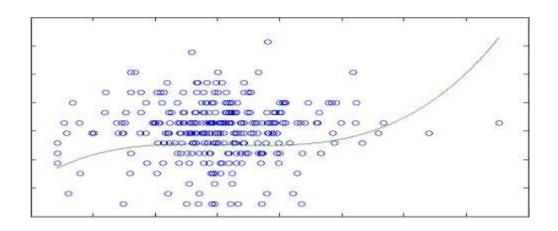
WarpPLS User Manual: Version 7.0

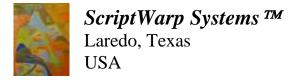


Ned Kock

WarpPLS[©] User Manual: Version 7.0

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A. Introduction

Structural equation modeling (SEM) employing the partial least squares (PLS) method, or PLS-based SEM for short, has been and continue being extensively used in a wide variety of fields (Kock, 2010; 2014a; 2015d; 2019a). Examples of fields in which PLS-based SEM has been used are: cliodynamics (Kock, 2015d), global environmental change (Brewer et al., 2012), information systems (Guo et al., 2011; Kock & Lynn, 2012; Kock & Moqbel, 2021; Kock et al., 2018), international business (Ketkar et al., 2012), marketing (Biong & Ulvnes, 2011; Kock, 2019b), medicine (Berglund et al., 2012; Melton et al., 2016), nursing (Kim et al., 2012), organizational leadership (Kock et al., 2019), and sustainable tourism (Rasoolimanesh et al., 2017).

This software provides users with a wide range of features, several of which are not available from other SEM software. For example, this software is the first and only (at the time of this writing) to explicitly identify nonlinear functions connecting pairs of latent variables in SEM models and calculate multivariate coefficients of association accordingly. Functions whose first and second derivatives are lines are modeled, covering a wide variety of noncyclical and monocyclical functions (Kock, 2010; 2016c).

Additionally, this software is the first and only (at the time of this writing) to provide classic PLS algorithms together with factor-based PLS algorithms for SEM (Kock, 2017; 2019a). Factor-based PLS algorithms generate estimates of both true composites and factors, fully accounting for measurement error (Kock, 2015b; 2017; 2019a; 2019b; 2019c). They are equivalent to covariance-based SEM algorithms; but bring together the "best of both worlds", so to speak.

Factor-based PLS algorithms combine the precision of covariance-based SEM algorithms under common factor model assumptions with the nonparametric characteristics of classic PLS algorithms (Kock, 2017; 2019a; 2019b; 2019c). Moreover, factor-based PLS algorithms address head-on a problem that has been discussed since the 1920s – the factor indeterminacy problem. Classic PLS algorithms yield composites, as linear combinations of indicators, which can be seen as factor approximations. Factor-based PLS algorithms, on the other hand, provide estimates of the true factors, as linear combinations of indicators and measurement errors (Kock, 2015b; 2017).

All of the features provided have been extensively tested with both "real" data, collected in actual empirical studies; as well as simulated data generated through Monte Carlo procedures, whereby data is created based on "true" parameter values that the software is expected to replicate (Kock & Gaskins, 2016; Kock & Moqbel, 2016; Robert & Casella, 2010). Future tests, however, may reveal new properties of these features, and clarify the nature of existing properties.

A.1. Software installation and uninstallation

The software installs automatically from a self-extracting executable file. There are two components to the software: the MATLAB Compiler Runtime, and the main software (i.e., WarpPLS). The first is a set of free-distribution MATLAB libraries with code that is called by the main software. Because the MATLAB Compiler Runtime is used, you do not have to have MATLAB (the main MATLAB program) installed on your computer to run WarpPLS.

Minimal and harmless changes to the operating system registry are made by the MATLAB Compiler Runtime, which are easily reversed upon uninstallation. To uninstall, normally the following or equivalent steps (depending on the operating system version used) can be taken: go the "Control Panel", click on "Add or Remove Programs" or "Programs and Features", and uninstall the MATLAB Compiler Runtime.

The **MATLAB** Compiler Runtime 7.14 is used in this version of WarpPLS. This is the same MATLAB Compiler Runtime that has been used since version 2.0. The MATLAB Compiler Runtime used in version 1.0 is a different one, and thus will *not* work properly with this version of WarpPLS.

In most cases, previous versions of WarpPLS and of the MATLAB Compiler Runtime may be retained on a user's computer. Different versions of WarpPLS and of the MATLAB Compiler Runtime generally do not interfere with one other.

To uninstall the main software program, normally all you have to do is to simply delete the main software installation folder. This folder is usually "C:\Program Files\WarpPLS 7.0" or "C:\Program Files (x86)\WarpPLS 7.0", unless you chose a different folder for the main software program during the installation process. Then delete the shortcut created by the software from the desktop.

Both programs, the MATLAB Compiler Runtime and the main software, may be retained without harm to your computer. They will not normally interfere with other programs; not even with MATLAB (the main MATLAB program), if you have it installed on your computer.

A.2. Stable version notice

This version was initially released as a beta version and was later upgraded to stable. As you will see below, it incorporates a number of new features, when compared with the previous version. It had undergone extensive focused testing in-house prior to its release as a beta version, and had been in the hands of users for comprehensive applied testing with user-specific empirical datasets prior to its upgrade to stable. Nevertheless, given the new features, and the inherent interconnectedness of features, it is possible that this stable version will still contain some software bugs, which we expect to be minor.

A.3. New features in version 7.0

HTMT ratios. The sub-option "Discriminant validity coefficients (extended set)", under the menu option "Explore additional coefficients and indices", now allows you to inspect the heterotrait-monotrait (HTMT) ratios calculated by the software. These ratios have been proposed for discriminant validity assessment, particularly in the context of composite-based SEM via classic PLS algorithms; as opposed to factor-based SEM via modern algorithms that estimate factors (which have been available from this software for quite some time now). Discriminant validity is a measure of the quality of a measurement instrument; the instrument itself is typically a set of question-statements. A measurement instrument has good discriminant validity if the question-statements (or other measures) associated with each latent variable are not confused by the respondents, in terms of their meaning, with the question-statements associated with other latent variables.

Discriminant validity coefficients (extended set). The HTMT ratios are provided along with other coefficients that are useful for discriminant validity assessment, in one single combined set of outputs. These other coefficients are correlations among latent variables and square roots of AVEs, structure loadings and cross-loadings, and full collinearity VIFs. For the HTMT ratios, the following coefficients are also provided: P values, and 90% confidence intervals.

Graphical user interface optimization. Several elements of the graphical user interface, such as screens and warning messages, have been optimized so that users can perform SEM analysis tasks with only a few clicks – and in a straightforward fashion. For example, automatic reanalyses are now conducted whenever any of the several SEM analysis settings are changed, with the results becoming immediately available to users. Also, new menu options are now available to facilitate tasks; e.g., users can now open or create a project through the "Open or create project (Step 1)" menu option available under the "Project" menu option. This new "Open or create project (Step 1)" option allows users to open or create a project file, providing an alternative path for executing Step 1.

Fractional splits for 2D moderating effects graphs. Users can now set "fractional" splits for 2D moderating effects graphs, through a new "Split" menu option. The default is 0.5, which splits the sample in the middle when drawing the lines for the effects and the "low" and "high" values of the moderating variable. For instance, if you set the fractional split to 0.1, the software splits the sample in 10% (of the sample) to the left and 90% to the right, respectively for the "low" and "high" values of the moderating variable. This new and powerful fractional split feature enables users to significantly expand their options for illustrating moderating effects in 2D graphs. In the previous version of the software the split was set at 0.5 (i.e., in the middle), with no way to modify it.

New moderating effects calculation options. Users can now choose among three options for moderating effects calculation: "Two Stages", "Variable Orthogonalization", and "Indicator Products". This is done through the new "View or change moderating effects settings" menu option, under the "Settings" menu option on the software's main window. The default moderating effects calculation option is "Two Stages", whereby latent variable scores are calculated first and then used in a second stage for the creation of the interaction variable that implements the moderating effect. The "Variable Orthogonalization" option implements a similar procedure, but stochastically departs from a random variable, which is fully orthogonal to the latent variables in the model, for the creation of the interaction variable that implements the moderating effect. The "Indicator Products" option employs indicator products for the creation

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of the interaction variable that implements the moderating effect; this was the only option available in the previous version of the software.

Incremental code optimization. This is conducted in each new version of this software. At several points the code was optimized for speed, stability, and coefficient estimation precision. This led to incremental gains in speed even as a number of new features were added. Several of these new features required new and complex calculations, mostly to generate coefficients that were not available before.

A.4. Note regarding features

The vast majority of the features implemented by the software **have been extensively vetted** by a variety of researchers, many of whom have published studies employing the software in highly selective publication outlets. Having said that, it should be also noted that some of the features provided by the software are still at an experimental stage, and may change in the future as more tests are conducted. Normally this is indicated in this user manual whenever it is the case.

Other novel features of this software may prove useful for applications different from the ones they were originally intended for. For example, an extensive set of causality assessment coefficients is provided by the software. Yet, the topic of causality assessment in the context of SEM is controversial (Kock, 2015e; Kock & Gaskins, 2016; Pearl, 2009). A causality assessment coefficient that is provided to inform the user of the possibility of a reverse link may prove in the future to be useful to identify a specific type of bias due to measurement error.

Finally, while this software aims at providing a wide range of features and outputs, the complexity inherent in SEM analyses and their dependence on theory that is constantly being refined would tend to make strong and sweeping claims regarding accuracy and statistical power likely to be proven exaggerated.

Researchers analyzing empirical data typically **do not know the underlying distributions of their data and of error terms**. Data analysis **software tools help researchers uncover characteristics of those distributions, with incomplete information**. Given this, it seems reasonable to conclude that all SEM algorithms and software tools that implement these algorithms have limitations in their accuracy, avoidance of false positives, and statistical power (i.e., avoidance of false negatives).

Accuracy and statistical power seem to suffer particularly when very small samples and deviations from normality are observed in the context of small effect sizes (Kock & Hadaya, 2018). Some exaggerated claims about PLS-based SEM's performance under these conditions have opened a door for criticism that would otherwise have been tightly closed. For example, Goodhue et al.'s (2012) extensive analysis of various SEM algorithms illustrates related limitations, although its negative results may have been exacerbated by the fairly low path coefficients that they used for small and medium effect sizes. Those path coefficients were based on effect sizes that were calculated using the stepwise regression procedure proposed by Cohen (1988) for the calculation of *f*-squared coefficients, which is generally not compatible with PLS-based SEM algorithms (Kock, 2014a). This theme is further explored later in this user manual.

This software attempts to ameliorate this situation in connection with accuracy and statistical power by providing an extensive set of features and outputs that can be used by researchers to reveal as many aspects of the underlying relationships as possible.

Some of the features provided are specifically aimed at increasing accuracy and statistical power. For example, jackknifing, one of the resampling methods provided, tends to generate relatively low standard errors, more in line with the true values, with small samples and medium to high effect sizes. This could increase statistical power with small samples and medium to high effect sizes, making the use of jackknifing more appropriate than bootstrapping in these cases. The same may be true for the "stable" methods, particularly the "Stable3" method (Kock, 2018b). In fact, Monte Carlo simulations suggest that the "stable" methods perform better than jackknifing and other resampling methods in this respect (Kock, 2018b).

This software's extensive range of features may also help further research on SEM methods in general.

B. The main window

Prior to displaying the software's main window, a command prompt window may be shown and kept open for the duration of the SEM analysis session. Whether this window is shown or not depends on the operating system being used and its settings. If it is not shown, that is not a problem.

However, do not try to close this command prompt window if it is shown, because it will list warnings and error messages that will likely be very useful in troubleshooting. Moreover, those warnings and error messages will indicate where in the source code they are happening, which will help the software developer correct any possible problems in future versions of the software.

In very slow computers, with limited computing power, only the command prompt window may be displayed for as long as a few minutes. The reason for this is that the computer needs to load a large runtime module prior to actually running this software. Users should not try to do anything during this time, as that will only delay the launch of the software's main window.

B.1. The SEM analysis steps

The software's main window (see Figure B.1) is where the SEM analysis starts. The top-left part of the main window contains a brief description of the five steps through which the SEM analysis takes place. The steps are executed by pressing each of the push buttons on the top-right part of the window. Not all menu options and push buttons become available right away. Menu options and push buttons become available as the analysis progresses.

WarpPLS 7.0 - Project file: C:\Uner\nedko\Documents\WarpPLS_6_0\01_ECollabMod...\01_L_PLSR_ECollabModStudyData.prj Project Data Modify Explore Settings Help Welcome to WarpPLS 7.0, a software developed by Ned Kock using MATLAB, C++ and Java. Proceed to Step 1 Proceed to Step 4 This software will help you conduct a structural equation modeling (SEM) analysis using various composite-based and factor-based methods including the "warped" partial least squares (PLS) method. The analysis will Proceed to Step 2 Proceed to Step 5 be conducted through the following steps: Step 1: Open or create a project file to save your work. Step 2: Read the raw data used in the SEM analysis. Proceed to Step 3 View/save analysis results Step 3: Pre-process the data for the SEM analysis Step 4: Define the variables and links in the SEM model. Step 5: Perform the SEM analysis and view the results. Press a "Proceed to Step ..." button when you are ready to continue. (Unavailable steps are grayed out; they will be made available as you progress through the steps.) For more help, click on the "Help" menu option at the top of this window. Status of SEM analysis steps (* = completed): *Step 1: Open/create project file Project file: 01: L. PLSR: ECollabModStudyData.prj Path: C: Users'nedko'Documents:WarpPLS_6_0/01_ECotabMod_1 Step 2: Read raw data Raw data file Kock_2014_ECollabModStudyData xlsx Path: C:\Users\nedkock\Documents\WarpPLS_6_0\01_ECollabM...\ Step 3: Pre-process data ep 4. Define variables/links in SEM model Step 5: Performiview SEM analysis/results

Figure B.1. The main window showing the steps (after a complete analysis was conducted)

The steps must be carried out in the proper sequence. For example, Step 5, which is to perform the SEM analysis and view the results, cannot be carried out before Step 1 takes place, which is to open or create a project file to save your work. This is the main reason why steps have their push buttons grayed out and deactivated until it is time for the corresponding steps to be carried out.

The bottom-left part of the main window shows the status of the SEM analysis; after each step in the SEM analysis is completed, this status window is updated. A miniature version of the SEM model graph is shown at the bottom-right part of the main window. This miniature version is displayed without results after Step 4 is completed. After Step 5 is completed, this miniature version is displayed with results.

