

SMARTPLS 3: SPECIFICATION, ESTIMATION, EVALUATION AND REPORTING

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ABSTRACT

The structural equation modelling with partial least squares estimation (PLS-SEM) has been used in a wide variety of research areas, increasing exponentially the number of articles published using this method. There are several reasons for this to be happening, but one of them is the fact that the SmartPLS software facilitated the use of PLS-SEM. This article aims to present seven didactic examples with real data sets available to those who want to learn or teach PLS-SEM, dealing with such topics as measurement model evaluation, structural model evaluation, multicollinearity, second-order latent variable, mediation, moderation with numerical and categorical variables (MGA - multi-group analysis).

Keywords: Structural Equations Modeling, SmartPLS 3, Partial Least Squares.

INTRODUCTION

The structural equation modeling with partial least squares estimation (PLS-SEM) in the social sciences and behavior areas has been shown as an excellent possibility for the evaluation of relations among constructs (or factors, components, latent variables, unobserved variables, subscales, etc.), since it is robust to the lack of multivariate normality and is feasible for small samples (less than ~ 100 cases). These aspects are very present in the use of attitude scales. There is an alert that is worth repeating: do not justify using SmartPLS 3 only because the sample is small (GUIDE; KETOKIVI, 2015). The complexity of the model, the lack of multivariate normality of the data or the need to use constructs with formative indicator are other reasons to justify the use of PLS-SEM.

In addition, when collecting data with attitude scales it should be borne in mind that many responses will not be of good quality for a variety of reasons, and thus the minimum sample size (RINGLE et al., 2014a, 2014b) should be doubled or triplicate to prevent “low” quality data from jeopardizing the analysis and results.

PLS-SEM is a “flexible” technique capable of estimating complex models (many constructs, many variables, many causal relationships between constructs – arrows – and formative models), so it has a great “tuning” with field knowledge and the nature of the problems and data coming from human social relations.

It fits very well in situations where the theory that underlies causal relationships does not yet have great “sedimentation” and can be used in a more “exploratory” way. In this sense, the complexity of the problems and the social processes does not allow (yet) to have theories with a degree of generalisation as in other areas of knowledge, such as in Physics and Chemistry, for example, a fact that reinforces the use of the statistical technique in question.

The primary goal of this paper is to present some advanced and complementary techniques and to serve as reference material for those interested in learning, teaching and using the structural equation modelling with

partial least squares estimation (PLS-SEM), so all data and models were available in Bido and Silva (2019).

It should be noted that in Ringle et al. (2014a, 2014b) there are more general and primary explanations (formative and reflective indicators, endogenous and exogenous variables, sample size definition, use of the software, etc.) than the present article, in this sense, it is recommended as a preliminary reading.

The focus of this article is more on the use of SmartPLS 3 software than on previous activities and decisions (definitions, hypotheses, etc.). In this way, the present work was structured as seven examples, and to make the best use of this material, it is suggested a complete reading followed by the modelling of each example from the datasets (.csv or .txt).

Because SmartPLS 3 has many outputs and space in the articles is always very limited, formatting the results as explained in this article can be a useful exercise.

EXAMPLE 1 - CONFIRMATORY COMPONENT ANALYSIS (CCA)

In the structural equation modelling covariance based (LISREL, AMOS, EQS, SAS, Stata, lavaan) it is recommended to run the two-step analysis (ANDERSON; GERBING, 1988), first the CFA (confirmatory factor analysis), which is a model in which all the latent variables (VL) are correlated with each other, to evaluate the measurement model and then another model including the structural relations (hypotheses).

In the context of PLS-SEM this approach is not recommended because the algorithm is “partial” (the iteration occurs in stages: measurement → structural → measurement → .until there is the convergence, that is, the results of a step are practically equal the previous one). This means that if the two-step approach is used, it may happen that a suitable model is obtained in the first stage (CCA), but inadequate in the second step because the structural part is different from that used in the CCA. Thus, it is recommended to run the structural model directly in PLS-SEM, even if the measurement evaluation is done separately from the structural model.

Therefore, this model (CCA) has not been widely used, but it can be useful when the objective is only to evaluate the LV measurement model and to obtain factor scores for use in further analyses.

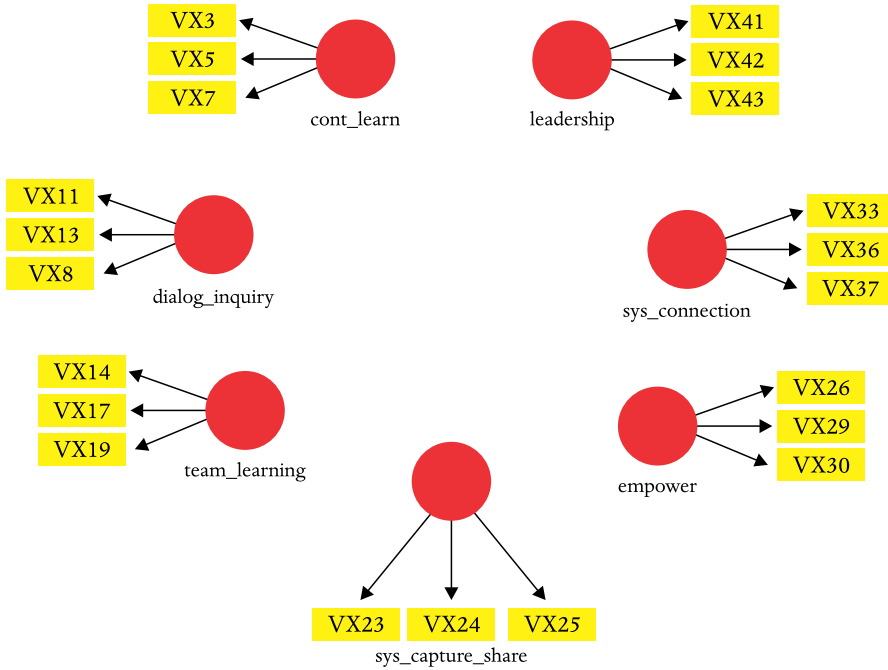
Specification

To exemplify confirmatory component analysis (CCA), the DLOQ (Dimensions of the Learning Organization Questionnaire) model of Marsick and Watkins was used, which has been replicated so many times that it had a special number in *Advances in Developing Human Resources* (v.15, n.2, 2013) and in Brazil the DLOQ-A (A of abbreviated) was validated, which instead of using six indicators by LV, uses three indicators by LV) by Menezes et al. (2011).

From this comment, it is concluded that SEM-CB (SEM covariance based, with software like LISREL, AMOS, EQS, Mplus and lavaan) is the most appropriate method, but it was decided to use this model as an example because the data were available and because it is an illustrative example

of the decisions that are made during the analysis (do not do this in your article - use PLS-SEM, when the correct would be SEM covariance based). In Figure 1 are the seven dimensions of DLOQ-A, which contents are explained in the article by Menezes et al. (2011, p.27-29).

Figure 1 Indicators by latent variable

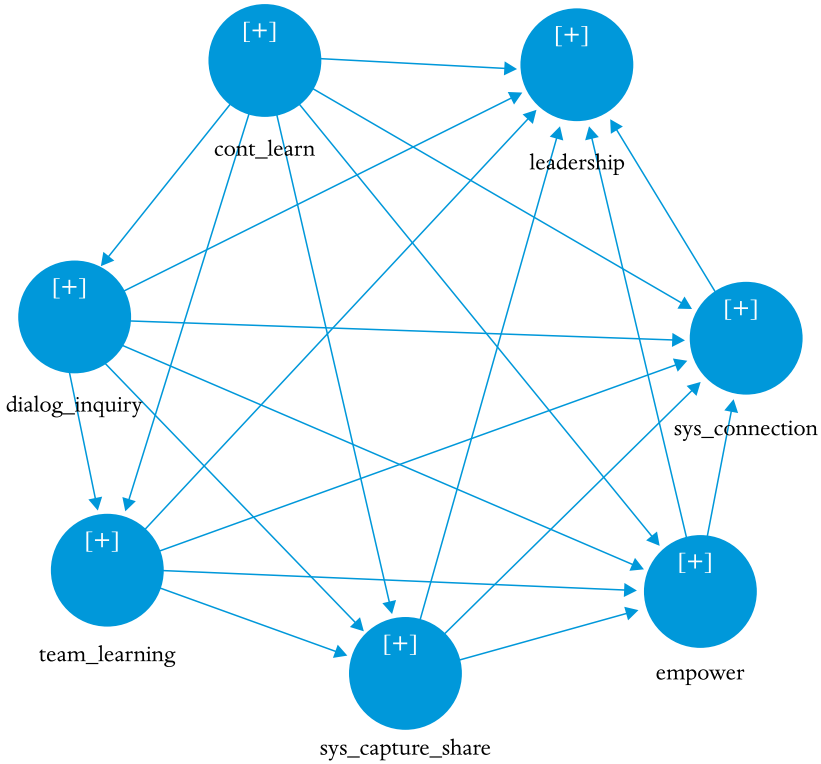


Note 1: Indicators available in Menezes et al. (2011).

Estimation

In the SEM-CB all exogenous LV are correlated by default, but in PLS-SEM it is necessary to include these relations (Figure 2), because the algorithm is “partial”, that is, it needs the measurement and structural relations to have the iterations (BIDO et al., 2010, p.252). The results presented in the arrows (path coefficients) will not be used at all in this analysis, therefore, no matter the sequence in which the LV is connected.

Figure 2 Connecting all latent variables to each other



Note 1: All LVs must be connected to all others, and although the direction of the arrows is not important here, there can be no feedbacks (non-recursive model). In this model it was started from the LV “cont_learn”, sending arrows to all the others, then “dialog_inquiry”, continuing counterclockwise until all LV have six arrows connected to them (arriving or leaving). Observed or measured variables (reflective indicators or scale items) were hidden (hide/show function) to make the figure clearer.

In the PLS algorithm we select the option “factor weighting scheme” (Figure 3) and from the output is analysed the correlations between the LV and the factor loadings (outer loadings and cross-loadings).

Figure 3 Weighting scheme in the PLS algorithm for the CCA

The screenshot shows the 'Weighting' tab in the SmartPLS 3 software. Under the 'Basic Settings' section, the 'Weighting Scheme' is set to 'Factor' (indicated by a selected radio button). The 'Maximum Iterations' is set to 300, and the 'Stop Criterion (10^{-X})' is set to 7.

