, the ideal being triple this value. This example has a database with 80 participants.

Researchers may organize their data in a spreadsheet in their preferred software, which they must save in the *.*csv format. Its first row should contain the labels (names) of the evaluated variables.

After starting the program, choose "new project" and name it according to your research. Next, a project folder will open in the left menu with two options: "import data" and "create model" (Figure 3A). Start with the first option and choose the *.*csv worksheet with the research data. Once the data are imported, SmartPLS opens a new window for researchers to adjust their data measurement and report any code for missing data (Figure 3B). Click "import" and the datasheet will be loaded with the option to identify sample groups, if relevant (Figure 3C). Once imported correctly, the data will be identified in the project folder in green.

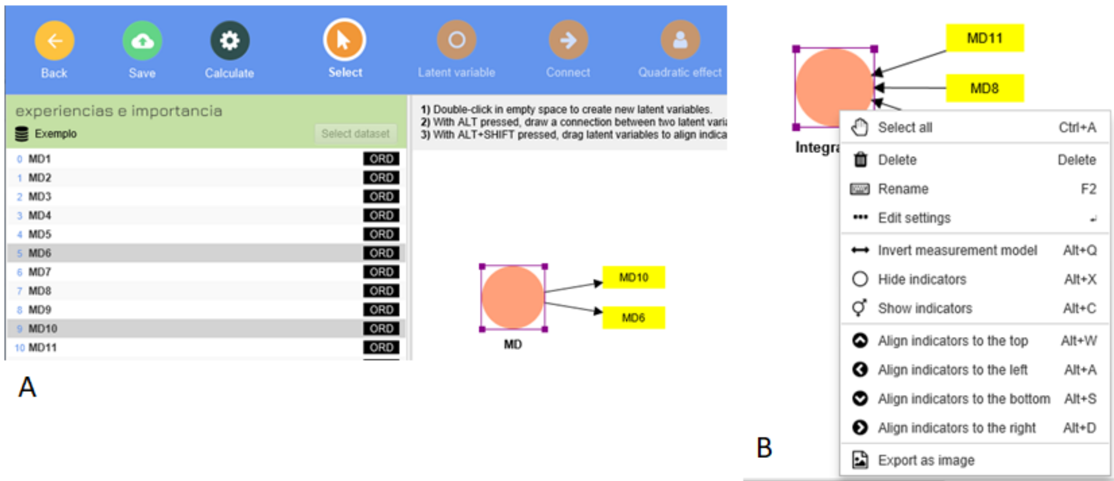
Figure 3 — Importing the database into the software



Source: Elaborated by the authors, 2022.

Now choose the second option, "create model." A window will open for the template to be named and the template type to be chosen. To analyze structural equations, choose "PLS-SEM." Click "Save." The menu on the left will identify the observable variables and model indicators. Select all that reflect or form the same latent variable (in our example, we selected items MD1, MD2, MD3 for the latent variable Mission) and drag them to the right (graphic window), already positioning it according to your hypothetical model. A text window will open to correctly name the latent variable. Press "enter" (Figure 4A). The left mouse button can open a menu to adjust the latent variable, including model type (whether formative or reflective), observable variable positioning, among other options (Figure 4B).