The following menu options are available under "Project": "Open or create project (Step 1)", "Save project", "Save project as ...", and "Exit". The "Open or create project (Step 1)" option allows users to open or create a project file, providing an alternative path for executing Step 1. Through the "Save project" option you can save the project file that has just been created or that has been created before and is currently open. To open an existing project or create a new project you need to execute Step 1, by pressing the "Proceed to Step 1" push button. The "Save project

as ..." option allows you to save an existing project with a different name and in a different folder from ones for the project that is currently open or has just been created. This option is useful in the SEM analysis of multiple models where each model is a small variation of the previous one. Finally, the "Exit" option ends the software session. If your project has not been saved, and you choose the "Exit" option, the software will ask you if you want to save your project before exiting. In some cases, you will not want to save your project before exiting, which is why a project is not automatically saved after each step is completed. For example, you may want to open an existing project, change a few things and then run a SEM analysis, and then discard that project. You can do this by simply not saving the project before exiting.

Initially, before Step 5 is completed, the menu option "Explore" becomes available from the main window with limited functionality available under it; it only allows users to explore statistical power and minimum sample size requirements. Extra functionality under "Explore" becomes available after Step 5 is completed. After Step 3 is completed, whereby the data used in the SEM analysis is pre-processed, three sets of menu options become available from the main window: "Data", "Modify", and "Settings".

The "Data" menu options refer primarily to data viewing and saving tasks. These menu options allow you to view or save data and various statistics, mostly descriptive statistics, into tab-delimited .txt files. The "tab-delimited .txt file" is the general file format used by the software to save most of the files containing analysis and summarization results. These files can be opened and edited using Excel, Notepad, and other similar spreadsheet or text editing software. These menu options are discussed in more detail later.

The "Modify" menu options refer primarily to data modification tasks. These menu options allow you to add new data labels and raw data to your dataset, redo missing data imputation, as well as add one or more latent variable scores (a.k.a. factor scores) to the dataset as new standardized indicators. Also available is the option of adding all latent variable scores at once to the dataset as new standardized indicators. Data labels can be shown on graphs as text next to data points, or as legends for data points using different markers. These menu options are discussed in more detail later.

The "Explore" menu options give you access to a variety of advanced ancillary analysis features. These allow you to estimate statistical power and minimum sample size requirements, view T ratios and confidence intervals for various coefficients, estimate complex probabilities via conditional probabilistic queries, conduct full latent growth analyses (Hubona & Belkhamza, 2021; Kock, 2020a), conduct multi-group and measurement invariance analyses, create analytic composites (Kock, 2021a; Kock et al., 2018) and instrumental variables (which can be used to address endogeneity and analyze reciprocal relationships), perform numeric-to-categorical and categorical-to-numeric conversions, view Dijkstra's consistent PLS outputs, view fit indices comparing indicator correlation matrices (shown together with other classic model fit and quality indices), and view new reliability measures generated in the context of factor-based PLS analyses. These menu options are discussed in more detail later.

The "Settings" menu options refer primarily to the settings used in an SEM analysis. You can view or change general SEM analysis settings through the "Settings" menu options. Here you can select the analysis algorithms used in the SEM analysis, the resampling method used to calculate standard errors and P values, as well as other elements that will define how the SEM analysis will be conducted. These menu options are discussed in more detail later.

The "Help" menu options give you access to help resources. There are several help menu options available on the main window, as well as on several other windows displayed by the

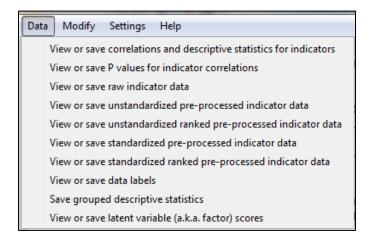
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software. The "Open User Manual file (PDF)" option opens this document as a PDF file from a Web location. The "Open Web page with video for this window" option opens a Web page with a video clip that is context-specific, in this case specific to the main window. The "Open Web page with links to various videos" option is not context-specific, and opens a Web page with links to various video clips. The "Open Web page with WarpPLS blog" option opens a Web page with the WarpPLS blog. Similar help options are available from several other windows in this software.

B.2. Data

The "**Data**" menu options allow you to view or save data and various statistics, mostly descriptive statistics (see Figure B.2). These menu options are discussed individually below. Some of them are discussed in more detail later in this document.

Figure B.2. Data menu options



The "View or save correlations and descriptive statistics for indicators" option allows you to view or save general descriptive statistics about the data. These include the following, which are shown at the bottom of the table that is displayed through this option: means, standard deviations, minimum and maximum values, medians, modes, skewness and excess kurtosis coefficients, results of unimodality and normality tests, and histograms. The unimodality tests for which results are provided are the Rohatgi- Székely test (Rohatgi & Székely, 1989) and the Klaassen-Mokveld-van Es test (Klaassen et al., 2000). The normality tests for which results are provided are the classic Jarque-Bera test (Jarque & Bera, 1980; Bera & Jarque, 1981) and Gel & Gastwirth's (2008) robust modification of this test. Since these tests are applied to individual indicators, they can be seen as "univariate" or "bivariate" unimodality and normality tests.

These descriptive statistics are complemented by the option "View or save P values for indicator correlations". This option may be useful in the identification of candidate indicators for latent variables through the anchor variable procedure discussed by Kock & Verville (2012). This can be done prior to defining the variables and links in a model. This can also be done after the model is defined and an analysis is conducted, particularly in cases where the results suggest outer model misspecification. Examples of outer model misspecification are instances in which indicators are mistakenly included in the model by being assigned to certain latent variables, and instances in which indicators are assigned to the wrong latent variables (Kock & Lynn, 2012; Kock & Verville, 2012).

The "View or save raw indicator data" option allows you to view or save the raw data used in the analysis. This is a useful feature for geographically distributed researchers conducting collaborative analyses. With it, those researchers do not have to share the raw data as a separate file, as that data is already part of the project file. That data can be viewed and easily replicated, if this is needed, through this option.

Two menu options allow you to view or save unstandardized pre-processed indicator data. This pre-processed data is not the same as the raw data, as it has already been through the

automated missing value correction procedure in Step 3. The options that allow you to view or save unstandardized pre-processed indicator data are: "View or save unstandardized pre-processed indicator data" and "View or save unstandardized ranked pre-processed indicator data". The latter option refers to ranked data.

When data is ranked, typically the value distances that typify outliers in data on ratio scales, whether standardized or unstandardized, are significantly reduced. This effectively eliminates outliers from the data, without any decrease in sample size. Often some information is lost due to ranking – e.g., the distances among data points based on answers on ratio scales. Ranked data can be saved and then selectively read into the project file (e.g., only one or a few columns) and used in only one or a few latent variables, if it appears that relationships involving those variables are being significantly and pathologically influenced by the existence of outliers.

Two related menu options allow you to view or save standardized pre-processed indicator data: "View or save standardized pre-processed indicator data" and "View or save standardized ranked pre-processed indicator data". The latter option ranks the data prior to standardizing it. Ranking often has little effect on ordinal data (e.g., data on Likert-type scales), and a major impact on ratio data (e.g., yearly income).

The options that refer to unstandardized data allow you to view or save pre-processed data prior to standardization. The options that refer to standardized data allow you to view or save pre-processed data after standardization; that is, after all indicators have been transformed in such a way that they have a mean of zero and a standard deviation of one.

The "View or save data labels" option allows you to view or save data labels. These are text identifiers that are entered by you separately, through one of the "Modify" menu options. Like the original numeric dataset, the data labels are stored in a table. Each column of this table refers to one data label, and each row to the corresponding row of the original numeric dataset. Data labels can later be shown on graphs, either next to each data point that they refer to, or as part of a graph's legend.

The "Save grouped descriptive statistics" option is a special option that allows you to save descriptive statistics (means and standard deviations) organized by groups defined based on certain parameters. This option is discussed in more detail at the end of this section. This could be considered a "legacy" option, which has been useful in the past but whose usefulness decreased as newer versions of this software have been released. As of this writing, other more advanced features of the software largely obviate the need for the functionality offered through this option.

The "View or save latent variable (a.k.a. factor) scores" option allows you to view or save the latent variable scores generated by the software. There is another option that allows you to save latent variable scores, available as a menu option on the window used to view and save model analysis results; which becomes available later, after Step 5 is completed. These two options return the same latent variable scores in most cases.

The exception to the general rule above is a situation in which you specified a range restriction for your analysis. In this case, only the latter option will return the range-restricted latent variable scores. These latent variable scores will generally have a smaller number of rows than the original dataset (because they are range-restricted), and thus will not be exactly matched to the original dataset.

B.2.1. Grouped descriptive statistics

When the "Save grouped descriptive statistics" option is selected, a data entry window is displayed (see Figure B.2.1.1). There you can choose a grouping variable, number of groups, and the variables to be grouped. This option is useful if one wants to conduct a comparison of means analysis using the software, where one variable (the grouping variable) is the predictor, and one or more variables are the criteria (the variables to be grouped).

Figure B.2.1.1. Save grouped descriptive statistics window

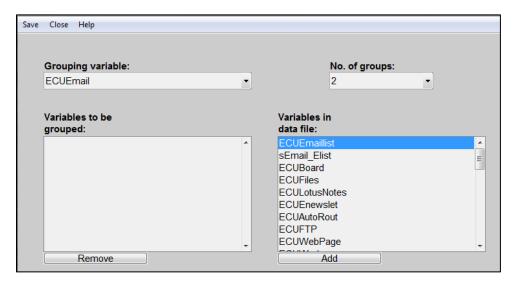


Figure B.2.1.2. Grouped descriptive statistics bar chart

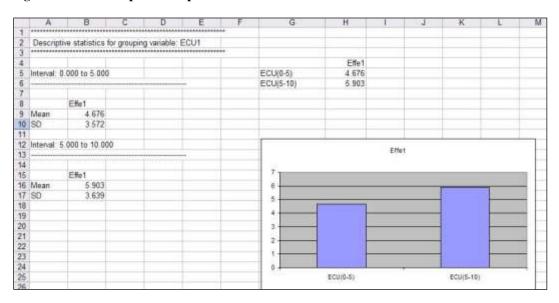


Figure B.2.1.2 shows the grouped statistics data saved through the window shown in Figure B.2.1.1. The tab-delimited .txt file was opened with a spreadsheet program, and contained the data on the left part of the figure.

The data on the left part of Figure B.2.1.2 was organized as shown above the bar chart; next the bar chart was created using the spreadsheet program's charting feature. If a simple

comparison of means analysis using this software (see, e.g., Kock, 2013) had been conducted in which the grouping variable (in this case, an indicator called "ECU1") was the predictor, and the criterion was the indicator called "Effe1", those two variables would have been connected through a path in a simple path model with only one path. Assuming that the path coefficient was statistically significant, the bar chart displayed in Figure B.2.1.2, or a similar bar chart, could be added to a report describing the analysis.

Some may think that it is overkill to conduct a comparison of means analysis using a SEM software package such as this, but there are advantages in doing so (Kock, 2013). One of those advantages is that this software calculates P values using a nonparametric class of estimation techniques, namely resampling and "stable" estimation techniques. (Resampling techniques are sometimes referred to as bootstrapping techniques, which may lead to confusion since bootstrapping is also the name of a type of resampling technique.) Nonparametric estimation techniques do not require the data to be normally distributed, which is a requirement of other comparison of means techniques (e.g., ANOVA).

Another advantage of conducting a comparison of means analysis using this software is that the analysis can be significantly more elaborate than with traditional comparison of means methods, even nonparametric ones. For example, the analysis may include control variables (or covariates), which would make it equivalent to an ANCOVA test. Finally, the comparison of means analysis may include latent variables, as either predictors or criteria (see, e.g., Kock & Chatelain-Jardón, 2011). This is not usually possible with ANOVA or commonly used nonparametric comparison of means tests (e.g., the Mann-Whitney U test).

An even more extreme situation is that discussed by Kock (2013) where data on only "one group and one condition" is available. This situation is illustrated through a scenario in which a researcher obtains empirical data by asking questions to gauge the effect of a technology on task performance, but does not obtain data on the extent to which the technology is used. Because of this, the researcher ends up with only one column of data to analyze.

Two other scenarios are also discussed by Kock (2013). These two scenarios are discussed to set the stage for the discussion of the "one group and one condition" scenario. The first is a typical study scenario in which the researcher measures the degree to which the technology is used, or the degree to which specific features of the technology are used, as well as team performance and/or related variables expected to be influenced by technology use.

In the second scenario the researcher does not have data on the extent to which the technology is used, but has data related to team performance and/or other variables expected to be influenced by technology use before and after the technology is introduced. This is a longitudinal data collection scenario for which a comparison of means test could be used. Data analyses for all three scenarios are discussed by Kock (2013) based on this software, showing the versatility of the software. The main reason for this versatility is that most of the data analysis methods used in behavioral research can be conceptually seen as special cases of SEM.

B.3. Modify

The "**Modify**" menu options allow you to add new data labels and raw data to your dataset, redo missing data imputation, as well as add one or more latent variable scores (a.k.a. factor scores) to the dataset as new standardized indicators (see Figure B.3). Also available is the option of adding all latent variable scores at once to the dataset as new standardized indicators. Data labels can be shown on graphs as text next to data points, or as legends for data points using different markers. These menu options are discussed individually below. Some of them are discussed in more detail later in this document.

Figure B.3. Modify menu options

Add data labels from clipboard

Add data labels from file

Add raw data from clipboard

Add raw data from file

Redo missing data imputation (via data pre-processing)

Add one or more latent variable (a.k.a. factor) scores as new standardized indicators

Add all latent variable (a.k.a. factor) scores as new standardized indicators

The menu options "Add data labels from clipboard" and "Add data labels from file" allow you to add data labels into the project file. Data labels are text identifiers that are entered by you through these options, one column at a time. Like the original numeric dataset, the data labels are stored in a table. Each column of this table refers to one data label, and each row to the corresponding row of the original numeric dataset. Data labels can later be shown on graphs, either next to each data point that they refer to, or as part of the legend for a graph.

Data labels can be read from the clipboard or from a file, but **only one column of labels can be read at a time**. Data label cells cannot be empty, contain spaces, or contain only numbers; **they must be combinations of letters, or of letters and numbers**. Valid examples are the following: "Age>17", "Y2001", "AFR", and "HighSuccess". These would normally be entered without the quotation marks, which are used here only for clarity. Some invalid examples: "123", "Age > 17", and "Y 2001".