Note: In the SmartPLS 3 Menu use: Calculate> PLS algorithm> Factor> Start calculation

The bootstrap is used to obtain the p-values of the correlations between the LVs and the factor loadings in SmartPLS 3 as follows:

- *Calculate > Bootstrapping > Complete bootstrapping (Figure 4) > Start Calculation*
- *Output of the Bootstrapping > Quality Criteria > Latent variable correlations (Note 2 in the footnote in Table 1)*
- *Output of the Bootstrapping > Final Results > Outer loadings (Footnote in Table 2)*

Figure 4 Bootstrapping to obtain the p-values

The screenshot shows the 'Weighting' tab in the SmartPLS 3.2.8 software. The 'Basic Settings' section is expanded, showing the following options:

- Subsamples:** 5000
- Do Parallel Processing:**
- Amount of Results:**
 - Basic Bootstrapping
 - Complete Bootstrapping

The 'Advanced Settings' section is also visible, showing:

- Confidence Interval Method:**
 - Percentile Bootstrap
 - Studentized Bootstrap
 - Bias-Corrected and Accelerated (BCa) Bootstrap
- Test Type:**
 - One Tailed
 - Two Tailed
- Significance Level:** 0,05

A callout box points to the 'Basic Bootstrapping' option with the text: "Basic option, when p-values of the correlations between the LVs are not necessary".

Note 1: In versions prior to SmartPLS 3.2.8 there were options for dealing with signal changes, which caused bimodality in bootstrapping results, but of the three options, two of them (no sign and individual sign changes) sometimes did not resolve or worsen the problem, so they have been withdrawn in the most current version.

Note 2: For each round of the bootstrapping algorithm, the results will be somewhat different (standard error, t-value, p-value) because it is based on random resampling and with replacement, but if a coefficient is significant ($p < 0.05$) this should not change from one round to another. Compare the p-values of Table 4 with yours (these are different rounds of bootstrapping).

Evaluation and reporting

In the CCA, only the measurement model (there is no structural model) is evaluated, what is done in the following section, based on the estimated model in the SmartPLS 3 software (RINGLE et al., 2015).

SmartPLS 3 produces several results, but some work is needed to format them. Two tables (Table 1 and 2) are required to evaluate the measurement model. The first is used for the analysis at the LV level and the second for the analysis at the indicator's level, it is recommended that they are evaluated simultaneously.

Table 1 was prepared as follows:

- *Output PLS algorithm > Quality Criteria:*
 - *Discriminant validity > Fornell-Larcker Criterion > Excel format*
 - Paste in an Excel spreadsheet
 - *Construct reliability and validity > Excel format*
 - Paste in the same Excel spreadsheet (anywhere)
 - Copy the reliability results, which were pasted > Right-Click (just below the correlation matrix) > Paste special > Transpose
 - Number the LVs and replace the names in the header with numbers.
 - Include note 1 in the footnote.

- *Output Bootstrapping > Quality Criteria:*
 - *Latent variable correlations*
 - Include note 2 in the footnote.

Table 1 Matrix of correlations between latent variables (n = 200)

| Latent variables | 1 | 2 | 3 | 4 | 5 | 6 | 7 |
|----------------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| 1 - team_learning | 0.831 | | | | | | |
| 2 - empower | 0.644 | 0.840 | | | | | |
| 3 - des_vis_sistem_org | 0.706 | 0.773 | 0.844 | | | | |
| 4 - sys_connection | 0.755 | 0.727 | 0.752 | 0.884 | | | |
| 5 - leadership | 0.673 | 0.758 | 0.740 | 0.742 | 0.831 | | |
| 6 - dialog_inquiry | 0.752 | 0.690 | 0.724 | 0.756 | 0.726 | 0.825 | |
| 7 - sys_capture_share | 0.663 | 0.675 | 0.717 | 0.662 | 0.648 | 0.675 | 0.868 |
| Cronbach's Alpha | 0.777 | 0.791 | 0.799 | 0.860 | 0.777 | 0.766 | 0.836 |
| rho_A | 0.778 | 0.793 | 0.812 | 0.865 | 0.784 | 0.766 | 0.840 |
| Composite reliability (CR) | 0.870 | 0.877 | 0.881 | 0.915 | 0.870 | 0.865 | 0.902 |
| Average Variance Extracted (AVE) | 0.691 | 0.705 | 0.713 | 0.781 | 0.690 | 0.680 | 0.753 |

Note 1: The values in the diagonal are the square root of the AVE.

Note 2: All correlations are significant at 1%.

Note 3: Here the three reliability measures were maintained to show the possibilities, but it is recommended to use composite reliability, as was done in Tables 5 and 7.

Table 2 was prepared as follows:

- *Output PLS algorithm > Quality Criteria:*
 - *Discriminant validity > Cross-loading > Excel format*
- Paste in an Excel spreadsheet (Figure 5)
 - Note that the indicators are listed in alphabetical order and not by LV, so the format in Figure 5b still needs to be rearranged.
 - Move the lines so that the indicators of the same LV stay together and the table should stand as a “ladder” (Table 2).
- *Output Bootstrapping > Final Results:*
 - *Outer loadings*
 - Include note 1 in the footnote.

Figure 5 Output PLS algorithm

| (a) SmartPLS 3 | | (b) Excel | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
|--|---------------|--------------|---------------|---------|------|-------|-------|------|-------|-------|------|--------------|-------|------|--------------|-------|------|--------------|-------|------|-------|-------|------|-------|-------|------|-------|-------|--|--|--|---------------|---------|------|-------|-------|------|-------|-------|------|--------------|-------|------|--------------|-------|------|--------------|-------|------|-------|-------|------|-------|-------|------|-------|-------|------|-------|--------------|------|-------|--------------|-----|-------|-------|------|-------|--------------|------|-------|-------|
| <p>Discriminant Validity</p> <p>Fornell-Larcker Criterion Cross Loadings</p> <table border="1"> <thead> <tr> <th></th> <th>team_learning</th> <th>empower</th> </tr> </thead> <tbody> <tr><td>VX11</td><td>0.631</td><td>0.656</td></tr> <tr><td>VX13</td><td>0.601</td><td>0.543</td></tr> <tr><td>VX14</td><td>0.866</td><td>0.560</td></tr> <tr><td>VX17</td><td>0.803</td><td>0.555</td></tr> <tr><td>VX19</td><td>0.824</td><td>0.484</td></tr> <tr><td>VX23</td><td>0.548</td><td>0.529</td></tr> <tr><td>VX24</td><td>0.611</td><td>0.618</td></tr> <tr><td>VX25</td><td>0.565</td><td>0.606</td></tr> </tbody> </table> | | | team_learning | empower | VX11 | 0.631 | 0.656 | VX13 | 0.601 | 0.543 | VX14 | 0.866 | 0.560 | VX17 | 0.803 | 0.555 | VX19 | 0.824 | 0.484 | VX23 | 0.548 | 0.529 | VX24 | 0.611 | 0.618 | VX25 | 0.565 | 0.606 | <table border="1"> <thead> <tr> <th></th> <th>team_learning</th> <th>empower</th> </tr> </thead> <tbody> <tr><td>VX11</td><td>0.631</td><td>0.656</td></tr> <tr><td>VX13</td><td>0.601</td><td>0.543</td></tr> <tr><td>VX14</td><td>0.866</td><td>0.560</td></tr> <tr><td>VX17</td><td>0.803</td><td>0.555</td></tr> <tr><td>VX19</td><td>0.824</td><td>0.484</td></tr> <tr><td>VX23</td><td>0.548</td><td>0.529</td></tr> <tr><td>VX24</td><td>0.611</td><td>0.618</td></tr> <tr><td>VX25</td><td>0.565</td><td>0.606</td></tr> <tr><td>VX26</td><td>0.588</td><td>0.823</td></tr> <tr><td>VX29</td><td>0.525</td><td>0.860</td></tr> <tr><td>VX3</td><td>0.612</td><td>0.651</td></tr> <tr><td>VX30</td><td>0.502</td><td>0.836</td></tr> <tr><td>VX33</td><td>0.650</td><td>0.699</td></tr> </tbody> </table> | | | team_learning | empower | VX11 | 0.631 | 0.656 | VX13 | 0.601 | 0.543 | VX14 | 0.866 | 0.560 | VX17 | 0.803 | 0.555 | VX19 | 0.824 | 0.484 | VX23 | 0.548 | 0.529 | VX24 | 0.611 | 0.618 | VX25 | 0.565 | 0.606 | VX26 | 0.588 | 0.823 | VX29 | 0.525 | 0.860 | VX3 | 0.612 | 0.651 | VX30 | 0.502 | 0.836 | VX33 | 0.650 | 0.699 |
| | team_learning | empower | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX11 | 0.631 | 0.656 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX13 | 0.601 | 0.543 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX14 | 0.866 | 0.560 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX17 | 0.803 | 0.555 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX19 | 0.824 | 0.484 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX23 | 0.548 | 0.529 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX24 | 0.611 | 0.618 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX25 | 0.565 | 0.606 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| | team_learning | empower | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX11 | 0.631 | 0.656 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX13 | 0.601 | 0.543 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX14 | 0.866 | 0.560 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX17 | 0.803 | 0.555 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX19 | 0.824 | 0.484 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX23 | 0.548 | 0.529 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX24 | 0.611 | 0.618 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX25 | 0.565 | 0.606 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX26 | 0.588 | 0.823 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX29 | 0.525 | 0.860 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX3 | 0.612 | 0.651 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX30 | 0.502 | 0.836 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |
| VX33 | 0.650 | 0.699 | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | | |