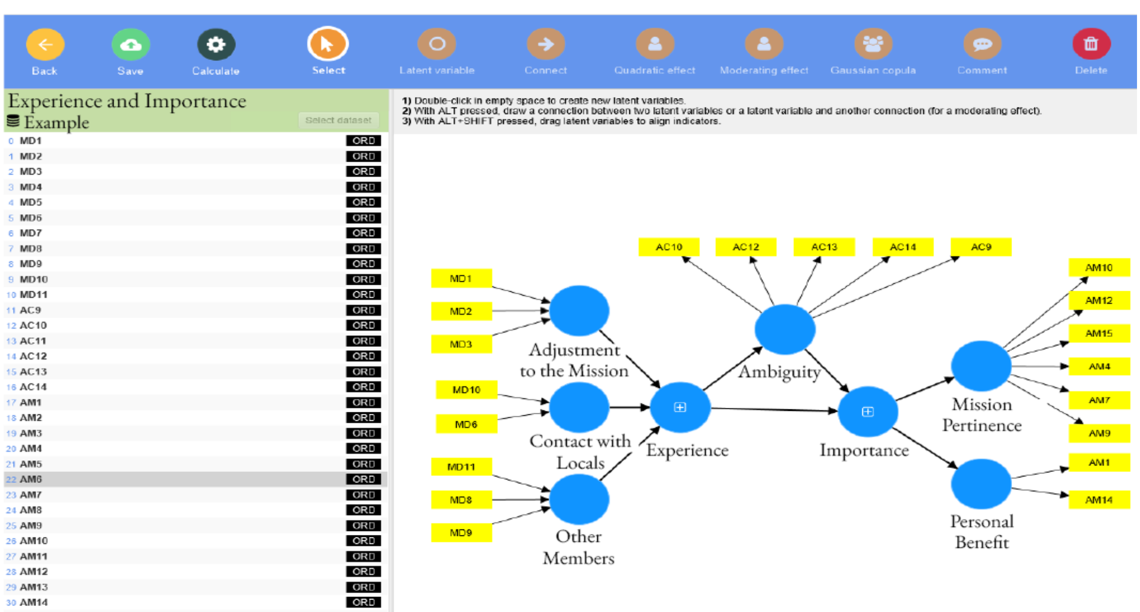
Figure 4 — Initial steps to configure measurement and structural models



Source: Elaborated by the authors, 2022.

To configure second-order latent variables, select all the observable variables that form/reflect first-order latent variables. Name and choose "hide indicators" to avoid polluting your model. Repeat this operation until you properly characterize all first- and second-order latent variables. Then, click the top menu under "connect" and determine the prediction paths between variables (Figure 5). Once these initial phases are complete, the model is ready to be analyzed.

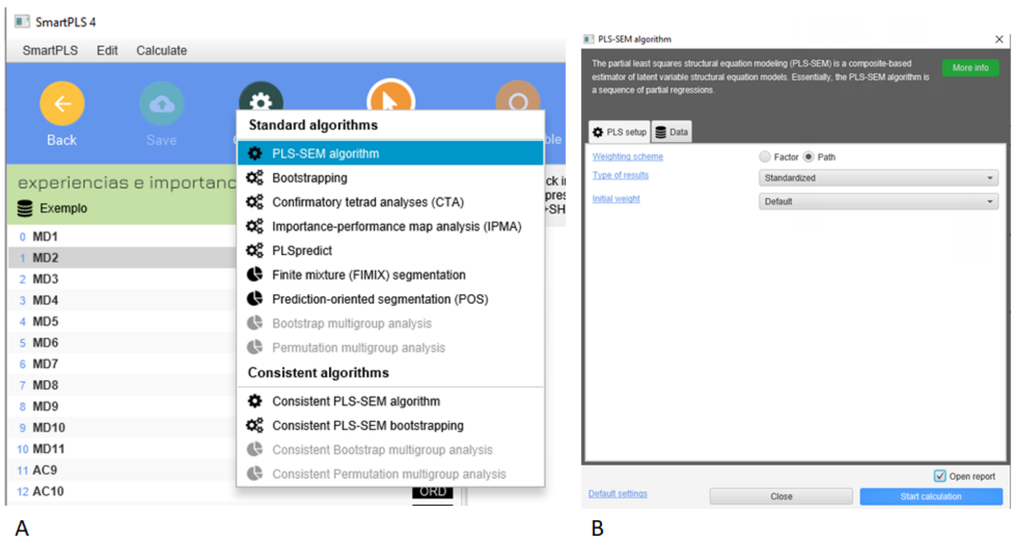
Figure 5 — Model ready for analysis



Source: Elaborated by the authors, 2022.

Our example has reflective and formative measurement models, and we chose the first option (Figure 6A). In the analysis configuration window, make sure to select "Path" for "Weighting Scheme" (Figure 6B).

Figure 6 — Starting the analysis



Source: Elaborated by the authors, 2022.

A new window will open with the analysis output and the menu on the left will make analysis results available. Above the graphical window, you will find options for which results to visualize in the measurement (outer) and structural models (inner model) and regarding latent variables. This analysis generates information of researchers' interest in the output "quality criteria."