Through the menu options "Add raw data from clipboard" and "Add raw data from file" users can add new data from the clipboard or from a file. This data then becomes available for use in models, without users having to go back to Step 2. These options relieve users from having to go through nearly all of the steps of a SEM analysis if they find out that they need more data after they complete Step 5 of the analysis. Past experience supporting users suggests that this is a common occurrence. These options employ the same data checks and data correction algorithms as in Step 2; please refer to the section describing that step for more details.

The option "Redo missing data imputation (via data pre-processing)" allows users to redo the missing data imputation process after choosing a method through the "View or change missing data imputation settings" option, which is available under the "Settings" menu options. The following missing data imputation methods are available: Arithmetic Mean Imputation (the software's default), Multiple Regression Imputation, Hierarchical Regression Imputation, Stochastic Multiple Regression Imputation, and Stochastic Hierarchical Regression

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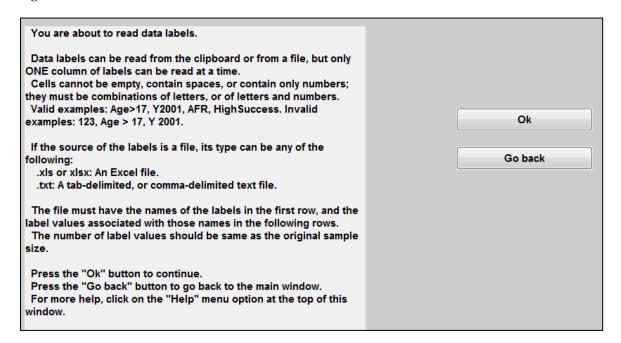
Imputation. Kock (2014c) and Kock (2018a) provide a detailed discussion of these methods and of a Monte Carlo simulation that assesses the methods' relative performances.

Latent variable scores can be easily added to the dataset via the options "Add one or more latent variable (a.k.a. factor) scores as new standardized indicators" and "Add all latent variable (a.k.a. factor) scores as new standardized indicators". These options allow users, after Step 5 is completed, to add one or more latent variables to the model as new standardized indicators, and also to add all latent variables as new indicators. Adding one or more latent variables at a time may be advisable in certain cases; for example, in hierarchical analyses using selected latent variables as indicators of second, third etc. order latent variables at each level. In such cases, adding all latent variables at once may soon clutter the set of indicators available to be used in the SEM model.

B.3.1. Data labels

Data labels can be added through the menu options "Add data labels from clipboard" and "Add data labels from file" (see Figure B.3.1). Data labels are text identifiers that are entered by you through these options, one column at a time. Like the original numeric dataset, the data labels are stored in a table. Each column of this table refers to one data label variable, and each row to the corresponding row of the original numeric dataset. Data labels can later be shown on graphs, either next to each data point that they refer to, or as part of the legend for a graph. Once they have been added, data labels can be viewed or saved using the "View or save data labels" option.

Figure B.3.1. Add data labels from file window



While data labels can be read from the clipboard or from a file, **only one column of labels can be read at a time**. Data label cells cannot be empty, contain spaces, or contain only numbers; **they must be combinations of letters, or of letters and numbers**. Valid examples are the following: "Age>17", "Y2001", "AFR", and "HighSuccess". These would normally be entered without the quotation marks, which are used here only for clarity. Some invalid examples are: "123", "Age > 17", and "Y 2001".

B.4. Explore

The "Explore" menu options allow you to estimate statistical power and minimum sample size requirements, view T ratios and confidence intervals for various coefficients, estimate complex probabilities via conditional probabilistic queries, conduct full latent growth analyses (Hubona & Belkhamza, 2021; Kock, 2020a), conduct multi-group and measurement invariance analyses, create analytic composites (Kock, 2021a; Kock et al., 2018) and instrumental variables (which can be used to address endogeneity and analyze reciprocal relationships), perform numeric-to-categorical and categorical-to-numeric conversions, view Dijkstra's consistent PLS outputs, view fit indices comparing indicator correlation matrices (shown together with other classic model fit and quality indices), and view new reliability measures generated in the context of factor-based PLS analyses. These menu options are discussed individually below.

Figure B.4. Explore menu options

Explore statistical power and minimum sample size requirements

Explore T ratios and confidence intervals

Explore conditional probabilistic queries

Explore full latent growth

Explore multi-group analyses

Explore measurement invariance

Explore analytic composites and instrumental variables

Explore categorical-numeric-categorical conversion

Explore Dijkstra's consistent PLS outputs

Explore additional coefficients and indices

Initially, before Step 5 is completed, the menu option "Explore" becomes available from the main window with limited functionality available under it. It only allows users to explore statistical power and minimum sample size requirements, through the menu option "Explore statistical power and minimum sample size requirements". Extra functionality under "Explore", via the other menu options, becomes available after Step 5 is completed.

B.4.1. Power and sample size requirements

The menu option "Explore statistical power and minimum sample size requirements" allows you to obtain estimates of the minimum required sample sizes for empirical studies based on the following model elements: the minimum absolute significant path coefficient in the model (e.g., 0.21), the significance level used for hypothesis testing (e.g., 0.05), and the power level required (e.g., 0.80). Figure B.4.1 illustrates this option. Two methods are used to estimate minimum required sample sizes, the inverse square root and gamma-exponential methods (Kock & Hadaya, 2018). These methods simulate Monte Carlo experiments, and thus produce estimates that are in line with the estimates that would be produced through the Monte Carlo method. The inverse square root method tends to slightly overestimate the minimum required sample size, while the gamma-exponential method provides a more precise estimate. Given this, users are advised to report both estimates, and try to meet the estimate generated by the more conservative of the two methods (i.e., the inverse square root method), which will ensure that the power level achieved by their study will be above the one sought.

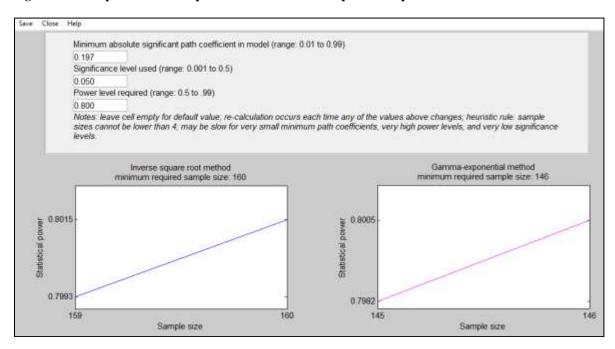


Figure B.4.1. Explore statistical power and minimum sample size requirements

Normally researchers have expectations regarding the results that they should obtain from their empirical studies, expectations that are based on extant theories that they may be empirically testing, as well as past empirical studies. If that is not the case, those researchers may find the default values provided by this software to be useful. The minimum required sample size estimates given by default by this software are 160 and 146. These estimates are generated based on the inverse square root and gamma-exponential methods, respectively, based on certain default values for model elements: 0.197 for minimum absolute significant path coefficient in the model, 0.05 for the significance level used, and 0.80 the power level required. In line with these estimates, the following general rule of thumb is recommended. Researchers who are uncertain about the results they should expect from their studies should aim for sample sizes of 160 or

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above, and no less than 146. The rationales for this general rule of thumb, as well as for the default values underlying it, are discussed in some detail by Kock & Hadaya (2018).

B.4.2. T ratios and confidence intervals

While P values are widely used in PLS-based SEM, as well as in SEM in general, the statistical significances of path coefficients, weights and loadings can also be assessed employing T ratios and/or confidence intervals (Kock, 2016b). These can be obtained through the menu option "Explore T ratios and confidence intervals", which allows you to set the confidence level to be used (see Figure B.4.2).

Figure B.4.2. Explore T ratios and confidence intervals

Save Close Help					
Confidence level used (ra 0.950 Notes: leave cell empty for directional hypotheses; in	or default value;	in a test with	n a T ratio, g erval, genera	enerally the	e hypothesis is supported othesis is supported if ze

Critical T ratios					

For one-tailed tests: 1.645.					
For two-tailed tests: 1.960.					

T ratios for path coefficients					

	ECollab	Projmgt	Success	JSat	ECollab*Projmgt
ECollab					
Projmgt	6.424				
Success	1.222	5.303		5.039	8.189
JSat					
ECollab*Projmgt					

Confidence intervals for path coefficients					

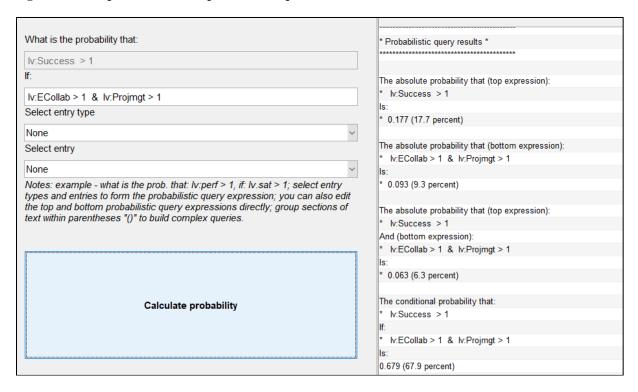
	ECollab			Projmgt	
ECollab					
Projmgt	0.244	0.458			

Generally speaking, the confidence level used should be the complement of the significance level used (i.e., 1 minus the significance level used). For example, if the significance level used is 0.05, then the confidence level used should be set at 0.95 (which is also the software's default). Critical T ratios are provided by the software based on the confidence level selected. The confidence intervals are also affected by the confidence level selected. Kock (2016b) discusses, with examples, how T ratios and confidence intervals can be used for hypothesis testing, either in place of P values or in conjunction with those values.

B.4.3. Conditional probabilistic queries

If an analysis suggests that two variables are causally linked, yielding a path coefficient of 0.25 for example, this essentially means in probabilistic terms that an increase in the predictor variable leads to an increase in the conditional probability that the criterion variable will be above a certain value. Yet, conditional probabilities cannot be directly estimated based on path coefficients; and those probabilities may be of interest to both researchers and practitioners. By using the "**Explore conditional probabilistic queries**" menu option, users of this software can estimate conditional probabilities via queries including combinations of latent variables, unstandardized indicators, standardized indicators, relational operators (e.g., > and <=), and logical operators (e.g., & and |). Figure B.4.3 illustrates this option.

Figure B.4.3. Explore conditional probabilistic queries

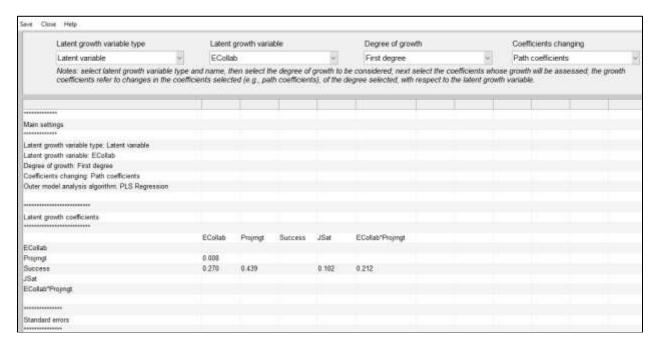


An example of conditional probabilistic query would be the following. What is the probability that: lv:Success > 0, if lv:ECollab > 1? Here the "lv" terms indicate that we are referring to the latent variables "Success" (level of success in a team project) and "ECollab" (level of use of an electronic collaboration technology in the project). Since the latent variables are standardized, this query translates to: What is the probability that a team will have an above average level of success in a project, if their level of use of the electronic collaboration technology is high?

B.4.4. Full latent growth

Sometimes the actual inclusion of moderating variables and corresponding links in a model leads to problems; e.g., increases in collinearity levels, and the emergence of instances of Simpson's paradox (Kock, 2015e; Kock & Gaskins, 2016). By using the menu option "Explore full latent growth" users can completely avoid these problems (see Figure B.4.4). This menu option allows you to estimate the effects of a latent variable or indicator on all of the links in a model (all at once), without actually including any links between the variable and other variables in the model (Kock, 2020a). Moreover, growth in coefficients associated with links among different latent variables and between a latent variable and its indicators, can be estimated; allowing for measurement invariance tests applied to loadings and/or weights. Finally, growth coefficients can be used in the assessment of moderated mediation effects (Hubona & Belkhamza, 2021; Kock, 2020a).

Figure B.4.4. Explore full latent growth

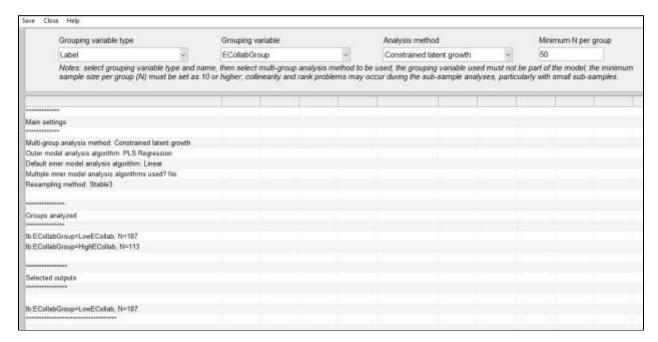


A full latent growth analysis could be seen as a comprehensive analysis of moderating effects where the moderating variable is "latent", in the sense that it does not "disrupt" the model in any way (Hubona & Belkhamza, 2021; Kock, 2020a). This is conceptually analogous to a multigroup analysis (see, e.g., Kock, 2014a). Two degrees of latent growth are provided through this menu option: first and second degree growth. An instance of second degree growth is equivalent to a double moderation, again with the moderating variable being "latent" (or "hidden" from the other variables in the model). If a link includes the latent growth variable itself, then the corresponding latent growth coefficient, if significant, suggests the existence of a nonlinear relationship (which is also equivalent to "self-moderation"; for a discussion of this equivalence in an action research context see: Kock et al., 2017). In such an instance (i.e., when the link includes the latent growth variable itself) the level of nonlinearity is likely "Warp2" if it is associated with significant first degree growth; and likely "Warp3" if it is associated with significant second degree growth.

B.4.5. Multi-group analyses

The menu option "Explore multi-group analyses" allows you to conduct analyses where the data is segmented in various groups, all possible combinations of pairs of groups are generated, and each pair of groups is compared (see Figure B.4.5). In multi-group analyses normally path coefficients are compared (Kock, 2014a). The grouping variables can be unstandardized indicators, standardized indicators, and labels. The sub-options available for group pair comparison refer to the following methods: constrained latent growth, Satterthwaite, and pooled standard error.