Table 2 Matrix of factor loadings (crossloadings) (n=200)

| Items | team_ learning | empower | sys_ connec- tion | leadership | cont_ learn | dialog_ inquiry | sys_ capture_ share |
|-------|----------------|--------------|-------------------|--------------|--------------|-----------------|---------------------|
| VX14 | 0.866 | 0.560 | 0.593 | 0.671 | 0.586 | 0.603 | 0.533 |
| VX17 | 0.803 | 0.555 | 0.624 | 0.641 | 0.574 | 0.633 | 0.631 |
| VX19 | 0.824 | 0.484 | 0.538 | 0.564 | 0.513 | 0.641 | 0.480 |
| VX26 | 0.588 | 0.823 | 0.654 | 0.609 | 0.685 | 0.591 | 0.658 |
| VX29 | 0.525 | 0.860 | 0.667 | 0.639 | 0.637 | 0.600 | 0.575 |
| VX30 | 0.502 | 0.836 | 0.621 | 0.578 | 0.578 | 0.543 | 0.452 |
| VX33 | 0.650 | 0.699 | 0.868 | 0.675 | 0.684 | 0.674 | 0.673 |
| VX36 | 0.435 | 0.592 | 0.807 | 0.518 | 0.508 | 0.494 | 0.577 |
| VX37 | 0.674 | 0.657 | 0.856 | 0.692 | 0.662 | 0.645 | 0.562 |
| VX41 | 0.651 | 0.639 | 0.632 | 0.872 | 0.612 | 0.652 | 0.600 |
| VX42 | 0.622 | 0.601 | 0.641 | 0.875 | 0.639 | 0.631 | 0.528 |
| VX43 | 0.724 | 0.683 | 0.717 | 0.904 | 0.713 | 0.718 | 0.623 |
| VX3 | 0.612 | 0.651 | 0.633 | 0.671 | 0.836 | 0.735 | 0.550 |
| VX5 | 0.448 | 0.608 | 0.539 | 0.577 | 0.813 | 0.449 | 0.402 |
| VX7 | 0.596 | 0.626 | 0.660 | 0.595 | 0.842 | 0.595 | 0.640 |
| VX11 | 0.631 | 0.656 | 0.696 | 0.623 | 0.634 | 0.790 | 0.655 |
| VX13 | 0.601 | 0.543 | 0.547 | 0.631 | 0.611 | 0.856 | 0.465 |
| VX8 | 0.624 | 0.491 | 0.528 | 0.613 | 0.542 | 0.827 | 0.530 |
| VX23 | 0.548 | 0.529 | 0.603 | 0.528 | 0.508 | 0.549 | 0.861 |
| VX24 | 0.611 | 0.618 | 0.672 | 0.583 | 0.598 | 0.626 | 0.887 |
| VX25 | 0.565 | 0.606 | 0.588 | 0.608 | 0.576 | 0.578 | 0.855 |

Note 1: All factor loadings are significant at 1%.

Note 2: High cross-loadings were formatted in red and italic.

With the results formatted in Tables 1 and 2, the evaluation of the measurement model is done in the following sequence (*):

- Convergent validity:
 - At the indicator's level: outer loading > 0.7 (Table 2)
 - At the LV level: AVE > 0.5 (Table 1)

- Discriminant validity:
 - At the LV level: $\sqrt{AVE} > r_{VL}$ (Table 1)
 - At the indicator's level: outer loadings > cross-loadings (horizontally and vertically in Table 2)
- Reliability
 - $CR > 0.7$ (Table 1)

(*) This sequence is suggested because one of the assumptions for the reliability assessment is that the construct is unidimensional, that is, its convergent and discriminant validity must be adequate, so if there is a problem of convergent or discriminant validity, it should not be continued to the reliability assessment.

Table 1 shows that for all LV, $AVE > 0.5$ and $\sqrt{AVE} > r_{VL}$, as well as $CR > 0.7$, therefore, the convergent validity, discriminant and reliability are adequate. However, the correlations between all LV are very high (about 0.65 to 0.75), which makes sense in the present model, since all LV are dimensions of the learning culture (MENEZES et al., 2011).

In Table 2 it can be observed that the factor loadings (in bold) are greater than the cross-loadings ("off-diagonal" loadings), confirming the discriminant validity, yet there are high cross-loadings (some of them about 0.7), which is consistent with the high correlations between LV (Table 1), but these high values raise some doubts:

- If the HTMT (heterotrait-monotrait ratio) matrix is used to evaluate the discriminant validity of this model, it is observed that some desattenuated correlations are greater than 0.85 (potential discriminant validity problem), but there are desattenuated correlations higher than 0.90, which indicates a lack of discriminant validity by this criterion (HAIR Jr. et al., 2016). This matrix is in the: *Output PLS algorithm > Discriminant Validity > heterotrait-monotrait ratio*. How does such a replicated scale still have this kind of problem? The focus of this article is not on the theoretical discussion of each model, but some answers would be:

- The LVs are organisational-level concepts, measured by individuals from the same organisation, so the unit of analysis would be the individual's perception of an organisational phenomenon, which is more homogeneous than if the unit of analysis were at the level of the organisations themselves (each case equals one organisation)
- The same person evaluating several constructs at the same time and with same assertive formats, there is a potential of the common method bias (CMB) (MACKENZIE; PODSAKOFF, 2012).
- Although the DLOQ and DLOQ-A are very replicated scales, in general, only Cronbach's alpha is analysed before the factor scores are generated by averaging the items. Both Menezes et al. (2011) and Yang (2003) had problems with full scale (DLOQ) when evaluating convergent and discriminant validity.
- These LV will be used in the next examples (structural models), then the consequences of keeping them separated or grouped will become more evident.

In this example, all factor loadings were high (greater than 0.8), but there are cases where recommended minimum values are not reached in the first round. Table 3 suggests some measures to improve the fit of the model.

Table 3 What to do when validity criteria are not met

| Results | Providence | Comment |
|--|--|---|
| Some loadings < 0.7 AVE > 0.5 CR > 0.7 | Keep the model | Whenever possible, it is recommended to maintain the maximum of indicators in the model so as not to jeopardise the validity of content [1] |
| Some loadings < 0.7 AVE < 0.5 CR > 0.7 | Delete indicator with lower loading and run again | These thresholds are not inflexible; sometimes it is better to keep more indicators, even with AVE just below 0.5 (LITTLE et al., 1999) |
| $\sqrt{AVE} < r_{VL}$ | Eliminating indicators with lower loadings (increases the AVE) | (i) If both providences are not enough, it is concluded that there is not discriminant validity between the LVs and it is decided to: (i) eliminate one of them from the model or |
| | Eliminating indicators with high cross-loadings (the correlation between the LV decreases) | (ii) Grouping them into a single LV, which may be inappropriate because it would require a revision of the conceptual definitions to maintain content validity. |

Note 1: When eliminating many indicators from the measurement, other problems can occur: chance capitalization raising doubts about the replicability of the results in a new sample, makes comparison with results of other studies unfeasible, and jeopardize the application of the scale in future studies (DEVELLIS, 2016; NETEMEYER et al., 2003). Hair Jr. et al. (2010, p.690) give a recommendation for SEM-covariance based, which applies to PLS-SEM: if the modification made in the model is not small (less than 20% of indicators were deleted), it should be replicated in another sample.

Legend: AVE = *average variance extracted*.

CR = *composite reliability*.

r_{VL} = *correlation between LV*.

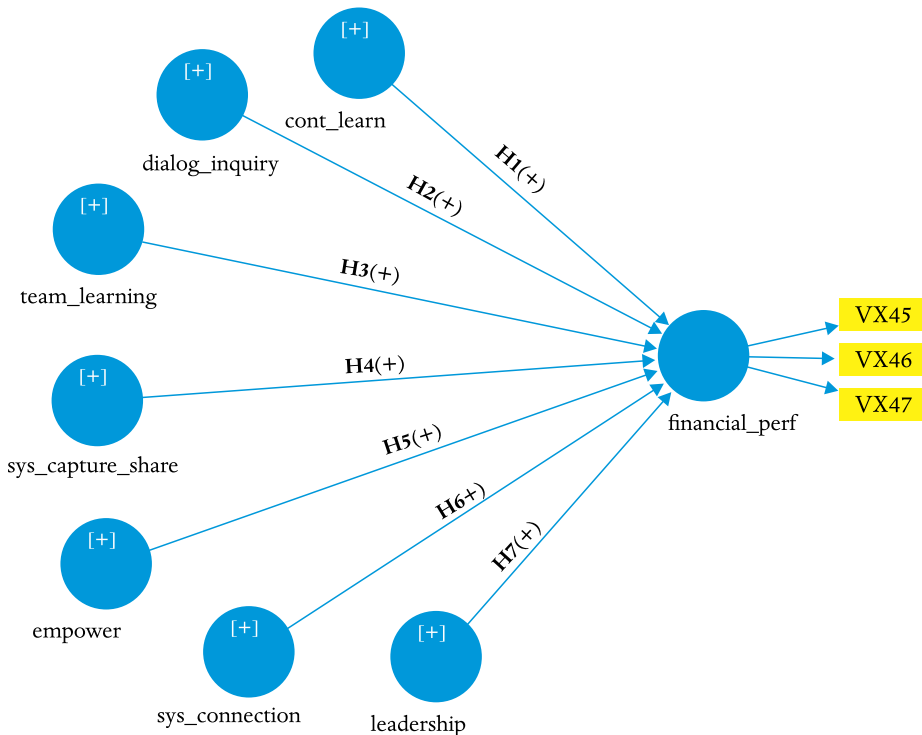
EXAMPLE 2 - SIMPLE STRUCTURAL MODEL

This example is based on the previous one, which was added a dependent variable, financial performance (Figure 6), there are now structural relationships (hypotheses H1 to H7).

Specification

DLOQ and DLOQ-A contain the seven dimensions used in Example 1 and two other performance dimensions, so the specification of the model presented in Figure 6 is based on the same theoretical framework (MENEZES et al., 2011).

Figure 6 Structural model

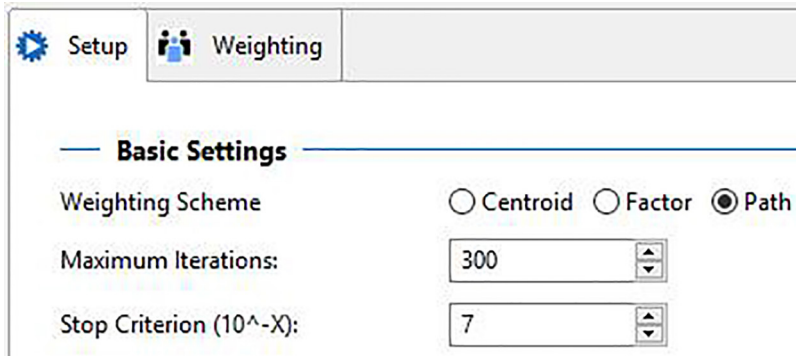


Note: Indicators available in Menezes et al. (2011).

Estimation

In the PLS algorithm, select the “path weighting scheme” (Figure 7), and from the output it will use the results: Collinearity Statistics (VIF), f Square and R square, to format the table with the results of the structural model (Table 4).