We initiated our analysis by the measurement model, as per the literature. In our example, we modeled the first-order domains on the experience scale as formative (contact with locations, adjustment to missions, and other personnel). We inspected its variability indicators and factor weights at this stage. We found that all indicators had adequate VIF values. The observable variable EXP6 had a non-significant factorial weight ($p = 0.057$) but a high factor loading ($\lambda = 0.59$). We decided to keep it in the model, assuming its importance to be absolute and non-relative (Table 2). Results indicated no correlation between indicators (which is highly desirable) and that all the indicators significantly contributed to form the construct of experience with peace missions.

Function ambiguity, mission pertinence, and personal benefit constitute the first-order latent variables in the analyzed example, which we modeled as reflective constructs. We observed that the observable variable AF11 of the latent variable Function Ambiguity ($\lambda = 0.44$); MI8, of the latent variable Personnel ($\lambda = 0.46$); and MI 2 ($\lambda = 0.25$), IM3 ($\lambda = 0.11$), and IM6 ($\lambda = 0.13$) of the latent variable Pertinence had low factor loadings. Thus, we removed them from our model. Researchers must remove each observable variable individually, performing a new estimation for each removed element. Researchers who remove observable variables from a first-order latent variable must also remove them from second-order latent variables. To remove a variable from the template, select “delete” from the top menu.

After removing those observable variables, we generated satisfactory evidence of convergent validity (AVE) and internal reliability (construct reliability). These results enable us to claim that the observable variables in each first-order latent variable adequately reflect them, that the measurement these scales made in the sample is free of random errors, and that we can consider these results as reliable (Table 2).

Table 2 — Quality indicators of measurement models for latent variables and first-order indicators

	λ/ω*	VIF	CC	AVE
Function ambiguity	0.51 – 0.83	n/a	0.84	0.52
Personal/career benefit (IMP)	0.55 – 0.86	n/a	0.73	0.57
Mission pertinence (IMP)	0.49 – 0.97	n/a	0.89	0.59
Locations (EXP)	*0.40 – 0.83	1.23 – 1.39	n/a	n/a
Mission Adjustment (EXP)	*0.36 – 0.57	1.06 – 1.61	n/a	n/a
Other peacekeepers (EXP)	*0.46 – 0.51	1.20 – 1.43	n/a	n/a

Note: IMP = importance of the mission; EXP = Experiences with peace missions; λ = factor loading; ω = factorial weight; VIF = multicollinearity indicator; CC = composite reliability; CVA = average variance extracted; n/a = not applicable. Values marked with * refer to ω.

Source: Elaborated by the authors, 2022.

Then, we only inspected evidence of discriminant validity for variables we modeled as reflexive. The analyzed data showed satisfactory evidence (Table 3), i.e., in this sample, the first-order latent variables in the model really differ from each other.

Table 3 — HTMT test values for first-order latent variables

	1	2	3
1) Function ambiguity	-		
2) Personal/career benefit (IMP)	0.77	-	
3) Mission pertinence (IMP)	0.72	0.30	-

Note: IMP = importance of the mission

Source: Elaborated by the authors, 2022.

It is also interesting to bring cross-loading analysis as evidence of discriminant validity (Figure 7), identifying the items in each predicted latent variable.