Figure B.4.5. Explore multi-group analyses

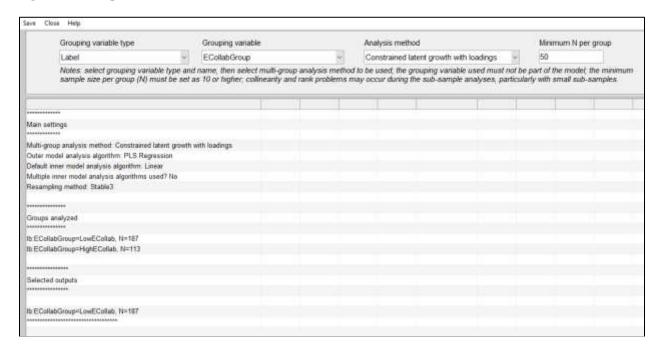


The constrained latent growth method is essentially the same method as that employed in a full latent growth analysis (Hubona & Belkhamza, 2021; Kock, 2020a), with the difference that here it is constrained to the subsample formed by the two groups being compared. The Satterthwaite and pooled standard error are classic methods that are widely used for multi-group analyses (for a detailed discussion of these methods, see: Kock, 2014a). One of the advantages of the constrained latent growth method is that the subsample it analyzes is larger than the subsamples analyzed by the Satterthwaite and pooled standard error methods. In most cases, multi-group analyses can be more easily and comprehensively conducted through a full latent growth analysis (Hubona & Belkhamza, 2021; Kock, 2020a).

B.4.6. Measurement invariance

The menu option "Explore measurement invariance" allows you to conduct analyses where the data is segmented in various groups, all possible combinations of pairs of groups are generated, and each pair of groups is compared (see Figure B.4.6). These analyses are similar, in several respects, to those conducted in multi-group analyses. However, while in multi-group analyses normally path coefficients are compared, in measurement invariance assessment the foci of comparison are loadings and/or weights (Kock, 2014a).

Figure B.4.6. Explore measurement invariance



As with multi-group analyses, the **grouping variables** can be **unstandardized indicators**, **standardized indicators**, and **labels**. The sub-options available for group pair comparison refer to the following methods: constrained latent growth, Satterthwaite, and pooled standard error. The constrained latent growth method is essentially the same method as that employed in a full latent growth analysis (Hubona & Belkhamza, 2021; Kock, 2020a), with the difference that here it is constrained to the subsample formed by the two groups being compared. The Satterthwaite and pooled standard error are classic methods that are widely used for measurement invariance testing (for a detailed discussion of these methods, see: Kock, 2014a). As noted earlier, one of the advantages of the constrained latent growth method is that the subsample it analyzes is larger than the subsamples analyzed by the Satterthwaite and pooled standard error methods. In most cases, measurement invariance assessment can be more easily and comprehensively conducted through a full latent growth analysis (Hubona & Belkhamza, 2021; Kock, 2020a).

B.4.7. Analytic composites

The menu option "Explore analytic composites and instrumental variables" allows you to create analytic composites (see Figure B.4.7). Analytic composites are weighted aggregations of indicators where the relative weights are set by you, usually based on one or more existing theories or the definition of the analytic composites. Relative weight values from -1 to 1 are allowed.

Figure B.4.7. Explore analytic composites

Save Close Help										
What to create?										
Analytic composite	~									
Notes, start by choosing what to co- past research, instrumental variable	eale, analytic compos es can be used in ma	ites are agg ny applicati	gregations of ons, such as	findicators v s controlling	with set weights, whe for endogeneity and	re the weights analyzing rec	s are defined ciprocal (no	f by the use wecursive)	r based on i relationship:	theory and s.
200 On On	- 4	4	1	T .	1		T.	1	T	1
Create analytic composite										
*** Available indicators										
Click to choose one or more.	JS#11	JSat2	JSit3	ECollab1	ECollab2	ECollab3	Projrigt1	Projmgt2	Projmgt3	Success
*** Indicators/weights to be used										
Indicator (click to remove):	JSat1	JSat2	JSat3							
Weight (click to change; -1 to +1)	1.000	0.500	-0.500							
*** Indicator coeffs										
Std. weight:	0.876	0.438	-0.438							
P value:	< 0.001	<0.001	< 0.001							
VF	1.277	1.339	1.315							
WLS:	1	1	-1							
ES	0.775	0.264	0.039							
*** Correls, with lat, vars, and reliabs										
Latent variable.	ECollab	Projrogt	Success	JS#.	ECollab Projingt	(CA)	(CR)			
Correlation/reliability	-0.056	0.076	0.239	0.572	-0.035	0.673	0.573			
*** Create analytic composite (click)?	Yes									

For example, an analytic composite may be defined as the aggregation of 10 stock prices weighted by values reflecting the relative market capitalization of their respective companies. In a case like this it makes no sense to let the software assign weights to indicators. The same is true when a construct is defined within the scope of a theory as being an aggregation of, say, 3 indicators with specific relative weights assigned to them.

Here **only relative weights matter**, because the actual standardized weights will be calculated by the software. For instance, in a three-indicator analytic composite, assigning the relative weights as 1, 0.5 and 0.25 (each weight being the preceding weight divided by 2) has the same effect as assigning them as 0.3, 0.15 and 0.075.

Analytic composites may also be used to reduce common structural variation in a model (Kock, 2021a) and in what-if analyses (Kock et al., 2018). In what-if analyses, analytic composites are designed as replacements for certain latent variables in simulations aimed at manipulating correlations with other latent variables to better reflect what would happen under certain conditions – e.g., if professional programmers were considered instead of students in software development tasks (Kock et al., 2018).

B.4.8. Instrumental variables: Endogeneity

The menu option "Explore analytic composites and instrumental variables" also allows you to create instrumental variables (see Figure B.4.8). Instrumental variables are variables that selectively share variation with other variables, and only with those variables. Instrumental variables can be used to test and control for endogeneity; a situation that occurs when the structural error term for an endogenous variable is correlated with one or more of the variable's predictors. For example, let us consider a simple population model (i.e., "true" model) with the following latent variable links: A > B and B > C.

Save Close Help What to create? Instrumental variable creation mode Instrumental variable Single stochastic variation sharing Notes: start by choosing what to create, analytic composites are aggregations of indicators with set weights, where the weights are defined by the user based on theory and past research, instrumental variables can be used in many applications, such as controlling for endogeneity and analyzing reciprocal (nonrecursive) relationships. Mode: Single stochastic variation sharing Available (click to choose only one): Selected (click to remove) ** Avadable instruments Lat. vars. (click to choose one or more): Indicators (click to choose one or more) " Instruments to be used Selected (click to remove): D Lat. var Lat. var Std. regression coeff. 0.248 0.098 Pisalue < 0.001 < 0.001 Correla with lat yers 0.098 Correlation 0.104 -0.0360.248 0.101 0.024 Create instrumental variable (click)?

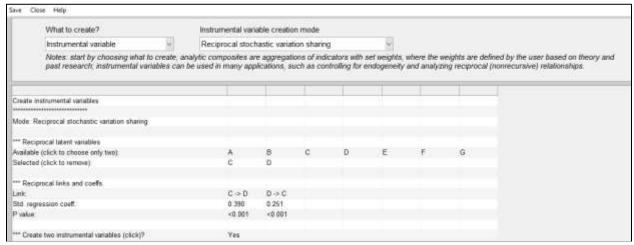
Figure B.4.8. Using instrumental variables to address endogeneity

This model presents endogeneity with respect to C, because variation flows from A to C via B, leading to a biased estimation of the path for the link B > C via ordinary least squares regression. Adding a link from A to C could be argued as "solving the problem", but in fact it creates an even more problematic scenario: the possibility of a type I error, since the link A > C does not exist at the population level. A more desirable solution to this problem is to create an instrumental variable iC, incorporating only the variation of A that ends up in C and nothing else, and revise the model so that it has the following links: A > B, B > C and iC > C. The link iC > C can be used to test for endogeneity, via its P value and effect size. This link (i.e., iC > C) can also be used to control for endogeneity, thus removing the bias when the path coefficient for the link B > C is estimated via ordinary least squares regression. To create instrumental variables so that you can test and control for endogeneity you should use the sub-option "Single stochastic variation sharing". The underlying technique, variation sharing, is discussed by Kock & Sexton (2017).

B.4.9. Instrumental variables: Reciprocity

Instrumental variables can also be used to estimate **reciprocal relationships** (see Figure B.4.9). For this, you should use the sub-option "**Reciprocal stochastic variation sharing**" (Morrow & Conger, 2021). A third sub-option, labeled "Instrument variables composite", is available for completeness but is not recommended. (This third sub-option refers to an old method used in econometrics to address endogeneity that unfortunately tends to add massive collinearity to almost any model.)

Figure B.4.9. Using instrumental variables to estimate reciprocal relationships



To illustrate the sub-option "Reciprocal stochastic variation sharing" let us consider a population model with the following latent variable links: A > C, B > D, C > D and D > C. To test the reciprocal relationship (Morrow & Conger, 2021) between C and D you should first control for endogeneity in C and D, due to variation coming from B and A respectively, by creating two instrumental variables iC and iD via the sub-option "Single stochastic variation sharing" and adding these variables to the model. Next you should create two other instrumental variables through the sub-option "Reciprocal stochastic variation sharing", which we will call here iCrD and iDrC, referring to the conceptual reciprocal links C > D and D > C respectively. (No links between C and D should be included in the model graph, since reciprocal links cannot be directly represented in this version of this software.)

The final model, with all the links, will be as follows: A > C, iC > C, B > D, iD > D, iDrC > D and iCrD > C. Here the link iDrC > D represents the conceptual link C > D, and can be used to test this conceptual link; and the link iCrD > C represents the conceptual link D > C, and can be used to test this conceptual link. In this example it is possible that significant collinearity may be added to the model -e.g., between iDrC and C, and/or iCrD and D – particularly for reciprocal effects of medium to large sizes. Given this, the model should be tested for full collinearity (through the inspection of full collinearity variance inflation factors) prior to the inclusion of the reciprocal instrumental variables, and only for vertical collinearity (through the inspection of block variance inflation factors) after those instrumental variables are included in the model.

B.4.10. Categorical-numeric-categorical conversion

The menu option "**Explore categorical-numeric-categorical conversion**" allows you to perform categorical-to-numeric and numeric-to-categorical conversions (see Figure B.4.10). In a **numeric-to-categorical** conversion one or more of the following numeric variables are converted into a single data label variable: latent variable, standardized indicator, and/or unstandardized indicator. This option is useful in multi-group analyses (Kock, 2014a) where the investigator wants to employ more than one numeric field for grouping. For example, let us assume that the following two unstandardized indicators are available: C, with the values 1 and 0 referring to individuals from the countries of Brazil and New Zealand; and G, with the values 1 and 0 referring to females and males. By using a numeric-to-categorical conversion a researcher could create a new data label variable to conduct a multi-group analysis based on four groups: "C=1G=1" (females from Brazil), "C=1G=0" (males from Brazil), "C=0G=1" (females from New Zealand), and "C=0G=0" (males from New Zealand).

Save Close Help Conversion type Categorical-to-numeric conversion mode Categorical-to-numeric Anchor-factorial with fixed variation Notes: start by selecting a conversion type, categorical variables are stored as label variables, each categorical to-numeric conversion employs at least one anchor latent variable, possible anchor latent variables are priority-ordered from left to right, numeric-to-categorical conversions can be useful in multi-group analyses Categorical-to-numeric conversion Mode: Anchor-factorial with fixed variation Current categorical variables Click to choose (only one) JSatGroup ECollabGroup Categorical variable to be convened Selected inlick to remove? JSatGroup (2 catgs.) (N=300) Possible anchor latent variables ECollab*Projmgt Click to chaose one or more Success ECellab. Abs. correl, with categorical variable 0.822 0.209 0.008 0.007 0.005 Latent variables to be used (None selected) (None pelected) * Create numeric variable (click)?

Figure B.4.10. Explore categorical-numeric-categorical conversion

In a **categorical-to-numeric** conversion a user can convert a categorical variable, stored as a data label variable, into a numeric variable that is then added to the dataset as a new standardized indicator. This new variable can subsequently be used as a new indicator of an existing latent variable, or as a new latent variable with only one-indicator (i.e., as a structural variable, making up the inner model). Three **categorical-to-numeric conversion modes** are available: anchorfactorial with fixed variation, anchor-factorial with variation diffusion (Kock, 2020b), and anchor-factorial with variation sharing. The following general rules of thumb are recommended for the use of these modes. The **anchor-factorial with fixed variation** mode should be employed when the new variable is expected to be included in the model as a new indicator of an existing latent variable; here if more than one anchor is chosen, only the anchor with the highest correlation will be used. The **anchor-factorial with variation diffusion** mode (Kock, 2020b)

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should be employed when the new variable is expected to be included in the model as a control variable; this option may be useful in multilevel analyses (Kock, 2020b), as a more sophisticated alternative to the group mean variable approach discussed by Kock & Hadaya (2018). The **anchor-factorial with variation sharing** mode should be employed when the new variable is expected to be included in the model as a one-indicator latent variable (i.e., as a structural variable with one single indicator) that is expected to significantly influence and/or be influenced by other latent variables in the model.

B.4.11. Consistent PLS outputs

The menu option "Explore Dijkstra's consistent PLS outputs" (see Figure B.4.11) allows you to obtain key outputs generated based on Dijkstra's consistent PLS (a.k.a. PLSc) technique, so named in honor of its developer – Theo K. Dijkstra. These outputs include PLSc reliabilities for each latent variable, also referred to as Dijkstra's rho_a's, which appear to be, in many contexts, better approximations of the true reliabilities than the measures usually reported in PLS-based SEM contexts – the composite reliability and Cronbach's alpha coefficients.

Figure B.4.11. Explore Dijkstra's consistent PLS outputs

ave Close Help						
	y for default value d if T ratio > critic	these outp			sts employing PLSc reliabilite I for directional hypotheses, i	
				18		

PLSc reliabilities (Dijkstra's rho_a's)						

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	0.706	0.672	0.651	0.691	1,000	

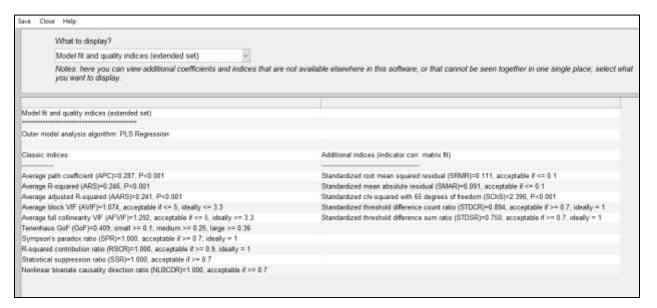
PLSc loadings						
	EColtab .	Projringt	Success	JSat	ECollab*Projmgt	
EColab1	0.575					
ECollab2	0.443					
ECollab3	0.820					
Projingt1		0.597				
Projmgt2		0.649				
Projmgt3		0.661				
Success1			0.623			
Success2			0.599			
Success3			0.633			
JSat1				0.768		
JSat2				0.574		
JS#3				0.560		
TOTAL BARBON COMME				1000	4.000	

Also included in the outputs generated via this menu option are PLSc loadings; along with the corresponding standard errors, one-tailed and two-tailed P values, T ratios, and confidence intervals. Given that some of these outputs depend on the confidence level used, this menu option allows you to set that confidence level. As noted earlier, normally the confidence level used is the complement of the significance level used (i.e., 1 minus the significance level used). For instance, if the significance level used is 0.05, then the confidence level used should normally be set at 0.95 (which is also the software's default).