Figure 7 Weighting scheme in the PLS algorithm for the structural model

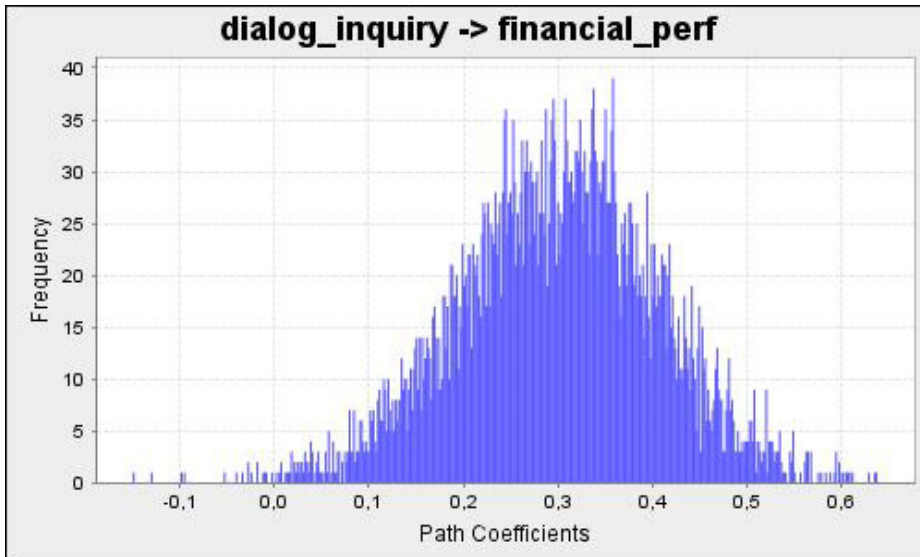


The bootstrapping algorithm is used in the same way as in Example 1 (Figure 4), and from the output it will use the results: Path coefficients and Path coefficients Histogram, to format the Table 4 with the results of the structural model.

Evaluation and reporting

The evaluation of the model should be done in two separate sections: (i) one for the measurement model (in the same way as was done in Exercise 1, but will not be presented here because of space constraints); (ii) and another for the structural model, which is the focus of this example.

Before starting the formatting of the results, it is necessary to evaluate if the bootstrapping histograms are unimodal (Figure 8), if they are not, we must go back to the beginning and assess the presence of outliers, indicators with little variability, binary indicators etc.

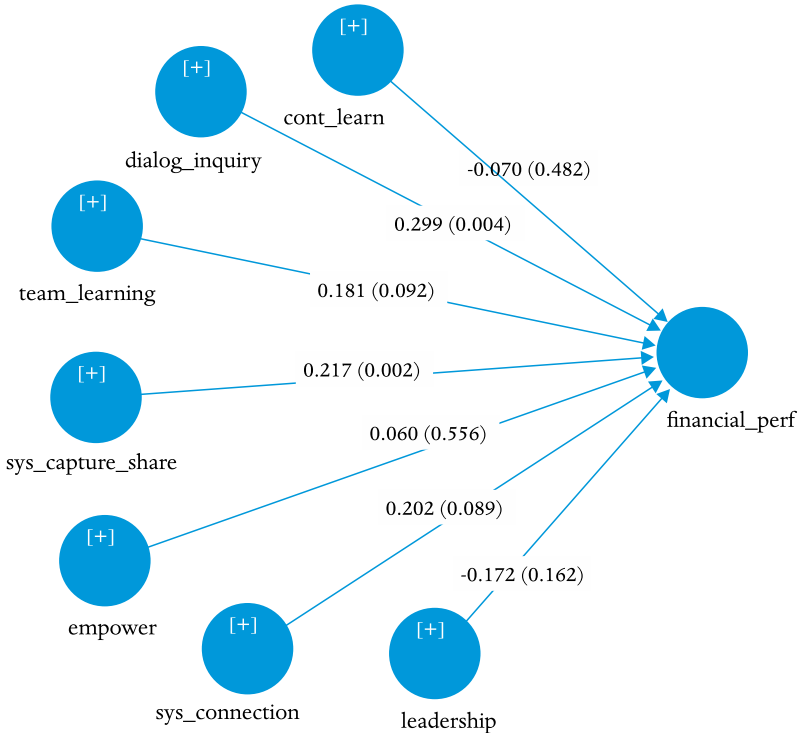
Figure 8 Histogram from bootstrapping

Note: A histogram for each structural coefficient is shown in bootstrapping output. If this chart presents bimodality, we must verify if there are outliers or LV measured by a few dichotomous indicators.

These graphs are presented in bootstrapping output: *Histograms > Path coefficients histograms*.

The results can be presented in the figure or table form. Figure 9 may be a good choice for presentation purposes in the form of PPT and group discussion, but for article it takes up a lot of space and contains little information (in SmartPLS 3 it is possible to select what should be displayed in the arrows and in the LV, for example, factor loadings, structural coefficients, t-value, p-value, R^2 or adjusted R^2). Table 4 is the recommended format for articles, dissertations, and theses.

Figure 9 Results of the structural model in bootstrapping



Note: Values outside the parentheses are standardised structural coefficients (betas), and the values within the parentheses are p-values (there is an option to present the t-values).

SmartPLS 3 contains many results of the structural model, to facilitate their presentation, it is recommended to format a table as follows:

- *Output Bootstrapping > Final Results:*
 - *Path coefficients > Excel format*
 - *Paste in an Excel spreadsheet*
 - Delete column “Sample Mean (M)”
 - Include columns for Hypothesis, VIF, f² and R² adjusted
- *Output PLS algorithm > Quality Criteria:*
 - Copy the results to the Excel spreadsheet (Table 4):

- *Collinearity Statistics (VIF) > Inner VIF Values*
- *f Square*
- Reorder the rows by grouping them by endogenous variable (unnecessary in this example because there is only one endogenous variable) and paste the adjusted R^2 values for each endogenous variable.
- Reorder the lines to put the hypotheses in a sequence.

With the results formatted in Table 4, it is easier to analyse them simultaneously, taking into account the following criteria:

- Multicollinearity
- If $VIF > 5$ consider excluding predictors or group them into a second-order LV (HAIR Jr. et al., 2016).
- Relative importance of predictors:
 - Effect size: $f^2 = 0.02 =$ small; $f^2 = 0.15 =$ medium; $f^2 = 0.35 =$ large (COHEN, 1988)
 - Structural coefficients (such as beta of the regression)
 - Correlations between exogenous and endogenous variables: comparing the correlations with the structural coefficients gives a more complete evaluation of the relative importance of the predictor.
- Explained variance of endogenous variables
 - $R^2 = 2\% =$ small; $R^2 = 13\% =$ medium; $R^2 = 26\% =$ large (COHEN, 1988)

Table 4 shows that only two of the seven hypotheses were confirmed ($p < 0.05$) and the effect size (f^2) is small in both relations, although the explained variance is large (adjusted $R^2 = 40.6\%$). The inconsistency between these results can be explained by multicollinearity, even if VIF is below 5:

- The correlations between the predictors and endogenous LV vary from 0.48 to 0.59 (values are very close to those shown in Table 5a), i.e., from the bivariate point of view all the predictors

Table 4 Results of the structural model (n=200)

| Structural relations | Hypothesis | VIF | F ² | Structural coefficient | Standard error | t-value | p-value | R ² adjusted |
|-------------------------------------|------------|-------|----------------|------------------------|----------------|---------|---------|-------------------------|
| cont_learn -> financial_perf | H1(+) | 3.281 | 0.003 | -0.070 | 0.102 | 0.692 | 0.489 | |
| dialog_inquiry -> financial_perf | H2(+) | 3.370 | 0.046 | 0.299 | 0.107 | 2.796 | 0.005 | |
| team_learning -> financial_perf | H3(+) | 3.020 | 0.019 | 0.181 | 0.108 | 1.684 | 0.092 | |
| sys_capture_share -> financial_perf | H4(+) | 2.510 | 0.033 | 0.217 | 0.072 | 2.997 | 0.003 | 0.406 |
| empower -> financial_perf | H5(+) | 3.231 | 0.002 | 0.060 | 0.101 | 0.590 | 0.555 | |
| sys_connection -> financial_perf | H6(+) | 3.660 | 0.019 | 0.202 | 0.118 | 1.708 | 0.088 | |
| leadership -> financial_perf | H7(+) | 3.531 | 0.015 | -0.172 | 0.124 | 1.383 | 0.167 | |

Note 1: p-values estimated by bootstrapping with 5000 repetitions.

Note 2: If the table has many columns and small font size, some simplifications can be made, for example: (i) delete the VIF column and include a footnote reporting only the largest value of VIF; (ii) exclude the t-value column and retain only p-value.

Note 3: This example does not have control variables, but if it had, it is recommended to present the results of 3 models: (1st) only with the control variables and the endogenous variables, (2nd) complete model with the variables control, (3rd) complete model without the control variables.

Legend: F² = effect size of Cohen (1988), VIF = variance inflation factor.

are important since any predictor alone explains approximately 25% of the endogenous LV variance.

- Although the correlation between the predictors and the endogenous variable were all positive and about 0.5, it can be seen in Table 4 that the structural coefficient in H7 was non-significant ($p > 0.05$) and its negative result indicates suppression, which is one of the symptoms of multicollinearity (COHEN et al., 2003).
- A VIF equal to 3.66 means that 72.7% of the variance of a predictor is explained by the other predictors (there is an overlap between them).
- The correlations between the predictors (Table 5a) range from 0.64 to 0.77, that is, higher than their correlations with the endogenous VL.

To address this inconsistency, Hair Jr. et al. (2016) recommend eliminating predictors or grouping them into a second-order VL, which was done by Menezes et al. (2011) and will be developed in the next example.

EXAMPLE 3 - STRUCTURAL MODEL WITH SECOND-ORDER LATENT VARIABLE (REPEATING INDICATORS)

From the empirical point of view, it has been observed in the previous examples that the seven LV of the DLOQ are highly correlated, and from the theoretical point of view the seven dimensions have to do with the learning culture, therefore, to use it as the common cause among the seven dimensions makes sense from both points of view.