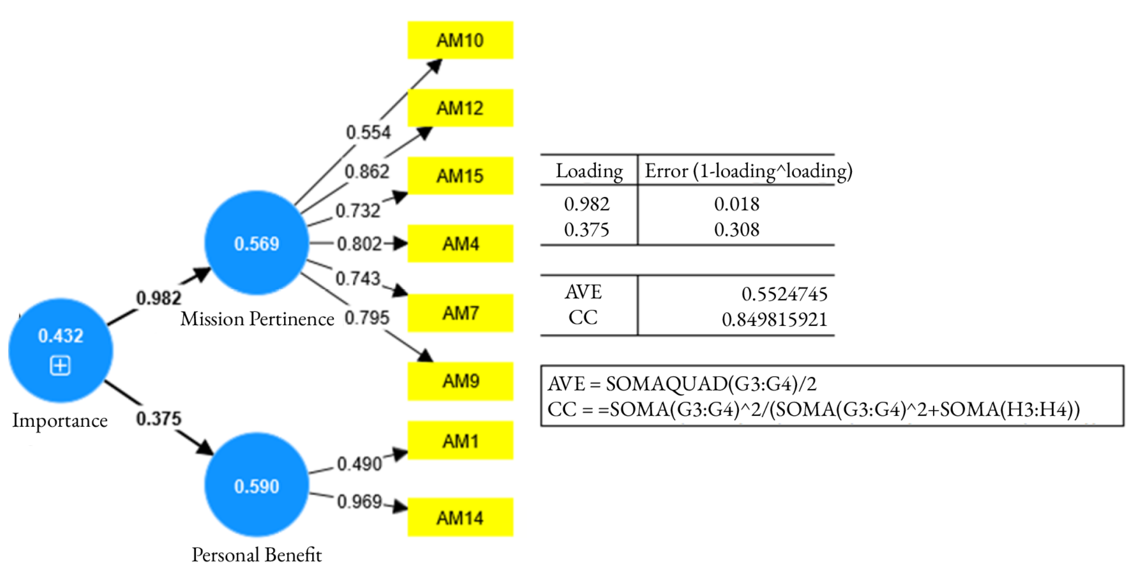
Figure 7 — Table with cross-factor loadings

	Ambiguity	Personal Benefit	Mission pertinence
AF10	0.734	-0548	-0.328
AF12	0.734	-0.316	-0.389
AF13	0.932	-0.391	-0.472
AF14	0.768	-0.264	-0.791
AF9	0.510	-0.371	-0109
IM1	-0.120	0.490	0.017
IM10	-0.551	0.199	0.554
IM12	-0.619	0.199	0.862
IM14	-0.512	0.969	0.213
IM15	-0.473	0.160	0.732
IM4	-0.484	0.167	0.802
IM7	-0.456	0.151	0.743
IM9	-0.401	0.026	0.795

Source: Elaborated by the authors, 2022.

The model has importance of the mission as a second-order latent variable measured as a formative model and a second-order domain, ground experience. We estimated the AVE (i.e., composite reliability) for the former. These calculations must be done by hand (or in an Excel table) as the software will do the calculations with observed repeated variables, rather than with first-order latent variable loadings (Figure 8).

Figure 8 — AVE and Composite Reliability calculation in the second-order latent variable



Source: Elaborated by the authors, 2022.

We avoided performing the HTHM test due to the absence of another latent variable measured as a reflective model from which it could differ. The presence of any such variable would require the test. For the ground experience domain, we observed multicollinearity between first-order domains (Table 4).

Table 4 — Quality indicators of latent variables and second-order domain

	VIF	CC	AVE
1) Importance of the mission	n/a	0.85	0.55
2) Ground experiences	1.32 – 1.36	n/a	n/a

Note: VIF = multicollinearity indicator; CC = composite reliability; Average variance extracted = mean variance extracted; n/a = not applicable

Source: Elaborated by the authors, 2022.

We found all values to be satisfactory, indicating that our adequate first-order variables (convergent validity) properly reflected second-order variables and generated reliable data (internal reliability) and that the formative construct had no unwanted correlations (multicollinearity). As these values were satisfactory, we analyzed structural models, testing the hypotheses of this study.

It is important to test collinearity before evaluating structural models. For this, we analyzed variance inflation factor (VIF) values for each latent variable in the structural model since the beginning of analysis. All values lie within those in Hair *et al*. (2017), i.e., below 5 (Table 5)

We used bootstrapping to investigate the significance of the indicators. It can be accessed in the top menu under "calculate." In the "PLS setup" tab, make sure to select "path" in "weighting scheme." Moreover, default settings can generally be maintained. The use of bootstrapping to analyze the significance of factorial loads obtained for observable variables is not only based on one estimation of the model, but also calculates estimates of parameters and their confidence intervals based on multiple estimates (HAIR *et al*., 2017; HAIR *et al*., 2017). The information of interest is in the "final results" topic of the bootstrapping analysis output.