B.4.12. Additional model fit and quality indices

The menu option "Explore additional coefficients and indices" allows you to obtain an extended set of model fit and quality indices (see Figure B.4.12). This extended set of model fit and quality indices includes the classic indices normally included in reports of SEM analyses employing this software, as well as new indices that allow investigators to assess the fit between the model-implied and empirical indicator correlation matrices (Kock, 2020c). These new indices are the standardized root mean squared residual (SRMR), standardized mean absolute residual (SMAR), standardized chi-squared (SChS), standardized threshold difference count ratio (STDCR), and standardized threshold difference sum ratio (STDSR).

Figure B.4.12. Extended set of model fit and quality indices



As with the classic model fit and quality indices, the interpretation of these new indices depends on the goal of the SEM analysis. Since these indices refer to the fit between the model-implied and empirical indicator correlation matrices (Kock, 2020c), they become more meaningful when the goal is to find out whether one model has a better fit with the empirical data than another model. In many cases additional insights can be obtained by using these indices in conjunction with the classic indices. When assessing the model fit with the data, several criteria are recommended. These criteria are discussed below, together with the discussion of these new model fit and quality indices (Kock, 2020c).

SRMR and **SMAR**. The SRMR index is calculated as the square root of the mean of the sum of the squared differences between the contents of non-redundant cells of the model-implied and empirical indicator correlation matrices. The SMAR index is calculated as the mean of the sum of the absolute differences between those matrices. The model-implied indicator correlation matrix is obtained based on the model parameters (e.g., weights and loadings) estimated by the software. The empirical indicator correlation matrix is simply the matrix containing the correlations among the indicators used in the model. The non-redundant cells of these matrices are the upper or lower triangular cells, excluding the diagonal cells. Generally **SRMR** and **SMAR** values lower than **0.1** indicate acceptable fit (Kock, 2020c).

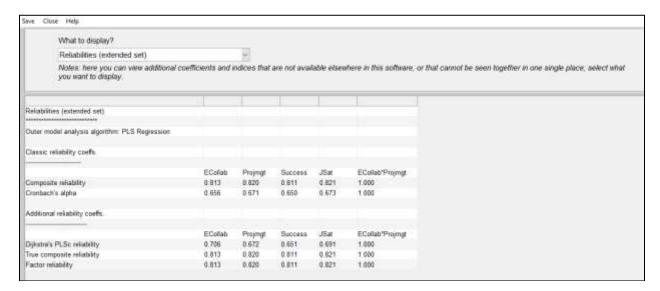
SChS. The SChS index is calculated as the chi-squared coefficient obtained from a test of independence comparing the contents of non-redundant cells of the model-implied and empirical indicator correlation matrices. Here the contents of non-redundant cells of the model-implied indicator correlation matrix are treated as the observed values in a chi-squared test of independence, whereas the corresponding values in the empirical indicator correlation matrix are treated as the expected values. The number of degrees of freedom is calculated as the number of non-redundant cells minus 1, in line with what is usually done in traditional chi-squared tests of independence. For simplicity and consistency of application with respect to other model fit and quality indices, the P value associated with each SChS is calculated as the complement of the P value generated by the chi-squared test of independence (i.e., 1 minus that P value). Normally acceptable fit is indicated by a P value associated with a SChS that is equal to or lower than 0.05; that is, significant at the 0.05 level (Kock, 2020c). This refers to the modified P value; the smaller it is, the better the fit.

STDCR and STDSR. The STDCR and STDSR indices are measures of the extent to which a model is free from instances in which the contents of non-redundant cells of the model-implied indicator correlation matrix differ significantly from the corresponding empirical indicator correlation matrix values. Here a heuristic threshold is used to establish whether two values differ significantly; this threshold is 0.2, twice the model-wide acceptable fit threshold for the SRMR and SMAR indices. The STDCR is calculated by dividing the number of non-redundant cells where significant differences do not exist by the total number of non-redundant cells. The STDSR index is calculated as the complement of the ratio obtained by dividing the sum of the absolute values of the differences between non-redundant cells where a significant difference exists by the total sum of the absolute values of the differences between non-redundant cells. These new STDCR and STDSR indices are calculated so that they can be used in ways analogous to other classic fit indices generated by this software. Generally values of the STDCR and STDSR equal to or greater than 0.7 indicate acceptable fit (Kock, 2020c).

B.4.13. Additional reliability coefficients

The menu option "Explore additional coefficients and indices" also allows you to obtain an extended set of reliabilities (or reliability coefficients). This extended set of reliabilities (see Figure B.4.13) includes the classic reliability coefficients normally included in reports of SEM analyses employing this software, plus the following, for each latent variable in your model: Dijkstra's PLSc reliability (also available via the menu option "Explore Dijkstra's consistent PLS outputs"), true composite reliability, and factor reliability.

Figure B.4.13. Extended set of reliability coefficients



When factor-based PLS algorithms are used in analyses, the **true composite reliability** and the **factor reliability** are produced as estimates of the reliabilities of the true composites and factors (Kock, 2015b; 2017; 2019a; 2019b; 2019c). They are calculated in the same way as composite reliabilities, but with different loadings. These reliabilities are calculated *after* the iterative estimation process is complete, based on the final true composite and factor estimates, whereas the composite reliabilities are calculated *during* the iterative estimation process. When classic composite-based (i.e., non-factor-based) algorithms are used, both true composites and factors coincide, and are approximated by the composites generated by the software. As such, true composite and factor reliabilities equal the corresponding composite reliabilities whenever composite-based algorithms are used.

B.4.14. Additional discriminant validity outputs

The menu option "Explore additional coefficients and indices" also allows you to obtain an extended set of discriminant validity coefficients (see Figure B.4.14). This extended set of discriminant validity coefficients includes the classic coefficients used in discriminant validity assessment normally included in reports of SEM analyses employing this software, namely the correlations among latent variables and the square roots of those latent variables' AVEs (shown on a table, with the square roots of AVEs along the diagonal). To these are added the following discriminant validity assessment coefficients: structure loadings and cross-loadings, full collinearity VIFs and HTMT ratios.

Save Close Help What to display? Discriminant validity coefficients (extended set) Notes: here you can view additional coefficients and indices that are not available elsewhere in this software, or that cannot be seen together in one single place, select what you want to display Full collinearity VFs ECollab "Projmgt **ECollab** JSat 1.154 1.126 1.279 1.587 1.312 HTMT meios (good # < 0.90, best if < 0.85) **ECollab** 0.530 Promat 0.229 0.472 Success 0.093 0.126 ECollat/Projmgt P values (one-tailed) for HTMT ratios Success JSst ECullab 'Projingt

Figure B.4.14. Extended set of discriminant validity coefficients

HTMT ratios have been proposed for discriminant validity assessment particularly in the context of composite-based SEM via classic PLS algorithms; as opposed to factor-based SEM via modern algorithms that estimate factors (which have been available from this software for quite some time now). Our simulations suggest that these HTMT ratios are not particularly useful when used in combination with factor-based algorithms; the classic correlations among latent variables and square roots of AVEs seem to be a better choice. For the HTMT ratios, the following coefficients are also provided: P values, and 90% confidence intervals.

B.5. Settings

The "**Settings**" menu options allow you to view or change general SEM analysis settings (see Figure B.5). Here you can select the analysis algorithm used in the SEM analysis, the resampling method used to calculate standard errors and P values, as well as other elements that will define how the SEM analysis will be conducted. These menu options are discussed individually below. Several of them are discussed in more detail later in this document.

Figure B.5. Settings menu options

View or change general settings

View or change individual inner model analysis algorithm settings

View or change moderating effects settings

View or change missing data imputation settings

View or change data modification settings

View or change individual latent variable weight and loading starting value settings

The "View or change general settings" option allows you to set the outer model analysis algorithm, default inner model analysis algorithm, resampling method, and number of resamples. Through these sub-options, users can set outer and default inner model algorithms separately. Users are also allowed to set inner model algorithms for individual paths through a different option. If users choose not to set inner model algorithms for individual paths in an analysis of a new model (i.e., a model that has just been created), their choice of default inner model algorithm is automatically used for all paths.

The "View or change individual inner model analysis algorithm settings" option allows you to set inner model algorithms for individual paths. That is, for each path a user can select a different algorithm from among the following choices: "Linear", "Warp2", "Warp2 Basic", "Warp3", and "Warp3 Basic". This option is particularly useful in empirical investigations where researchers have solid theoretical reasons to expect certain paths to be associated with nonlinear relationships of particular types (for an example of nonlinear theorizing in an action research context see: Kock et al., 2017). Those researchers may also have solid theoretical reasons to expect certain paths to be associated with linear relationships. Given that one of the main goals of SEM is to test theory, theoretical considerations should be given a very high priority in the selection of algorithms to be used for each path in a model.

The "View or change moderating effects settings" option allows you to set the moderating effects calculation option to be used by the software. You can choose among three options for moderating effects calculation: **Two Stages**, **Variable Orthogonalization**, and **Indicator Products**. The default moderating effects calculation option is **Two Stages**. All of these options apply to moderating effects that are explicitly included in the model, Moderating effects involve moderating variables and moderating links; the latter occurring between the moderating variables and direct links to which the variables point. Another test of similar effects, which complements these three options, is the full latent growth test (Hubona & Belkhamza, 2021; Kock, 2020a). This test could be seen as a comprehensive analysis of moderating effects where the moderating variable is "latent", in the sense that it does not "disrupt" the model in any way. That is, in a full latent growth test, the moderating links are not explicitly included in the model, which makes its

results similar to those of multi-group analyses where no sample segmentation occurs (Kock, 2020a).

The "View or change missing data imputation settings" option allows you to set the missing data imputation method to be used by the software, from among the following methods: Arithmetic Mean Imputation (the software's default), Multiple Regression Imputation, Hierarchical Regression Imputation, Stochastic Multiple Regression Imputation, and Stochastic Hierarchical Regression Imputation. The missing data imputation method chosen will be used prior to execution of Step 3, and also after that when the option "Redo missing data imputation (via data pre-processing)" under the "Modify" menu option is selected. Kock (2014c) and Kock (2018a) provide a detailed discussion of these methods, as well as of a Monte Carlo simulation whereby the methods' relative performances are investigated.

The "View or change data modification settings" option allows you to select a range restriction variable type, range restriction variable, range (min-max values) for the restriction variable, and whether to use only ranked data in the analysis. Through these sub-options, users can run their analyses with subsamples defined by a range restriction variable, which is chosen from among the indicators available. They can also conduct their analyses with only ranked data, whereby all of the data is automatically ranked prior to the SEM analysis. When data on a ratio scale is ranked, typically the value distances that typify outliers are significantly reduced, effectively eliminating outliers without any decrease in sample size.

The "View or change individual latent variable weight and loading starting value settings" option allows you to set the initial values of the weights and loadings for each latent variable. The default is 1 for all weights and loadings. With this option, latent variables measured in a reversed way, as well as formative latent variables with most of their weights and loadings ending up being negative, can be more easily operationalized.

Several of the options above, and their component elements, are discussed in more detail in the subsections below, still in this section describing the main window options. These subsections include further discussions about data labels, general settings, data modification settings, individual inner model analysis algorithm settings, as well as individual latent variable weight and loading starting value settings. A further discussion of grouped descriptive statistics, which can be saved through a sub-option under the "Data" options, is also provided.

B.6. General settings

The "View or change general settings" option allows users to set the outer model analysis algorithm, default inner model analysis algorithm, resampling method, and number of resamples (see Figure B.6). Through these sub-options, users can set outer and default inner model algorithms separately. Users are also allowed to set inner model algorithms for individual paths, but through a different settings option. If users choose not to set inner model algorithms for individual paths, their choice of default inner model algorithm is automatically used for all paths.

Factor-Based PLS Type CFM3 Factor-Based PLS Type CFM2 Factor-Based PLS Type REG2 Warp2 Factor-Based PLS Type PTH2 Warp2 Basic Factor-Based PLS Type CFM1 Warp3 Factor-Based PLS Type REG1 Warp3 Basic Factor-Based PLS Type PTH1 **PLS** Regression Outer model analysis algorithm: PLS Mode M PLS regression PLS Mode M Basic PLS Mode A PLS Mode A Basic Default inner model analysis algorithm: PLS Mode B PLS Mode B Basic Robust Path Analysis Resampling method: Stable2 No. of resamples=sample size Stable3 Bootstrapping Jackknifing Blindfolding Parametric

Figure B.6. View or change general settings window

The settings chosen for each of the options can have a dramatic effect on the results of a SEM analysis. At the same time, the right combinations of settings can provide major insights into the data being analyzed. As such, the settings' options should be used with caution, and normally after a new project file (with a unique name) is created and the previous one saved. This allows users to compare results and, if necessary, revert back to project files with previously selected settings. Given that one of the main goals of SEM is to test theory, theoretical considerations should be given a very high priority in the selection of combinations of settings.

A key criterion for the calculation of the weights, observed in virtually all classic PLS-based algorithms, is that the regression equation expressing the relationship between the indicators and the latent variable scores has an error term that equals zero. In other words, in classic PLS-based algorithms the latent variable scores are calculated as exact linear combinations of their indicators. This is not the case with the "Factor-Based PLS" algorithms provided by this software, as these algorithms estimate latent variable scores fully accounting for measurement error (Kock, 2017; 2019a; 2019b; 2019c).

In nonlinear SEM analyses, the warping takes place during the estimation of path coefficients, and after the estimation of all weights, latent variable scores, and loadings in the model. The weights and loadings of a model with latent variables make up what is often referred to as the

outer model (a.k.a. measurement model), whereas the path coefficients among latent variables make up what is often called the **inner model (a.k.a. structural model)**.