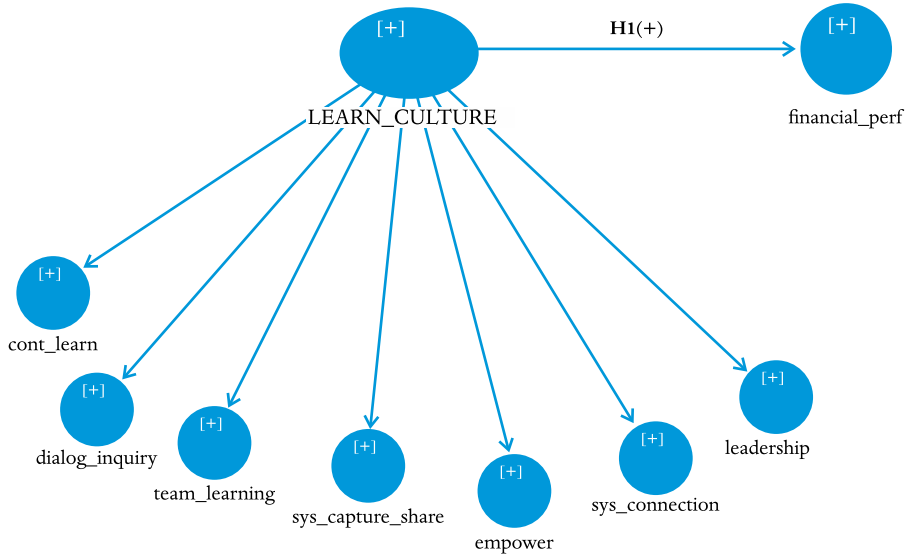
Specification

A second-order latent variable is measured by two or more first-order LVs and is thus modelled when using SEM based on covariance, but in the case of PLS-SEM, if the LV has no measured variables connected to it does not start the iterations. In these cases, one of the options is to reuse the indicators of the first-order LV in the second-order LV.

This option is recommended when the number of indicators per LV is approximately equal (in this example, the seven first-order LVs have three indicators each); otherwise, the LV that has more indicators will result in a larger factor loading simply because it has more repeated indicators in the second-order LV.

The relationships between the second-order LV and its dimensions (first-order LV) should be interpreted and used as factor loadings (not hypotheses). In this model, the only hypothesis (structural relationship) is between the learning culture and performance (Figure 10).

Figure 10 Specification of the structural model in SmartPLS 3



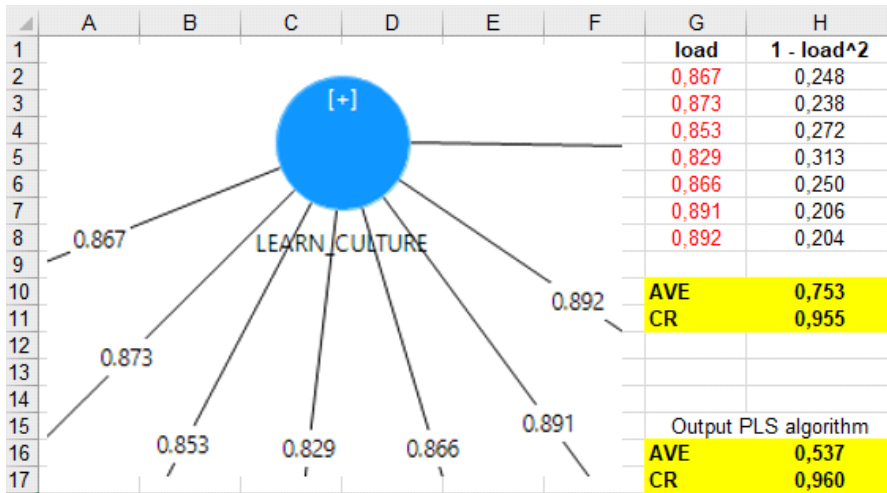
Note 1: Learning Culture is a second-order LV.

Note 2: The LV Learning Culture contains 21 indicators (the indicators of the 7 LV were repeated in it), but were hidden to make it easier to see the model.

Estimation

The estimation (PLS algorithm and bootstrapping) is done exactly as was done in example 2, but a care that must be taken is that the relationships between the second-order VL and its first-order LV will be in the output of structural relations (path coefficients), so a formatting job is required (to separate these results), as well as to calculate AVE (average variance extracted) and CR (composite reliability) by hand, because SmartPLS 3 does these calculations with the indicators that were repeated in the second-order LV (Figure 11).

Figure 11 AVE and CR calculation for the second-order LV in the Excel spreadsheet



Note: To calculate the AVE = H10 = SUMSQ(G2:G8)/7
 To calculate the CR = SUM(G2:G8)^2/(SUM(G2:G8)^2+SUM(H2:H8))

Evaluation and reporting

For models with second-order LV, it is recommended to present the results in three steps: (i) measurement model of the first-order LV (as was done in Tables 1 and 2), (ii) measurement model of the LVs that are in the structural model (in Table 5), (iii) structural model as was done in Table 4 (below, in Table 6).

The formatting of the tables is done in the same way as was done in the previous examples, but now has one more step, which is explained below:

- *Output PLS algorithm > Quality Criteria:*
- *Discriminant validity > Fornell-Larcker Criterion > Excel format*
 - Paste in the Excel spreadsheet and include the AVE and CR values as done in the previous examples, pass the endogenous variables to the end of the table (last row and column on the right).
 - Copy and paste this table into another Excel spreadsheet

- In the first table: delete the second-order LV
- In the second table: remove the first-order LVs that were used to measure the second-order LV and correct the AVE values (square root of the AVE in the diagonal) and the CR for the second-order LV.

Table 5 Matrix of correlations between LV's (n = 200)

| (a) First-order LV | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 |
|----------------------------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|--------------|
| 1 - team_learning | 0.832 | | | | | | | |
| 2 - deleg_pod_resp | 0.643 | 0.840 | | | | | | |
| 3 - empower | 0.704 | 0.772 | 0.844 | | | | | |
| 4 - sys_connection | 0.754 | 0.726 | 0.751 | 0.884 | | | | |
| 5 - leadership | 0.671 | 0.757 | 0.738 | 0.742 | 0.831 | | | |
| 6 - cont_learn | 0.752 | 0.688 | 0.721 | 0.755 | 0.723 | 0.825 | | |
| 7 - sys_capture_share | 0.662 | 0.674 | 0.716 | 0.661 | 0.647 | 0.672 | 0.868 | |
| 8 - financial_perf | 0.549 | 0.508 | 0.559 | 0.477 | 0.471 | 0.588 | 0.565 | 0.885 |
| Composite reliability (CR) | 0.870 | 0.878 | 0.882 | 0.915 | 0.870 | 0.865 | 0.902 | 0.915 |
| Average variance extracted (AVE) | 0.692 | 0.705 | 0.713 | 0.781 | 0.690 | 0.681 | 0.753 | 0.782 |

| (b) LV of the structural model | 1 | 2 |
|----------------------------------|--------------|--------------|
| 1 - LEARN_CULTURE | 0.868 | |
| 2 - financial_perf | 0.612 | 0.885 |
| Composite reliability (CR) | 0.955 | 0.915 |
| Average variance extracted (AVE) | 0.753 | 0.782 |

Note 1: The values in the diagonal are the square root of the AVE.

Note 2: All correlations are significant at 1%. This information is displayed in the bootstrapping output when the "complete" option is run.

Note 3: Culture_Apren is a second-order LV.

In order to evaluate the cross-loadings (as was done in Table 2), the second-order LV and the repeated indicators should be excluded. It was not presented here due to space constraints.

The structural model is now quite simple, although at first glance it seems that the inclusion of second-order LV would increase the complexity of the model. The results are presented in Table 6.

Table 6 Results of the structural model (n = 200)

| Structural relation | f ² | Structural coefficient | Standard error | t-value | p-value | R ² |
|------------------------------------|----------------|------------------------|----------------|---------|---------|----------------|
| LEARN_CULTURE -> financial_perf | 0.597 | 0.612 | 0.046 | 13.187 | 0.000 | 0.374 |

Note: p-values estimated by bootstrapping with 5000 repetitions.

In this example, the seven dimensions of the DLOQ-A were used to measure the learning culture, and this variable explained 37.4% of the variance of the performance, confirming the only hypothesis proposed (remembering that in this model, the other relationships are measurement).

When the number of indicators/LV is equal for all LVs (as in this example), the approach of the repeated indicators can be used, but when the quantities of indicators/LV in the first-order LV are very different, this approach is not recommended because the first-order LV that has more indicators will result in a stronger relationship with the second-order LV (factor loading), simply because it had more repeated indicators in the second-order LV, and the LV that has fewer indicators, will have a lower factor loading.

When the number of indicators/VL varies, it is recommended the two-step approach to model second-order LV, which will be presented in the next example.

EXAMPLE 4 - STRUCTURAL MODEL WITH SECOND-ORDER LATENT VARIABLE (TWO STEPS APPROACH)

This option must be chosen to model second-order LV when the number of indicators per LV is very different (in first-order LVs). It is necessary to obtain the first-order LV factor scores, to save these scores in the original data set, to import them into SmartPLS 3 and to model the second-order LV as if it were a first-order LV, using these scores for its measurement.

Specification

For this example, the model of example 1 was run, and the factor scores were copied/pasted to the original data set. These scores are in the Output PLS algorithm:

- *Final results > Latent variable > Latent variable*

Other possibilities for generating the factor scores of each first-order LV are:

- To perform a principal component analysis (PCA) for each LV, to evaluate if the indicators are with adequate loadings and must be kept in the model, to generate the factor score in the PCA itself;
- Using an older method (summated rating scales), which consists of generating the score for each LV as the average of its indicators. A previous analysis of Cronbach's alpha or PCA's for each LV can help decide whether to maintain all indicators to obtain the scores or not. This procedure can also be related to the literature on "item parcels" (LITTLE et al., 2002).

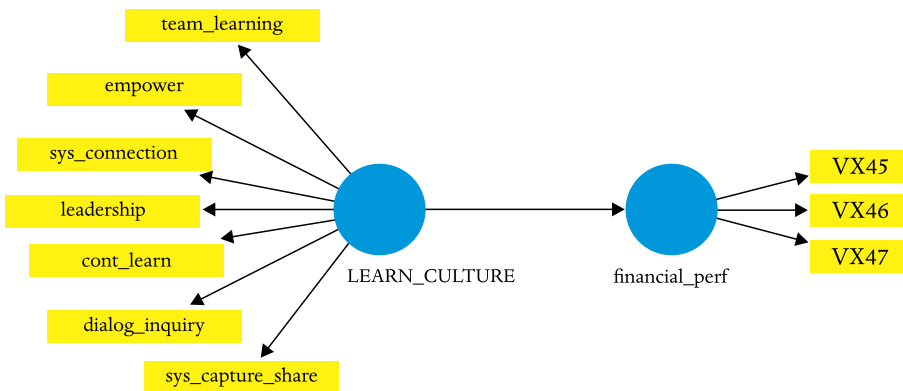
Sometimes in the copy and paste action formatting problems can occur (UK and USA format use dot as decimal point and in Brazilian many European countries use comma), if this occurs, a simple solution is to copy from SmartPLS 3 (click in "Excel Format") and paste in the notepad and to replace the dots by commas, and then copy/paste to Excel. Save as .csv (character separated by comma) and import it into SmartPLS 3: right-click

on project name > import data file > ...> right-click on dataset name > Select Active Data File.