Table 5 — Direct, specific indirect, and total effects

Effect	Structural Recovery	VIF	β	*t*	p
Direct	Function ambiguity → Importance of the mission	0.00	−0.74	8.41	<0.001
Direct	Ground experience → Function ambiguity	1.00	0.26	1.96	0.05
Direct	Ground experience → Importance of the mission	0.00	-0.10	0.94	0.35
Indirect	Ground experience → Function ambiguity → Importance of the mission	n/a	0.20	1.91	0.06
Total	Ground experience → Importance of the mission	n/a	0.11	0.72	0.47

Source: Elaborated by the authors, 2022.

The Student's t-test analyzes the hypothesis that correlation coefficients equal zero. Results above 1.96 reject hypotheses and show a significant correlation (HAIR *et al.*, 2017). Researchers should avoid considering values attributed to first-order latent variables. In the output, the results of interest are in the "final results" topic. Table 5 shows coefficient values between constructs and their Student's t-test.

We only observed a direct and statistically significant effect of function ambiguity on mission importance ($\beta = -0.74$; $p < 0.001$). This indicates that role ambiguity negatively predicts the perception of mission importance.

We observed the coefficient of determination (R^2) to evaluate the extent to which the model explained dependent variables. It was based on the analyses in Cohen (1988), which determines that values equal to 2%, 13%, and 25% are considered small, medium, and large, respectively. Analyses showed that function ambiguity (predicted by ground experience) obtained an $R^2 = 0.06$ (considered small) and that importance of the mission, an $R^2 = 0.51$ (considered large). This enables us to infer that the prediction model explains 51% of the importance given to the mission by military personnel (both regarding their perception of its value to their career and the mission itself). However, the explanation of function ambiguity by ground experience is very poor (about 6%), indicating to the researcher that other factors should be considered in a future model to explain the manifestation of this variable more comprehensively.

In addition to evaluating the magnitude of R^2 values as a criterion of predictive accuracy, it is necessary to evaluate the variable effect size (i.e., their explanatory importance in the model) by the Cohen indicator (f^2). This indicator evaluates whether the construct, when omitted, importantly impacts other endogenous constructs. F^2 values equal to 0.02, 0.15, and 0.35 are considered small, medium, and large effects, respectively (Cohen, 1988), of an exogenous latent variable. Results indicated that the relation Function ambiguity →Mission importance has a large effect size ($f^2 = 0.98$) and that Ground experience →Mission importance has a small effect size ($f^2 = 0.02$), as does Ground experience →Function ambiguity ($f^2 = 0.08$), understandable given the non-significance of these last two predictive relations. Function ambiguity constitutes an important exogenous variable for the model. R^2 and f^2 results can be accessed after the PLS-algorithm analysis request in the "quality criteria" topic of the analysis output.

The Stone Geisser indicator (Q^2) indicates the predictive relevance of a model. It evaluates the contribution of an exogenous construct to the Q^2 of an endogenous latent variable. It can be calculated by "blindfolding" or "PLS-predict," which is based on a series of interactions. SmartPLS4 performs only the latter (the third version of the software still does both). It can be chosen from the top menu under "calculate." In the output, the results of interest are in the "final results" topic (LV prediction sumary). Specifically, when a PLS-SEM model has predictive relevance, it accurately predicts the endogenous variables of the model. Values equal to or greater than zero indicate model accuracy (Table 6).

Table 6 — Stone-Geisser Indicator values for the endogenous variables of the model

Endogenous variables	MAE	Q^2_predict
Function ambiguity	0.82	0.04
Importance of the mission	0.83	0.00

Note: MAE = mean absolute error; Q^2 = Stone Geisser indicator.

Source: Elaborated by the authors, 2022.

This example of PLS-SEM estimation process only brought its main analyses to evaluate measurement and structural models[3]. We kept the database small and made a simple model so researchers who is still a novice at this statistical technique can use it under the free license of the software.

7 CONCLUSION

We sought to describe a multivariate statistical technique that can help military science researchers to propose new theories based on quantitative data. We hope this theoretical-methodological essay instigates other researchers to consider this exploratory approach to explain military science, international security, and defense phenomena. A robust approach to the attitudes determining individuals' behavior toward security perception, threat, power projection, and economic investments can benefit not only the understanding of our local reality but also the complexities of these phenomena.

3 The database can be requested from the first author of the article by e-mail.

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