B.6.1. Outer model analysis algorithms

The outer model analysis algorithms available are Factor-Based PLS Type CFM3, Factor-Based PLS Type CFM2, Factor-Based PLS Type REG2, Factor-Based PLS Type PTH2, Factor-Based PLS Type CFM1, Factor-Based PLS Type REG1, Factor-Based PLS Type PTH1, PLS Regression, PLS Mode M, PLS Mode M Basic, PLS Mode A, PLS Mode A Basic, PLS Mode B, PLS Mode B Basic, and Robust Path Analysis. All of these outer model algorithms share a common characteristic. They calculate latent variable scores as exact linear combinations of their indicators, or of their indicators and measurement errors. With the exception of the Robust Path Analysis algorithm, all of these algorithms perform iterations until they converge to a solution.

There has been a long and in some instances fairly antagonistic debate among proponents and detractors of the use of Wold's original PLS algorithms (Adelman & Lohmoller, 1994; Kock, 2015b; 2019a; 2019b; 2019c; Lohmöller, 1989; Wold, 1980) in the context of SEM. This debate has been fueled by one key issue, which is analogous to the issue underlying the related principal components versus factor analysis debate. **Wold's original PLS algorithms do not deal with actual factors**, as covariance-based SEM algorithms do; **but with composites**, which are exact linear combinations of indicators (Kock, 2015a; 2015b; 2017; 2019a; 2019b; 2019c). **The "Factor-Based PLS" algorithms** provided by this software **have been developed specifically to address this perceived limitation** of Wold's original PLS algorithms.

The Factor-Based PLS Type CFM3, Factor-Based PLS Type CFM2 and Factor-Based PLS Type CFM1 algorithms generate estimates of both true composites and factors, in two stages, explicitly accounting for measurement error (Kock, 2015b; 2017). Like covariance-based SEM algorithms, these algorithms are fully compatible with common factor model assumptions, including the assumption that all indicator errors are uncorrelated. In their first stages, these algorithms employ a new "true composite" estimation sub-algorithm, which estimates composites based on mathematical equations that follow directly from the common factor model. The second stage employs a new "variation sharing" sub-algorithm, which can be seen as a "soft" version of the classic expectation-maximization algorithm (Dempster et al., 1977; Kock, 2015b; Kock & Sexton, 2017) used in maximum likelihood estimation, with apparently faster convergence and nonparametric properties. The Factor-Based PLS Type **CFM3** algorithm employs both loadings and reliabilities from Dijkstra's consistent PLS (a.k.a. PLSc) technique; the former (i.e., loadings) to improve computation efficiency, and the latter (i.e., reliabilities) to estimate measurement error and true composite weights. The Factor-Based PLS Type CFM2 algorithm employs reliabilities from Dijkstra's consistent PLS technique, but not loadings. The Factor-Based PLS Type CFM1 algorithm does not employ Dijkstra's consistent PLS technique at all, instead using Cronbach's alpha coefficients to estimate measurement error and true composite weights.

Factor-Based PLS Type REG2, Factor-Based PLS Type PTH2, Factor-Based PLS Type REG1 and Factor-Based PLS Type PTH1 are also factor-based PLS algorithms that generate estimates of both composites and factors, in two stages, fully accounting for measurement error. The Factor-Based PLS Type REG2 and Factor-Based PLS Type REG1 algorithms first estimate composites via PLS Regression (discussed below), and then estimate factors employing variation sharing (Kock, 2015b; 2017; Kock & Sexton, 2017). Among the factor-based algorithms available in this software, these Factor-Based PLS Type REG2 and Factor-Based PLS Type REG1 algorithms can be seen as the closest to Wold's original PLS design. The Factor-Based PLS Type REG2 algorithm employs reliabilities from Dijkstra's consistent PLS

technique to estimate measurement error and true composite weights; the **Factor-Based PLS Type REG1** algorithm employs Cronbach's alpha coefficients for that purpose.

The Factor-Based PLS Type PTH2 and Factor-Based PLS Type PTH1 algorithms first estimate composites via Robust Path Analysis (discussed below), and then estimate factors employing variation sharing (Kock, 2015b; 2017; Kock & Sexton, 2017). By doing so, these algorithms address several of the concerns about Wold's original PLS algorithms raised in an important critical article by Rönkkö & Evermann (2013). These algorithms can also be seen as addressing the call for simplicity made in a thought-provoking article on PLS by Rigdon (2012). These algorithms share a common characteristic with the algorithms discussed above. The Factor-Based PLS Type PTH2 algorithm employs reliabilities from Dijkstra's consistent PLS technique to estimate measurement error and true composite weights; while the Factor-Based PLS Type PTH1 algorithm employs Cronbach's alpha coefficients to estimate those weights.

Unlike the Factor-Based PLS Type CFM3, Factor-Based PLS Type CFM2 and Factor-Based PLS Type CFM1 algorithms; the **Factor-Based PLS Type REG2**, **Factor-Based PLS Type PTH2**, **Factor-Based PLS Type REG1** and **Factor-Based PLS Type PTH1** algorithms **do not impose certain common factor model assumptions** that some researchers have claimed do normally hold in practice, such as the assumption that all indicator errors are uncorrelated.

PLS Regression has been the default outer model algorithm since the software's inception, and is maintained as such as a matter of tradition. This algorithm iterates until the outer model weights become stable with the following calculations being performed in successive iterations for each latent variable in the model: (a) the outer model weights are calculated through a least squares regression where the latent variable is the predictor and the indicators are the criteria; and (b) the latent variable is calculated as an exact linear combination of the indicator scores (Kock & Mayfield, 2015; Kock & Moqbel, 2016). In the PLS Regression algorithm, the inner model does not influence the outer model. That is, the weights are not influenced by the links connecting latent variables, which are created by the user in Step 4.

The following outer model algorithms are similar to PLS Regression, but in them the inner model influences the outer model: PLS Mode M, PLS Mode M Basic, PLS Mode A, PLS Mode A Basic, PLS Mode B, and PLS Mode B Basic. These are classic PLS algorithms that have been historically associated with PLS-based SEM software (Chatelin et al., 2002; Kock, 2016a; Kock & Mayfield, 2015; Kock & Moqbel, 2016; Temme et al., 2006). In them, the iterative process leading to the calculation of latent variable scores involves the intermediate calculation of path coefficients, correlations, and signs of correlations. These are used as inputs in the calculation of weights in successive iterations, typically leading to the addition of collinearity among latent variables that are linked.

The above collinearity inflation that occurs when the inner model influences the outer model often has the effect of strengthening associations among linked latent variables, but not enough to overcome to underestimation bias inherent in composite-based SEM algorithms (Kock, 2015a; 2015b). This tendency toward collinearity inflation is a relatively small but real phenomenon that has been presented as a weakness of PLS-based SEM, and that has been referred to as the "capitalization on error" problem of PLS-based algorithms (see, e.g., Goodhue et al., 2012; Kock & Hadaya, 2018). This problem is generally overstated, as PLS-based algorithms in general tend to also reduce collinearity compared to covariance-based SEM. That is, when the inner model influences the outer model collinearity is indeed increased, but often not to the extent that the increase offsets the previous collinearity decrease that normally results from the use of PLS-

based algorithms. Moreover, capitalization on error is only a problem in cases where minimum sample size requirements are significantly underestimated (Kock & Hadaya, 2018).

PLS Mode M is often referred as the "MIMIC" or "mixed" mode. In it, the inner model influences the outer model through path coefficients. The outer model is estimated employing factor-to-indicators or indicators-to-factor causality stances, depending on whether latent variables are defined as formative or reflective (Kock & Mayfield, 2015; Kock & Moqbel, 2016). PLS Mode M in fact uses either PLS Mode A or PLS Mode B, based on whether latent variables are defined as reflective or formative, respectively. The PLS modes A and B are discussed below.

PLS Mode M Basic is a variation of PLS Mode M in which the inner model influences the outer model through the signs of correlations among latent variables. This corresponds to what Lohmöller (1989) refers to as a "basic scheme", also referred to as a "centroid scheme" (Kock & Mayfield, 2015; Kock & Moqbel, 2016; Tenenhaus et al., 2005).

For the purposes of PLS-based SEM, the schemes known as "centroid" and "factorial" are largely redundant (Kock & Mayfield, 2015; Kock & Moqbel, 2016; Tenenhaus et al., 2005), but they share a common property. They tend to reduce the number of instances of Simpson's paradox (Kock, 2015e; Kock & Gaskins, 2016; Wagner, 1982) in the SEM analysis results. Because of this property and the fact that these two schemes are redundant, this software implements only one of them, the "centroid" scheme. This scheme is referred to as "basic", for simplicity and consistency with prior seminal publications that set the foundations of PLS-based SEM (see, e.g., Kock & Mayfield, 2015; Kock & Moqbel, 2016; Lohmöller, 1989).

PLS Mode A is often referred to as the "reflective" mode, which is arguably incorrect because both reflective and formative latent variables can be used with this algorithm (Kock & Mayfield, 2015; Kock & Moqbel, 2016). In other words, using PLS Mode A does not make a formative latent variable become a reflective latent variable (Kock & Mayfield, 2015). In it, the inner model influences the outer model through path coefficients and correlations, depending on whether the links go into or out from each latent variable, respectively. In this mode the outer model weights are calculated through a least squares regression where the latent variable is the predictor and the indicators are the criteria. PLS Mode A Basic is a variation of PLS Mode A in which the inner model influences the outer model through the signs of the correlations among latent variables.

PLS Mode B is often referred to as the "formative" mode. This is arguably incorrect for the same reason discussed above, namely that both reflective and formative latent variables can be used with this algorithm (Kock & Mayfield, 2015; Kock & Moqbel, 2016). In other words, using PLS Mode B does not turn a reflective latent variable into a formative latent variable. However, PLS Mode B is often less stable than PLS Mode A, and also tends to cause a significant increase in collinearity among linked latent variables (Kock, 2021a; Kock & Mayfield, 2015). In it, the inner model influences the outer model through path coefficients and correlations, depending on whether the links go into or out from each latent variable, respectively. In this mode the outer model weights are calculated through a least squares regression where the indicators are the predictors and the latent variable the criterion. **PLS Mode B Basic** is a variation of PLS Mode B in which the inner model influences the outer model through the signs of the correlations among latent variables.

The **Robust Path Analysis** algorithm is a simplified algorithm in which latent variable scores are calculated by averaging the scores of the indicators associated with the latent variables. That is, in this algorithm weights are not estimated through PLS Regression. This algorithm is called

"robust" path analysis, because a standard path analysis (where all latent variables are measured through single indicators) can be conducted through it, and the P values can be calculated through the nonparametric resampling or stable methods implemented through the software. If all latent variables are measured with single indicators, the Robust Path Analysis algorithm will yield latent variable scores and various parameters that are identical to those generated through the other algorithms, but with greater computational efficiency.

B.6.2. Inner model analysis algorithms

Many relationships in nature, including relationships involving behavioral variables, are nonlinear (Kock, 2010; 2016c; Kock & Gaskins, 2016) and follow a pattern known as U-curve (or inverted U-curve). In this pattern a variable affects another in a way that leads to a maximum or minimum value, where the effect is either maximized or minimized, respectively (Kock, 2010; 2016c; Kock & Gaskins, 2016). This type of relationship is also referred to as a J-curve pattern; a term that is more commonly used in economics and the health sciences. For an example of nonlinear theorizing in an action research context see: Kock et al. (2017).

The term "U-curve" is used here also to refer to nonlinear relationships that can be represented as sections of a U curve. As such, it covers all noncyclical nonlinear relationships. These relationships include the logarithmic, hyperbolic decay, exponential decay, exponential, and quadratic relationships, among others. That is, these relationships can be conceptually modeled as variations of U-curve relationships (Kock, 2010; 2016c; Kock & Gaskins, 2016; Kock et al., 2017).

The **default inner model analysis algorithms** available are the following: **Linear, Warp2, Warp2 Basic, Warp3, and Warp3 Basic**. All of these inner model algorithms share a common characteristic. They calculate path coefficients through least squares regression algorithms based on the latent variable scores calculated through one of the outer model analysis algorithms available.

The **Linear** algorithm does not perform any warping of relationships. The **Warp2** algorithm tries to identify U-curve relationships among linked latent variables, and, if those relationships exist, the algorithm transforms (or "warps") the scores of the predictor latent variables (Kock, 2010; 2016c) so as to better reflect the U-curve relationships in the estimated path coefficients in the model. Here the signs of the path coefficients are initially (i.e. prior to the inner model least squares regressions) assigned as the signs of the corresponding path coefficients obtained without any warping. Similarly to the outer model "basic" versions, the **Warp2 Basic** algorithm is a variation of the Warp2 algorithm that tends to reduce the number of instances of Simpson's paradox (Kock, 2015e; Kock & Gaskins, 2016; Wagner, 1982) in the final results. This happens because in this basic version the signs of path coefficients are initially assigned as the signs of the corresponding correlations obtained without any warping.

The **Warp3** algorithm, the default algorithm used by the software, tries to identify relationships among latent variables defined by functions whose first derivatives are U-curves (Kock, 2010; Kock & Gaskins, 2016). These types of relationships follow a pattern that is more similar to an S-curve (or a somewhat distorted S-curve). An S-curve can be seen as a combination of two connected U-curves, one of which is inverted (Kock, 2010). Examples of S-curve functions are the sigmoid, hyperbolic sine and hyperbolic tangent. The logistic function is a type of sigmoid function, and thus is also an example of S-curve function. Similarly to the Warp2 Basic algorithm, the **Warp3 Basic** algorithm is a variation of the Warp3 algorithm that tends to reduce the number of instances of Simpson's paradox (Kock, 2015e; Kock & Gaskins, 2016; Wagner, 1982) in the final results. Again, here this happens because the signs of path coefficients are initially assigned as the signs of the corresponding correlations obtained without any warping.

In summary, with the exception of the "Linear" algorithm, all of the default inner model analysis algorithms perform nonlinear transformations on the predictor latent variable scores prior to the calculation of path coefficients. In other words, except for the "Linear" algorithm, these algorithms "warp" the predictor latent variable scores by finding best-fitting nonlinear

functions that minimize sums of squared residuals on a bivariate basis (Kock, 2010; Kock & Gaskins, 2016). This process can be seen as another least squares minimization stage that is "in between" those used in the calculation of latent variable scores and path coefficients.