Another option is to use Excel features to import data: Paste > Use Text Import Wizard > My data has headers > Next > Tab > Next > Advanced > Decimal separator = dot; Thousands separator = comma > Ok > Finish.

Comparing Figure 12 with Figure 10 it is observed that the structural model is the same; only the measurement of the second-order LV is different.

Figure 12 Structural model with second order LV modelled in two steps



Note 1: Learning Culture is a second order LV.

Note 2: The indicators of LV learning culture are factor scores saved in the first step, in the confirmatory component analysis.

Estimation

At this point, there is no novelty; the estimation (PLS algorithm and bootstrapping) was the same as example 2.

Evaluation and reporting

As in Example 2, the results were formatted into two tables for the measurement model (Table 7a and 7b) and a table for the structural model (Table 8), which are presented following.

Table 7 Results of the measurement model (n = 200)

| (a) Indicators | LEARN_CULTURE | financial_perf |
|----------------------------------|---------------|----------------|
| team_learning | 0.857 | 0.549 |
| empower | 0.863 | 0.508 |
| sys_connection | 0.892 | 0.560 |
| leadership | 0.883 | 0.477 |
| cont_learn | 0.864 | 0.472 |
| dialog_inquiry | 0.881 | 0.589 |
| sys_capture_share | 0.834 | 0.565 |
| VX45 | 0.650 | 0.894 |
| VX46 | 0.485 | 0.895 |
| VX47 | 0.464 | 0.864 |
| (b) Latent variables | LEARN_CULTURE | financial_perf |
| LEARN_CULTURE | 0.868 | |
| financial_perf | 0.616 | 0.885 |
| Composite reliability (CR) | 0.955 | 0.915 |
| Average variance extracted (AVE) | 0.753 | 0.782 |

Note: Panel (a) = crossloading matrix

Panel (b) = matrix of correlations between the LV, with the square root of the AVE in the diagonal.

Table 8 Structural model results (n=200)

| Structural relation | f ² | Structural coefficient | Standard error | t-value | p-value | R ² |
|---------------------------------|----------------|------------------------|----------------|---------|---------|----------------|
| LEARN_CULTURE -> financial_perf | 0.613 | 0.616 | 0.044 | 13.959 | 0.000 | 0.380 |

Since all first-order LVs had three indicators (equal quantity of indicators/LV), the approach of repeating first-order LV indicators in second-order LV and the two-step approach yielded identical results for practical purposes (R^2 equal to 0.374 and 0.380, respectively).

Both approaches solved the problem of multicollinearity found in example 2, requiring a modification in the conceptual model: to define the second-order LV and to revise the hypothesis (structural relation).

This procedure (grouping multicollinear variables) is recommended by Hair Jr. et al. (2016, position 4541), but also uses the same logic of what is known as principal components regression (COHEN et al., 2003, p.428).

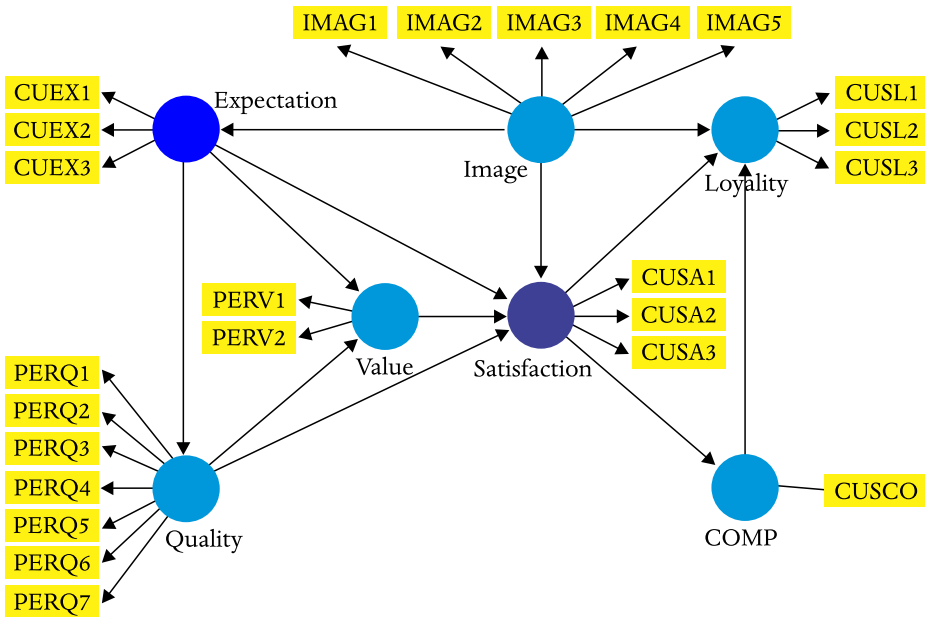
EXAMPLE 5 - STRUCTURAL MODEL WITH MEDIATION (DIRECT, INDIRECT AND TOTAL EFFECTS)

Examples 5 and 6 are based on the European Customer Satisfaction Index (ECSI) model, whose data and design are available on the SmartPLS 3 website (RINGLE et al., 2015) in the “Resources> SmartPLS Project Examples” tab. This example is already a “classic” because since 2005 it has been used for the teaching of PLS-SEM and has as reference the article by Tenenhaus et al. (2005).

Specification

This example will not be modified in any way (Figure 13), only the way in which the software estimates the indirect and total effects will be presented, so that it is possible to evaluate if the mediation is full (when indirect effect is significant but direct is null) or partial (when indirect and direct effects are significant).

Figure 13 ECSI model - direct and indirect effect of Expectation on Satisfaction



Source: Ringle et al. (2015).

Note 1: Direct effect: *Expectation* → *Satisfaction*

Indirect effect: *Expectation* → *Value* → *Satisfaction*

Indirect effect: *Expectation* → *Quality* → *Value* → *Satisfaction*

Indirect effect: *Expectation* → *Quality* → *Satisfaction*

Note 2: Expectation and Satisfaction are in different colour only to highlight that, in this example, the focus of the analysis is in the relationships (direct, indirect and total) between them.

Estimation

Strictly speaking, the measurement model and then the structural model should be evaluated. By limiting space, no adjustment will be made to the measurement model (on the one hand, if the objective is to compare the index - satisfaction score - from one survey to another, it is necessary that the measurement model be the same - configural invariance - and, on the other hand, if the analyzes presented in Example 1 are performed,

severe problems of convergent and discriminant validity will be identified, see for yourself).

For the purpose of this example, consider the following situation: the path coefficient between Expectation and Satisfaction is not significant (0.063, $p > 0.20$), so does Expectancy not influence Satisfaction?

Evaluation and reporting

To evaluate whether there is mediation and whether it is total or partial, direct, indirect and total effects are evaluated, as shown in Table 9.

Table 9 Mediation, direct and indirect effects

| Direct effect | Indirect effect | Mediation |
|--------------------------------|--------------------------------|-----------------------|
| Significant ($p < 0.05$) | Not significant ($p > 0.05$) | There is no mediation |
| Significant ($p < 0.05$) | Significant ($p < 0.05$) | Partial mediation |
| Not significant ($p > 0.05$) | Significant ($p < 0.05$) | Full mediation |

The formatting of Table 10 is made from the bootstrap results, highlighting that the amount of results (indirect effects) is large, so the work is more to select those that interest:

- *Output Bootstrapping > Final Results:*
 - *Path coefficients > Excel format*
 - Paste into an Excel spreadsheet
 - *Specific indirect effects > Excel format*
 - Paste into an Excel spreadsheet
 - *Total effects > Excel format*
 - Paste into an Excel spreadsheet
 - Copy/paste the necessary lines
 - Exclude the column “*Sample Mean (M)*”

Table 10 Specific indirect effects (detailed)

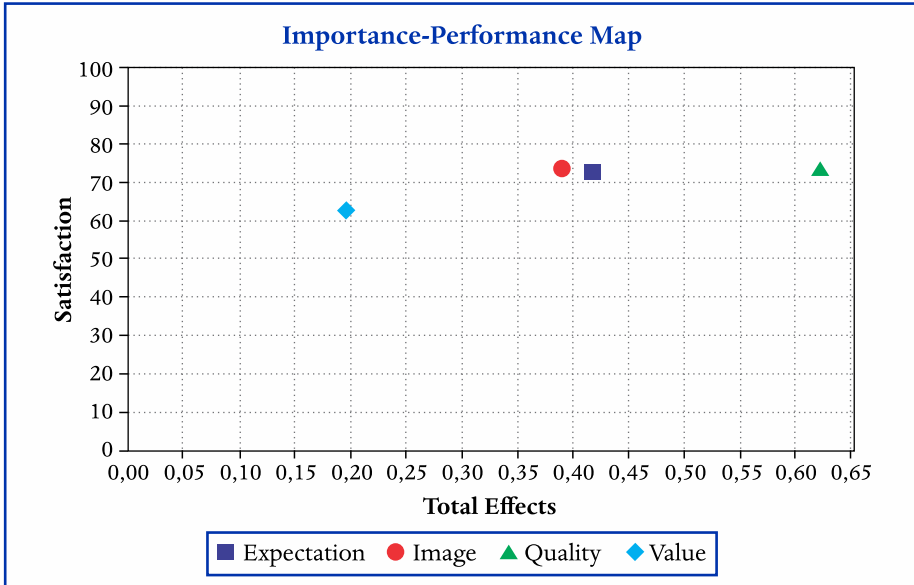
| | Effects | Coefficient | Standard error | t-value | p-value |
|----------|---|-------------|----------------|---------|---------|
| Direct | Expectation -> Satisfaction | 0.063 | 0.050 | 1.25 | 0.213 |
| Indirect | Expectation -> Quality -> Satisfaction | 0.285 | 0.044 | 6.41 | 0.000 |
| Indirect | Expectation -> Quality -> Value -> Satisfaction | 0.061 | 0.022 | 2.75 | 0.006 |
| Indirect | Expectation -> Value -> Satisfaction | 0.010 | 0.017 | 0.57 | 0.566 |
| Total | Expectation -> Satisfaction | 0.418 | 0.058 | 7.24 | 0.000 |

Note: In the bootstrap output the specific indirect effects option displays the results of all indirect effects, as in this table. The total indirect effects option is less detailed and shows only the total indirect effect (0.355, $p < 0.001$).

Responding to the question posed at the beginning of section 5, Expectation does not have a direct effect on Satisfaction, but has an indirect effect (0.355, $p < 0.001$), that is, it is a total mediation, so it is important to promote satisfaction.

The results can be complemented with Figure 14, which relates the total effects (importance) to performance (mean scores on a scale of 0 to 100). Here it is explicit that expectation, although not having a significant direct effect, has an important total effect, and only lags behind perceived quality in terms of priority, which can be improved from a score of 73 to 100.

Figure 14 Importance-performance map (or Priority map)



Note: To get this chart:

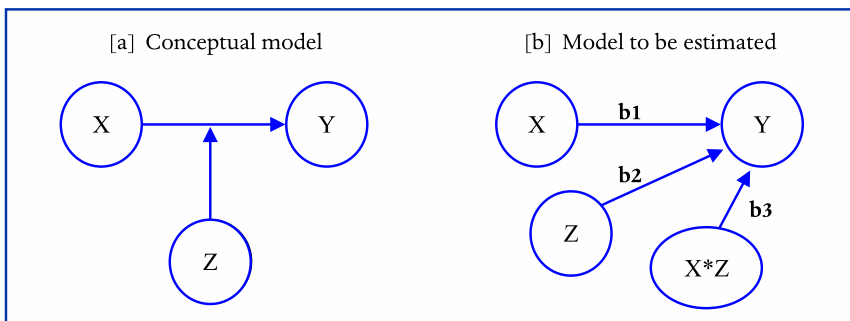
Calculate > Importance-Performance... > Select the LV Satisfaction > Start calculation.

The coordinates of each point can be obtained in the output in Final results > Performance / Index.

EXAMPLE 6 - STRUCTURAL MODEL WITH MODERATION OF A CONTINUOUS VARIABLE

A moderating variable strengthens or weakens the relationship between an independent variable (IV or predictor) and a dependent variable (DV or criterion or endogenous). This moderator variable can be continuous (at least interval or considered as such) or categorical. For the first case, follow this example (Figure 15), and for the case of categorical moderator follow the example 7 (MGA - Multi-group analysis).

Figure 15 Representation of the moderator variable



Note: To understand the need for the multiplicative term, simply compare the models with and without moderation:

Without moderation: $y = a + b_1x \rightarrow$ se $x = 0, y = a$

With moderation: $y = a + b_1x + b_2z + b_3xz \rightarrow$ se $x = 0, y = a + b_2z \rightarrow b_2$ moves the line vertically.

Without moderation: $y = a + b_1x \rightarrow \frac{\partial y}{\partial x} = b_1$

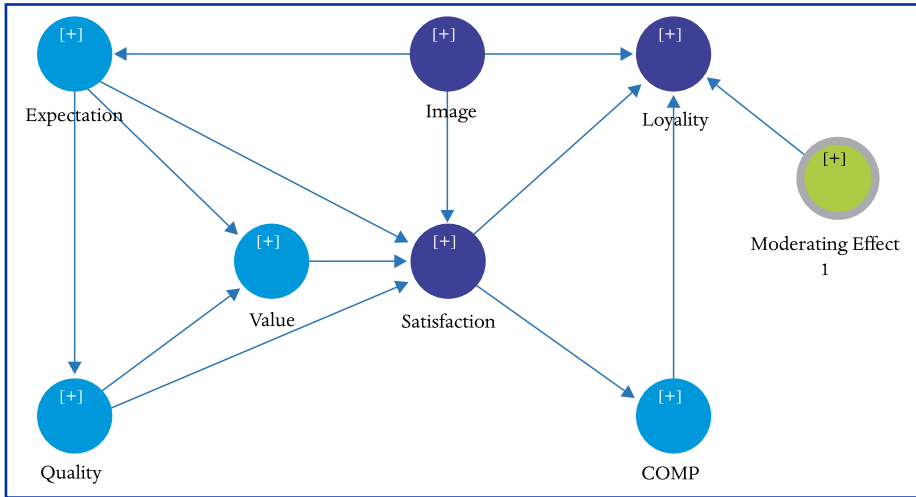
With moderation: $y = a + b_1x + b_2z + b_3xz \rightarrow \frac{\partial y}{\partial x} = b_1 + b_3z \rightarrow b_3$ changes the slope of the line.

Specification

The relationship between IV and DV may be positive or negative and the moderating variable may weaken or strengthen this relationship, Gardner et al. (2017) present several examples that may be useful to understand how a moderating variable would be justifiable in a model.

The model to be used in this example is the same ECSI, including a moderating effect of the Image on the relationship between Satisfaction and Loyalty, as was done in the presentation of the XLSTAT-PLSPM software (2017) and is shown in Figure 16.

Figure 16 Moderating effect of the Image on the Satisfaction-Loyalty relationship



Note 1: To create the multiplicative term in SmartPLS 3: Right-click on the dependent variable> Add Moderating Effect> Select the moderator variable and the independent variable> Select the calculation method (*)> Ok.

(*) The “orthogonalization” method is suggested because it guarantees that there will be no multicollinearity between the multiplicative term and the independent and moderating variable.

Note 2: Image, Satisfaction, and Loyalty are in different colour only to highlight that, in this example; the focus of the analysis is in the relationships (direct and moderate) among them.

Estimation

The estimation of this model is performed in the usual way, as is done in any model and as presented in the model of example 5. When specifying the multiplicative term in the previous step, SmartPLS 3 generates a sim-

ple slope analysis, which contains three lines: one for the average value of the moderator and another two with a standard deviation above and below the average.

For v.2 of SmartPLS, or other software that does not have this graph, it can be generated from the results of the bootstrap (structural coefficients) and the worksheets developed by Dawson (2014), which are recommended by Hair Jr. et al. (2016).

Evaluation and reporting

The result of the moderating effect is included in the structural model evaluation table, as was done in Tables 4, 6 and 8. Only the result of the moderating effect was shown in Table 11 because of space constraint.

Table 11 Results of the structural model

| Structural relation | Gardner et al. (2017, p.614) | f ² | Structural coefficient | Standard error | t-value | p-value |
|--------------------------|------------------------------|----------------|------------------------|----------------|-------------|--------------|
| Moderating Effect | | | | | | |
| 1 -> Loyalty | XZ | 0.030 | -0.103 | 0.036 | 2.88 | 0.004 |
| Satisfaction -> Loyalty | X | 0.193 | 0.468 | 0.085 | 5.48 | 0.000 |
| Image -> Loyalty | Z | 0.032 | 0.184 | 0.078 | 2.36 | 0.018 |
| COMP -> Loyalty | | 0.007 | 0.072 | 0.057 | 1.26 | 0.206 |

Legend: X = Independent variable; Z = Moderator variable; XZ = multiplicative term or term of interaction.

Note 1: Gardner et al. (2017, p.614) assist in the interpretation of the moderation results from the X, Z, and XZ signals.

Note 2: Incomplete table; it includes just the structural relations with loyalty (adjusted R² = 46.4%), which is the focus of this example.

As was quoted in Example 2, to evaluate the effect size of the structural coefficients is used the Cohen (1988) classification: f² = 0.02 = small; f² = 0.15 = medium; f² = 0.35 = large. However, when it comes to the moder-

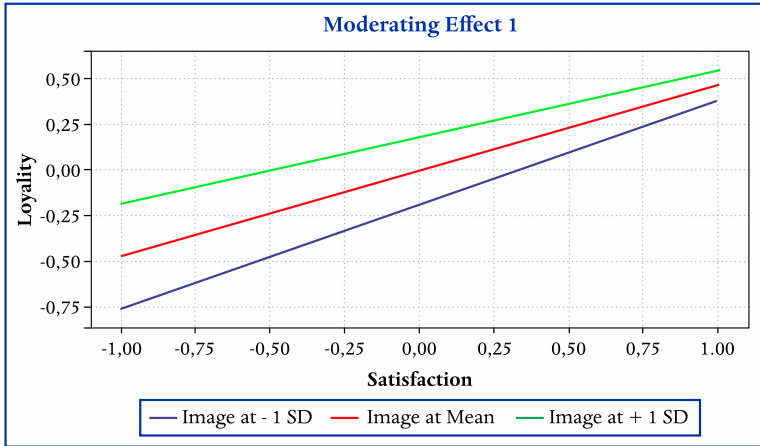
ating effect, Hair Jr. et al. (2017) suggest the classification of Kenny (2015): $f^2 = 0.005 = \text{small}$; $f^2 = 0.010 = \text{medium}$; $f^2 = 0.025 = \text{large}$. Therefore, the moderating effect in this example is significant and large.

Another important result of the moderating effect is the Figure 17a:

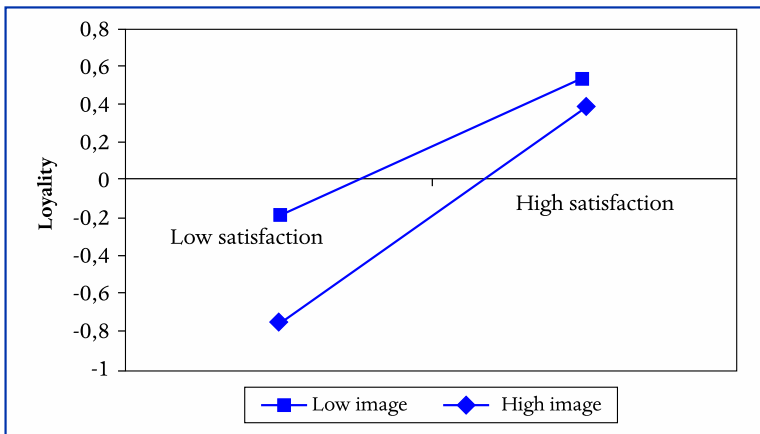
- the upper (green) line represents the relationship between satisfaction and loyalty when the image has high values (1 standard deviation above the mean). For high image values, the satisfaction-loyalty relationship is weaker. According to Gardner et al. (2017, p.614): “Weakening: Z moderates the positive (negative) relationship between X and Y, so that the relationship becomes weaker as Z increases.”
- the bottom line (blue) represents the relationship between satisfaction and loyalty when the image has low values (1 standard deviation below the mean). For low image values, the satisfaction-loyalty relationship is stronger.
- Figure 17b contains the same graph as Figure 17a, but may be more suitable than the first in the case of Black & White articles. To generate Figure 17b, the structural coefficients of Table 11 were entered in Dawson’s “two-way interactions – standardized” worksheet (2014).