B.6.3. Resampling methods

One of several resampling methods may be selected for the calculation of P values and related coefficients (e.g., standard errors). In the calculation of P values, a one-tailed test is generally recommended if the coefficient is assumed to have a sign (positive or negative), which should be reflected in the hypothesis that refers to the corresponding association (Kock, 2015a). Hence this software reports one-tailed P values for coefficients used in hypothesis testing (e.g., path coefficients); from which two-tailed P values can be easily obtained if needed (Kock, 2015a). The software also reports at several points, in addition to one-tailed P values: two-tailed P values, T ratios, and confidence intervals. The available **resampling methods** used to generate standard errors, which are in turn used in the calculation of P values and other hypothesis-testing coefficients (Kock, 2014b; 2016b; 2018b), are the following: **Stable1, Stable2, and Stable3, Bootstrapping, Jackknifing, Blindfolding, and Parametric**.

With the **Stable1** method, the software's default up until version 4.0 (when it was called simply the "stable" method), P values are calculated through nonlinear fitting of standard errors to empirical standard errors generated with the other resampling methods available. In other words, the Stable1 method could be viewed as a quasi-parametric method that yields P values that try to approximate the "average" P values generated by the software's other resampling methods.

The **Stable2** and **Stable3** methods have been developed as alternatives to the Stable1 method. Unlike the Stable1 method, they rely on the direct application of exponential smoothing formulas (for details, see: Kock, 2014b and Kock, 2018b), and that can thus be more easily implemented and tested by methodological researchers. Several Monte Carlo experiments show that the **Stable2** and **Stable3** methods yield estimates of the actual standard errors that are consistent with those obtained via bootstrapping, in many cases yielding more precise estimates of the actual standard errors (Kock, 2014b; 2018b; Kock & Hadaya, 2018). The more accurate of the two methods seems to be the Stable3 method, which also appears to be more accurate than the Stable1 method. As such, **the Stable3 method is set as the software's default** starting in version 5.0.

With the **Parametric** method, P values are calculated assuming multivariate normality and also that path coefficient estimates are distributed as expected based on the central limit theorem. Neither the **Parametric** method nor the three "stable" methods (**Stable1**, **Stable2** and **Stable3**) actually generates resamples, so calling them resampling methods is done here for simplicity in the grouping of settings options. Because no resamples are generated, these are the most efficient of the methods from a computing load perspective. These methods can be particularly useful in the analysis of large datasets, as in these cases creating resamples can be computationally very taxing. With the emergence of the concept of "big data", the need to analyze large datasets is becoming increasingly common.

Bootstrapping employs a resampling algorithm that creates a number of resamples (a number that can be selected by the user), by a method known as "resampling with replacement". This means that each resample contains a random arrangement of the rows of the original dataset, where some rows may be repeated. The commonly used analogy of a deck of cards being reshuffled, leading to many resample decks, is a good one; but not entirely correct because in Bootstrapping the same "card" may appear more than once in each of the resample "decks".

Jackknifing, on the other hand, creates a number of resamples that equals the original sample size, and where each resample has one row removed. That is, the sample size of each resample is the original sample size minus 1. Thus, **when Jackknifing is selected the number of resamples**

is automatically set as the sample size. This refers to the most common form of jackknifing, also known as "delete-1" and "classic" jackknifing, which is the one implemented through this software.

Blindfolding employs a resampling algorithm that creates a number of resamples (a number that can be selected by the user) by a method whereby each resample has a certain number of rows replaced with the means of the respective columns. The number of rows modified in this way in each resample equals the sample size divided by the number of resamples. For example, if the sample size is 200 and the number of resamples selected is 100, then each resample will have 2 rows modified. If a user chooses a number of resamples that is greater than the sample size, the number of resamples is automatically set to the sample size (as with Jackknifing).

The default number of resamples for Bootstrapping and Blindfolding is 100. It can be modified by entering a different number in the appropriate edit box. (Please note that we are talking about the number of resamples here, not the sample size of the original dataset.) **Leaving the number of resamples for Bootstrapping as 100 is recommended** because it has been shown that higher numbers of resamples lead to negligible improvements in the reliability of P values (see, e.g., Goodhue et al., 2012). In fact, according to the original developer of the Bootstrapping method, even setting the number of resamples at 50 is likely to lead to fairly reliable P value estimates (Efron et al., 2004).

Conversely, increasing the number of resamples well beyond 100 leads to a higher computation load on the software, making the software look like it is having a hard time coming up with the results. In very complex models, a high number of resamples may make the software run very slowly. Some researchers have suggested in the past that a large number of resamples can address problems with the data, such as the presence of outliers due to errors in data collection. This opinion is not shared by the original developer of the Bootstrapping method, Bradley Efron (see, e.g., Efron et al., 2004).

Not considering the "stable" methods, arguably Jackknifing is particularly good at addressing problems associated with the presence of outliers due to errors in data collection. Generally speaking, Jackknifing tends to generate more stable resample path coefficients (and thus more reliable P values) with small sample sizes (lower than 100), and with samples containing outliers (see, e.g., Chiquoine & Hjalmarsson, 2009). Monte Carlo simulations suggest that the "stable" methods perform better than Jackknifing in this respect (Kock, 2014b; 2018b).

Again, not considering the "stable" methods, Bootstrapping tends to generate more stable resample path coefficients (and thus more reliable P values) with larger samples and with samples where the data points are evenly distributed on a scatter plot. Monte Carlo simulations suggest that the "stable" methods perform better than Bootstrapping in this respect as well (Kock, 2014b; 2018b). The use of Bootstrapping with small sample sizes (lower than 100) has been discouraged (Nevitt & Hancock, 2001; Kock, 2018b).

Generally speaking, Bootstrapping and Jackknifing can be seen as complementary resampling methods, in that one tends to perform well in situations where the other does not, and vice-versa. Nevertheless, the "stable" methods provided by this software seem to be an improvement over them, as indicated by Monte Carlo simulations (Kock, 2014b; Kock, 2018b). A set of related Monte Carlo simulations reported by Kock & Hadaya (2018) suggests that the "stable" methods help avoid the "capitalization on error" problem, often associated with PLS-based SEM, when appropriate sample sizes are employed in empirical studies (see, also: Kock, 2018b).

Blindfolding tends to perform somewhere in between Jackknifing and Bootstrapping. If the number of resamples is set as very close to the sample size, particularly with small sample sizes

(lower than 100) and with samples containing outliers, Blindfolding performs similarly to Jackknifing. With larger samples and with samples where the data points are evenly distributed on a scatter plot, Blindfolding tends to performs more like Bootstrapping, especially when the number of resamples is set as the same for both algorithms.

Prior to the development of the "stable" methods, a recommendation was usually made in connection with Bootstrapping and Jackknifing. Since the warping algorithms are also sensitive to the presence of outliers, the recommendation was to estimate P values with both Bootstrapping and Jackknifing, which are complementary resampling methods, and use the P values associated with the most stable coefficients. An indication of instability is a high P value (i.e., statistically non-significant) associated with path coefficients that could be reasonably expected to yield low P values. For example, with a sample size of 100, a path coefficient of 0.2 could be reasonably expected to yield a P value that is statistically significant at the 0.05 level. If that is not the case, there may be a stability problem. Another indication of instability is a marked difference between the P values estimated through Bootstrapping and Jackknifing.

The recommendation above was based on the fact that P values can be easily estimated using two or more resampling methods by following the simple procedure outlined as follows. Run a SEM analysis of the desired model, using one of the resampling methods, and save the project. Then save the project again, this time with a different name, change the resampling method, and run the SEM analysis again. Then save the second project again. Each project file will now have results that refer to one of the resampling methods. The P values can then be compared, and the most stable ones used in a research report on the SEM analysis. While this is a perfectly valid approach for the calculation of P values, as the coefficients to which the P values refer do not change across analyses, it is very important to fully disclose this to the readers of the research report (or reports) written based on the SEM analyses.

An alternative to the above approach is the use one of the "stable" methods, particularly the Stable3 method (see, e.g., Kock, 2014b; 2018b; Kock & Hadaya, 2018), as these methods can be seen as yielding P values that are consistent with and often more precise than the P values generated by the software's other resampling methods. Using these "stable" methods has the advantage of requiring much less manual work from the user. Based on various tests in the context of PLS-based SEM, it seems that the Stable3 method yields fairly reliable results for path coefficients associated with direct effects (Kock, 2014b; 2018b; Kock & Hadaya, 2018). It is less clear if the Stable3 method, or any of the other "stable" methods, is advisable for the calculation of P values for path coefficients associated with indirect and total effects, and research in this area is ongoing.

B.7. Individual inner model algorithm settings

The "View or change individual inner model algorithm settings" option allows users to set inner model algorithms for individual paths (see Figure B.7). The algorithms available are the same as those that can be selected as default inner model analysis algorithms: Linear, Warp2, Warp2 Basic, Warp3, and Warp3 Basic.

Figure B.7. View or change individual inner model algorithm settings

	Natu	Perform	Fluency	Fluency*Natu	Warp2
Natu					
Perform	LN		LN	LN	Warp2 basic Warp3
Fluency	LN				
Fluency*Natu				Warp3 basic	

Individual inner model algorithms can be set for both regular and interaction effect latent variables; the latter are associated with moderating effects. Since **moderating effects** themselves **incorporate nonlinearity**, it is usually recommended that they be **set here as "Linear"**; otherwise **the nonlinearity inherent in moderation** is **captured by the nonlinear algorithm chosen**, in many cases rendering the **moderating effect non-significant** (Kock & Gaskins, 2016). If no choice is made for an individual inner model algorithm, the default inner model analysis algorithm is used. If a model is changed after an analysis is conducted, the individual inner model algorithms are set to the default inner model analysis algorithm.

This option allows users to customize their analyses based on theory and past empirical research. If theory or results from past empirical research suggest that a specific link between two latent variables is linear, then the corresponding path can be set to be analyzed using the Linear algorithm. Conversely, if theory or results from past empirical research suggest that a specific link between two latent variables should have the shape of a U curve (or J curve), the corresponding path can be set to be analyzed using the Warp2 algorithm or the Warp2 Basic algorithm. Kock et al. (2019) provide an example of explicit linear and nonlinear theorizing with respect to different links in the same model, leading to linear and nonlinear relationships being assessed simultaneously.

B.8. Moderating effects settings

The "View or change moderating effects settings" option allows you to set the moderating effects calculation option to be used by the software. You can choose among three options for moderating effects calculation: Two Stages, Variable Orthogonalization, and Indicator Products. The default moderating effects calculation option is Two Stages, whereby latent variable scores are calculated first and then used in a second stage for the creation of the interaction (or product) latent variable that implements the moderating effect. The Variable Orthogonalization option implements a similar procedure, but stochastically departs from a random variable, which is by definition fully orthogonal to all of the latent variables in the model, for the creation of the interaction variable that implements the moderating effect. This is done via a technique similar to the variation sharing method described by Kock (2019a), which is the foundation of modern factor-based SEM algorithms that go from composites to factors. The Indicator Products option employs indicator products for the creation of the interaction variable that implements the moderating effect, a classic approach used in PLS-based SEM.

Unless a model is improperly specified, and the improper specification leads to severe biases, the options Two Stages and Variable Orthogonalization should yield fairly similar results. An example of a situation in which this would not occur would be a model that suffers from severe endogeneity, in which case the Variable Orthogonalization option may yield more trustworthy results. These two options should also yield results similar to the Indicator Products option when classic composite-based PLS algorithms are used. On the other hand, if factor-based PLS algorithms are used, the results produced by the Indicator Products option should differ, particularly if the number of indicators of the interaction variable that implements the moderating effect is small (e.g., in the single digits). The reason for this is that the interaction variable that implements the moderating effect is treated as a factor by factor-based PLS algorithms.

If the Indicator Products option is used, the number of indicators of the interaction variable is the product of the number of indicators of the moderating variable and the number of indicators of the predictor variable in the link that is moderated. For example, if the number of indicators of the moderating variable is 3, and the number of indicators of the predictor variable in the link that is moderated is 4, then the number of indicators of the interaction variable is 12. When the number of indicators of the interaction variable becomes large, then the reliability of the corresponding true composite and factor converge. As this happens, the true composite and factor also converge (Kock, 2019a). This is a variation of the phenomenon sometimes referred to as "consistency at large" (Wold et al., 2001). This is why the results produced by the Indicator Products option should differ from the results yielded by the other options, if: (a) the number of indicators of the interaction variable that implements the moderating effect is small, and factor-based PLS algorithms are used.

All of the above options apply to moderating effects that are explicitly included in the model. Moderating effects involve moderating variables and moderating links; the latter occurring between the moderating variables and direct links to which the variables point. **Another test of similar effects, which complements the above options, is the full latent growth test** (also implemented by this software, but via a different menu option). This test could be seen as a comprehensive analysis of moderating effects where the moderating variable is "latent", in the sense that it does not "disrupt" the model in any way (Hubona & Belkhamza, 2021; Kock, 2020a). That is, in a full latent growth test, the moderating links are not explicitly included in the

model, which makes its results similar to those of multi-group analyses where no sample segmentation occurs (Kock, 2020a).

Of the options above, the one most likely to yield results similar to full latent growth (Kock, 2020a) is the Variable Orthogonalization option. The reason for this is that a latent variable that is fully orthogonal to the other latent variables in the model would "not be seen" by those other latent variables; i.e., it would not "disrupt" the model in any way. However, **there is a key difference between the Variable Orthogonalization option and full latent growth**. The Variable Orthogonalization option departs from a fully orthogonal variable, but this variable ends up being correlated with the endogenous variable to which its interaction (or product) latent variable points – unless the moderating effect is zero. Since the endogenous variable in question is likely correlated with other latent variables in the model, then the interaction (or product) latent variable also is correlated with those other latent variables.

B.9. Missing data imputation settings

The "View or change missing data imputation settings" option allows you to set the missing data imputation method to be used by the software, from among the following methods: Arithmetic Mean Imputation (the software's default), Multiple Regression Imputation, Hierarchical Regression Imputation, Stochastic Multiple Regression Imputation, and Stochastic Hierarchical Regression Imputation. Kock (2014c) and Kock (2018a) provide a detailed discussion of these methods, as well as of a Monte Carlo simulation whereby the methods' relative performances are investigated. The missing data imputation method chosen will be used prior to execution of Step 3, and also after that when the option "Redo missing data imputation (via data pre-processing)" under the "Modify" menu option is selected.