Figure 17 Graph of the moderating effect of the Image on the Satisfaction-Loyalty relation

(a) Graph generated in SmartPLS 3 when including a moderator variable



(b) Graph generated with the structural coefficients of Table 11 and Dawson worksheet (2014)



Note 1: Graph 17a is generated in SmartPLS 3 and is presented in the output of the PLS algorithm in the tab: Final Results > Simple slope analysis.

Note 2: The structural coefficients of Table 11 were entered in Dawson’s two-way interactions - standardized worksheet (2014) to provide graph 17b.

Note 3: The inclusion of quadratic effects in SmartPLS 3 is done similarly to the interaction term, but the software does not generate the graph for quadratic effect. It can be prepared with one of Dawson’s worksheets (2014).

EXAMPLE 7 - STRUCTURAL MODEL WITH MODERATION OF A CATEGORICAL VARIABLE – MGA

This type of analysis is used when there is a priori a variable that will be used to define the groups to be compared (observed heterogeneity), for example, gender, country, sector, etc.

The model used in this example remains the ECSI, but the data used are those available in the package `plspm` of the software R (SANCHEZ, 2013). They are from a Spanish research, which includes the gender variable and will be used as a categorical moderator in this example. To obtain the data, install the R software and run the following script:

```
install.packages("plspm", dep=T)
library(plspm)
data(satisfaction)
write.csv(satisfaction, "ECSI_mga.csv", row.names=F)
getwd() # to see in which folder the .csv file was saved
```

Specification

The structural model is the same as in Figure 13, except that there is no LV Complaint, and now the gender variable will be used as a categorical moderator in the multi-group analysis (MGA).

In this type of analysis the objective can be: (i) to show that the measurement model is invariant (or equivalent) between the groups, in the sense that the same construct is measured equally in different groups (MILLSAP, 2011), (ii) to assess if the relations between the constructs (structural coefficients) vary depending on the group (HAIR JR et al., 2016).

Estimation

The modelling is done in SmartPLS 3 like the previous ones but must be added the information of which variable will be used as a categorical moderator, which will define the groups to be compared. To do this, just do as in Figure 18: double-click on the data set icon > Generate data groups > Select the variable "gender" > Ok.

Figure 18 Defining the groups to be used in the multi-group analysis (MGA)

| Indicators: | Indicator Correlations | Raw File | Data Groups |
|-------------------|------------------------|----------|-------------|
| Name | | | Records |
| GROUP_gender(0.0) | | | 102 |
| GROUP_gender(1.0) | | | 148 |

Although it is not the recommended method for moderators that are numerical variables, if it is decided to discretize a numerical variable (dichotomize or polytomize) to use it as the variable that will define the groups, this can be done directly in SmartPLS 3 as follows:

double-click the dataset icon > Add data groups > Name the category of the group > Select the variable > Define the criteria for inclusion in the category > Ok (Figure 19), and repeat the same procedure for the other categories to include all the sample (collectively exhaustive and mutually exclusive categories).

Figure 19 Dichotomization of a numerical variable for use in the MGA

| Indicators: | Indicator Correlations | Raw File | Data Groups |
|-------------|------------------------|----------|-------------|
| Name | | | Records |
| older | | | 154 |
| younger | | | 156 |

Note: This dataset is not the same as that used in the MGA examples (n = 310).

After the groups are defined, it is possible to execute the MGA in two ways, permutation being the most recommended because it has a measurement invariance test (MICOM) to evaluate the invariance of the measurement model:

- i. MGA: Calculate > Multi-group Analysis (MGA) > Select a genre in each group > Start calculation.
- ii. Permutation: Calculate > Permutation > Select a genre in each group > Start calculation.

Evaluation and reporting

First, it is necessary to evaluate if the measurement model is invariant from one group to another. The invariance can be evaluated from a weaker form (configurational invariance, which means that the same indicators are used to measure the same constructs in different groups), to something more restricted as the indicators show the same factor loads in different groups etc. For further study on this topic, we suggest Henseler et al. (2016) for models estimated by PLS-SEM and Little (2013) for models estimated by SEM covariance based.

In this example, the configurational invariance is guaranteed from the beginning (step 1), since the two groups and their differences are estimated in the same round. In step 2 the compositional invariance (MICOM) is evaluated, which is accepted if the correlation between the scores for each construct is equal to 1, when using the outer weights of group 1 and group 2.

In Figure 20 it is observed that the compositional invariance was not obtained for the Value construct, and one of the following options must be chosen:

- If the difference is due to a few indicators, they could be excluded from the model;
- Define a priori weights for each indicator (fixed values);
- Exclude the entire construct from the model, with some post hoc justification/explanation;
- Do not continue the comparison and analyse the groups separately.

Figure 20 MICOM results

| | Original Correlation | Correlation Permutation Mean | 5.0% | Permutation p-Values |
|--------------|-------------------------|---------------------------------|-------|-------------------------|
| Expectation | 0.999 | 0.999 | 0.997 | 0.573 |
| Image | 0.996 | 0.997 | 0.991 | 0.292 |
| Loyalty | 0.995 | 0.996 | 0.990 | 0.303 |
| Quality | 0.999 | 0.999 | 0.998 | 0.465 |
| Satisfaction | 1.000 | 1.000 | 0.999 | 0.448 |
| Value | 0.994 | 0.999 | 0.996 | 0.008 ← |

Note: This result is displayed in the permutation output > Quality criteria > MICOM

To evaluate the indicators of each construct in the output of Permutation (Final results > outer loadings and outer weights) we observe the following significant differences between the groups:

- Outer loading: indicator val3 presented a difference equal to 0.306 ($p = 0.002$)
- Outer weight: indicator val3 presented a difference equal to 0.091 ($p = 0.013$) and val1 was equal to 0.115 ($p = 0.004$).

From these results, it was decided to exclude the indicator val3 and run the permutation again, which resulted in the acceptance of the compositional invariance for all constructs (configurational + compositional = partial invariance), which allows the comparison of the structural coefficients (in step 3 of the MICOM are compared the means and variances to establish the total invariance).

Finishing the analysis, it is observed in Figure 21 two structural coefficients that were different (Image \rightarrow Loyalty; Satisfaction \rightarrow Loyalty). The MGA analysis can complement the results of the Permutation because it presents the coefficients and p-values for the two groups.

Figure 21 Permutation results (difference of structural coefficients)

| Path Coefficients | | | | | | | |
|-----------------------------|---------|---------|--|---------|--------|-------|------------------------|
| Matrix | | | | | | | Copy to Clipboard: |
| | Path... | Path... | Path Coefficients Original Differenc... | Path... | 2.5% | 97.5% | Permutation p-Value |
| Expectation -> Quality | 0.858 | 0.837 | 0.021 | 0.000 | -0.089 | 0.080 | 0.618 |
| Expectation -> Satisfaction | 0.058 | -0.047 | 0.105 | 0.004 | -0.238 | 0.277 | 0.449 |
| Expectation -> Value | 0.080 | 0.170 | -0.090 | -0.001 | -0.315 | 0.304 | 0.551 |
| Image -> Expectation | 0.483 | 0.619 | -0.136 | 0.004 | -0.190 | 0.200 | 0.172 |
| Image -> Loyalty | 0.082 | 0.471 | -0.389 | 0.013 | -0.285 | 0.295 | 0.007 |
| Image -> Satisfaction | 0.162 | 0.220 | -0.057 | 0.004 | -0.206 | 0.213 | 0.588 |
| Quality -> Satisfaction | 0.028 | 0.234 | -0.206 | -0.002 | -0.382 | 0.330 | 0.252 |
| Quality -> Value | 0.616 | 0.678 | -0.062 | 0.002 | -0.311 | 0.331 | 0.708 |
| Satisfaction -> Loyalty | 0.716 | 0.260 | 0.456 | -0.010 | -0.325 | 0.275 | 0.001 |
| Value -> Satisfactio | 0.689 | 0.498 | 0.191 | -0.007 | -0.334 | 0.307 | 0.255 |

Note: This result is displayed in the permutation output > Final Results > Path coefficients.

If there are more than two groups to compare, multiple comparisons will be necessary. In this case, the Bonferroni correction is indicated, for example: if there are three groups to be compared (ABC), there will be three comparisons (AB, AC, BC), so the p-values should be multiplied by 3 (or the level of significance - α - should be divided by 3, for example, $0.05/3 = 0.0167$) to assert that the difference is significant at 5%. For four groups, there will be six comparisons (AB, AC, AD, BC, BD, CD), so the p-values should be multiplied by 6 or $\alpha = 0.05/6 = 0.00833$, to assert that the difference is significant 5% (HAIR JR et al., 2016).

More recommendation than the conclusion

The article presented does not have a “closure” or a set of the findings, because it had a basis of presentation of statistical techniques, thus forming an attempt to create a set of guidelines for the use of the PLS-SEM multivariate technique in other contexts and situations different from the more common ones.

The increasing use of PLS-SEM probably has as main reasons the types of research that are carried out in the areas of human, social and behavioral sciences, that is, they are data from attitude scales or Likert type (in many times) and such scales present data that are rarely adherent to the multivariate normal distribution; have models that do not have very solid or “sedimented” theoretical bases, because in the areas of knowledge indicated the problems are more complex and difficult to structure.

Thus, the higher “plasticity” in the assumptions that support the statistical technique presented here allows the inclusion of a wide range of models and variations of these that better meet the needs of the indicated areas.

Also, there is sometimes debate and some controversy over working with small samples, and in the introduction, a warning already has been added to not to use PLS-SEM with the only justification that the sample is small. But what is the problem of using a small sample if the effects found were significant? Briefly:

- If the sample is small, it will result in greater variation in results;
- When eliminating indicators with low loadings, it may be that the others (indicators), which are with high loadings present these values only because the sample is small, that is, if the sample was large, the variation would be smaller, and it would be observed that the loadings are not so high. This discussion has been made as overfitting and chance capitalisation;
- Therefore, Hair Jr. et al. (2010) suggest the use of a new sample if more than 20% of indicators are excluded.

Finally, it is understood that this article was an attempt to complement and advance in relation to the publication of Ringle et al. (2014a; 2014b), but learning is a work-in-process, so some videos have been prepared for the examples presented in this article and are available on the YouTube Channel (<https://bit.ly/2F7kgud>), from so that interested parties can send questions and suggestions on the Canal itself.

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