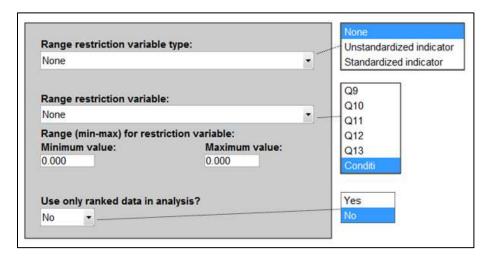
As noted above, a Monte Carlo simulation was conducted to assess the performance of five missing data imputation methods implemented through this software: Arithmetic Mean Imputation, Multiple Regression Imputation, Hierarchical Regression Imputation, Stochastic Multiple Regression Imputation, and Stochastic Hierarchical Regression Imputation. The detailed results are provided later in this document; see also: Kock (2014c) and Kock (2018a). In summary, Multiple Regression Imputation yielded the least biased mean path coefficient estimates, followed by Arithmetic Mean Imputation. When we look at mean loading estimates, Arithmetic Mean Imputation yielded the least biased results, followed by Stochastic Hierarchical Regression Imputation, and Hierarchical Regression Imputation.

Compared with the no missing data condition, none of the methods induced a reduction in standard errors for path coefficients. This is noteworthy since prior results outside the context of PLS-based SEM have tended to show a significant downward bias in standard errors, particularly for non-stochastic missing data imputation varieties. Such downward bias in standard errors has led to concerns regarding an inflation in type I errors, and warnings against the use of single missing data imputation methods in general (Enders, 2010; Kock, 2014c; 2018a; Newman, 2014). Our results strongly suggest that such concerns may not be warranted in the context of PLS-based SEM.

B.10. Data modification settings

The "View or change data modification settings" option allows users to run their analyses with subsamples defined by a range restriction variable, which is chosen from among the indicators available. (After Step 5 is completed, latent variable scores can also be added to the model as standardized indicators.). This option also allows users to conduct their analyses with only ranked data (see Figure B.10).

Figure B.10. View or change data modification settings



Two **range restriction variable types** are available: standardized and unstandardized indicators. This means that the range restriction variable can be either a standardized or unstandardized indicator. **Once a range restriction variable is selected, minimum and maximum values must be set (i.e., a range)**, which in turn has the effect of restricting the analysis to the rows in the dataset within that particular range.

The option of selecting a range restriction variable and respective range is useful in multi-group analyses (Kock, 2014a) "done by hand", as opposed to using the menu options "Explore multi-group analyses" or "Explore full latent growth". In a multi-group analysis "done by hand" separate analyses are conducted for group-specific subsamples, saved as different project files, and the results then compared against one another. One example would be a multi-country analysis, with each country being treated as a subsample, but without separate datasets for each country having to be provided as inputs.

Let us assume that an unstandardized variable called "Country" stores the values "1" (for Brazil), "2" (for New Zealand), and "3" (for the USA). To run the analysis only with data from Brazil one can set the range restriction variable as "Country" (after setting its type as "Unstandardized indicator"), and then set both the minimum and maximum values as "1" for the range.

This range restriction feature is also useful in situations where outliers are causing instability in a resample set, which can lead to abnormally high standard errors and thus inflated P values. Users can remove outliers by restricting the values assumed by a variable to a range that excludes the outliers, without having to modify and re-read a dataset.

Users can also select an option to conduct their analyses with only **ranked data**, whereby all of the data is automatically ranked prior to the SEM analysis (the original data is retained in

unranked format). When data measured on ratio scales is ranked, typically the value distances that typify outliers are significantly reduced, effectively eliminating outliers without any decrease in sample size. Contrary to popular belief, this cannot be achieved through standardization alone.

Often some information is lost due to ranking - e.g., the distances among data points based on answers on ratio scales. Thus a concomitant increase in collinearity may be observed, but typically not to the point of threatening the credibility of the results. The option of using only ranked data in the analysis can be very useful in assessments of whether the presence of outliers significantly affects path coefficients and respective P values, especially when outliers are not believed to be due to measurement error.

B.11. Weight and loading starting value settings

The "View or change individual latent variable weight and loading starting value settings" option allows users to set the initial values of the weights and loadings for each latent variable (see Figure B.11). This is a specialized option that will only rarely be used. The default starting value for all latent variables is 1. While any real number can be used here, normally only -1 and 1 are used.

Figure B.11. View or change individual latent variable weight and loading starting value settings

Natu	Perform	Fluency	Fluency*Natu
1.00	1.00	1.00	1.00
Note: do n	ot forget to sa	ve your settin	gs.

This option reflects a little known characteristic of classic PLS-based SEM analyses, which is that they do not always converge to the same solution. The estimated coefficients depend on the starting values of weights and loadings, thus leading to different solutions depending on the initial configurations of those starting values. Even in simple models, often at least two solutions exist – as long as latent variables are used, with multiple indicators. By convention the solution most often accepted as valid is the one associated with the default starting value for all latent variables, which is 1.

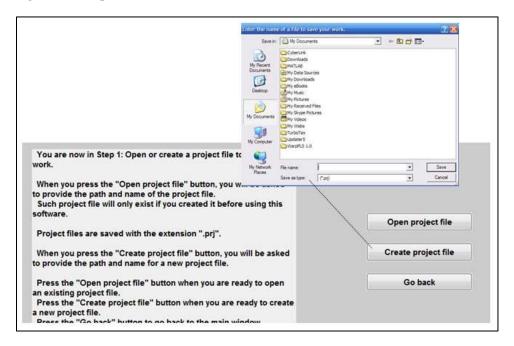
With this option, latent variables measured in a reversed way can be more easily operationalized. An example would be a latent variable reflecting boredom being measured through a set of indicators that individually reflect excitement. In this type of scenario, generally the starting value of weights and loadings for the latent variable should be set to -1.

This option can also be useful with formative latent variables for which most of the weights and loadings end up being negative after an analysis is conducted. In this case, paths associated with the latent variable may end up being reversed, leading to conclusions that are the opposite of what is hypothesized. The solution here would normally be a change in sign for starting value of weights and loadings, usually from 1 to -1.

C. Step 1: Open or create a project file to save your work

In Step 1 you will open or create a project file to save your work (see Figure C.1). **Project files are saved with the ".prj" extension, and contain all of the elements needed to perform a SEM analysis**. That is, they contain the original data used in the analysis, as well as information pertaining to the graphical model, the inner and outer model structures, and the results.

Figure C.1. Step 1 window



Once an original data file is read into a project file, the original data file can be deleted without effect on the project file. The project file will store the original location and file name of the data file so that this information is available in case it is needed in the future, but the project file will no longer use the data file.

Project files may be created with one name, and then renamed using Windows Explorer or another file management tool. Upon reading a project file that has been renamed in this fashion, the software will detect that the original name is different from the file name, and will adjust accordingly the name of the project file that it stores internally.

Different users of this software can easily exchange project files electronically if they are collaborating on a SEM analysis project. This way they will have access to all of the original data, intermediate data, and SEM analysis results in one single file. Project files are relatively small. For example, a complete project file of a model containing 5 latent variables, 32 indicators (columns in the original dataset), and 300 cases (rows in the original dataset) will typically be only approximately 200 KB in size. Simpler models may be stored in project files as small as 50 KB.

If a project file created with a previous version of the software is open, the software automatically recognizes that and converts the file to the new version. This takes placed even with project files where all of the five steps of the SEM analysis were completed. However, because each new version incorporates new features, with outputs stored within new or modified

software objects, normally **previous versions of the software cannot properly reuse project files created with more recent versions**.

D. Step 2: Read the raw data used in the SEM analysis

Through Step 2, you will read the raw data used in the SEM analysis (see Figure D.1). While this should be a relatively trivial step, it is in fact one of the steps where users have the most problems with other SEM software. Often a SEM software application will abort, or freeze, if the raw data is not in the exact format required by the SEM software, or if there are any problems with the data, such as missing values (empty cells).

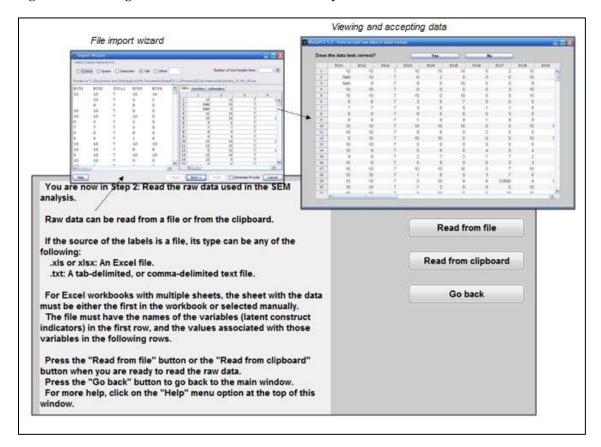


Figure D.1. Reading the raw data used in the SEM analysis

The buttons "Read from file" and "Read from clipboard" allow you to read raw data into the project file from a file or from the clipboard, respectively. This software employs an import wizard that avoids most data reading problems, even if it does not entirely eliminate the possibility that a problem will occur. Click only on the "Next" and "Finish" buttons of the file import wizard, and let the wizard do the rest. Soon after the raw data is imported, it will be shown on the screen, and you will be given the opportunity to accept or reject it. If there are problems with the data, such as missing column names, simply click "No" when asked if the data looks correct.

Raw data can be read directly from Excel files, with extensions ".xls" or ".xlsx", or text files where the data is tab-delimited or comma-delimited. When reading from an ".xls" or ".xlsx" file that contains a workbook with multiple worksheets, make sure that the worksheet that contains the data is the first on the workbook. If the workbook has multiple worksheets, the file import wizard used in Step 2 will typically select the first worksheet as the source or raw

data. If the desired worksheet is not the first in the workbook, in many cases the user will be able to select the proper worksheet through the wizard, but this selection can lead to mistakes when made by novice users. **Raw data files, whether Excel or text files, must have indicator names in the first row, and numeric data in the following rows**. They may contain empty cells, or missing values; these will be automatically replaced with values calculated by one of the missing data imputation algorithms available in a later step.

The "View or change missing data imputation settings" option under "Settings" allows you to set the missing data imputation method to be used by the software in the next step. Users may want to employ non-automated approaches to deal with missing data, such as deleting the rows with missing cells, or manually replacing them with the average of nearby values on the same column. The most widely used approach, and also a reasonably reliable one in the context of PLS-based SEM, is replacing the missing values with column averages. This missing data imputation method is called "Arithmetic Mean Imputation", and is automated by the software. It is in fact the software's default missing data imputation method. Kock (2014c) and Kock (2018a) provide a detailed discussion of various missing data imputation methods, as well as of a Monte Carlo simulation whereby the methods' relative performances are investigated.

While missing data imputation is done automatically by the software, you should not use datasets with too many missing values, as this will distort the results. A general rule of thumb is that your dataset should not have any column with more than 10 percent of its values missing; a more relaxed rule would be to set the threshold to 20 percent (Hair et al., 1987; 2009). On the other hand, Kock (2014c) and Kock (2018a) show that even 30 percent of missing data will still not lead to significant bias (from the perspective of theory testing) with any of the missing data imputation methods employed by this software. One can reduce the percentage of missing values per column by deleting rows in the dataset, where the deleted rows are the ones that refer to the columns with missing values.

One simple test can be used to try to find out if there are problems with a raw data file. Try to open it with a spreadsheet software program (e.g., Excel), if it is originally a text file; or try to create a tab-delimited text file with it, if it is originally a spreadsheet file. If you try to do either of these things, and the data looks corrupted (e.g., missing column names, misplaced columns, cells containing unrecognized symbols etc.), then it is likely that the original file has problems, which may be hidden from view. For example, a spreadsheet file may be corrupted, but that may not be evident based on a simple visual inspection of the contents of the file.

Common sources of problems are data files where variables storing numeric data are mixed in with data label variables. (The latter are often called "categorical variables", and store text or alphanumeric data). Users should make sure that numeric data is separated from text or alphanumeric data, and also separately read into the software. The latter (i.e., text or alphanumeric data) can be read into data label variables, but certain precautions must be taken. Check the discussion in connection with the "Modify" menu option for more details; the "Modify" menu option is available from the software's main window. When reading numeric data into the software, column names (i.e., headings) must not be numeric; in these cases, column names must be text or alphanumeric.

E. Step 3: Pre-process the data for the SEM analysis

In Step 3 the raw data will be pre-processed for the SEM analysis. This is mostly an automatic process, requiring only a few button clicks from you. This step will correct problems with the data, such as: identical column names, columns with zero variance, and missing data.

The "View or change missing data imputation settings" option allows you to set the missing data imputation method to be used by the software in this step. Missing data imputation can be redone after this step, if you later decide to use a different imputation method. To accomplish that you should use the option "Redo missing data imputation (via data pre-processing)" under the "Modify" menu option. Kock (2014c) and Kock (2018a) provide a detailed discussion of missing data imputation methods, as well as of a Monte Carlo simulation comparing the methods' relative performances.

This step will also let you know if the data has rank problems, which usually happens when the sample size is very small relative to the number of existing indicators. A related cause of rank problems is a sample with many repeated or linearly dependent values on different rows or columns, which sometimes is an indication of data fabrication. Please note that the term "rank" here comes from matrix algebra, and is unrelated to the same term used in the context of ranked data, as discussed earlier in connection with the software settings.

If there are rank problems, this does not mean that you cannot proceed with the SEM analysis. However, the results may be unstable and, in some cases, completely unreliable. On the other hand, it is not uncommon for rank problems to be reported and still the results of the ensuing SEM analysis turn out to be reliable. This is due to the general robustness methods for SEM analysis implemented by this software.

At the end of this step, a window will be displayed with the pre-processed data, which will be standardized. Standardized data columns have means that equal zero and standard deviations that equal one. If you use the Arithmetic Mean Imputation method for dealing with missing data (the software's default), previously missing values will be shown as zero, since they were replaced with the averages (or means) of the columns. Standardized data usually ranges from -4 to 4, with outliers assuming values toward the left or right end of those extremes, sometimes beyond -4 or 4.

Outliers can significantly change the shape of a nonlinear relationship, but this may also be the case with linear relationships. For example, one single outlier may change the sign of a linear association, from positive to negative (i.e., changing the relationship from direct to inverse). Because of this, there is invariably the temptation of removing outliers from analyses. This is often a mistake (Giaquinta, 2009; Hair et al., 2009; Kock, 2016a), as outliers can be invaluable in elucidating the true nature of an association (Kaiser, 2010; Kock, 2011b; Rosenthal & Rosnow, 1991; Wold et al., 2001). Generally speaking, outliers should only be removed if there are good reasons to believe that they are due to measurement error.

After the software displays the pre-processed and standardized data, typically you will accept the data and move on to the next step. If the data looks corrupted, do not accept it; click on the "No" button when asked if the data looks correct. If there are problems in this step, they will usually be related to problems with the raw data file. Check that file, and see if you can correct those problems.

As mentioned before in this manual, one simple test can be used to try to find out if there are problems with a raw data file. Try to open it with a spreadsheet program, if it is originally a text file; or to try to create a tab-delimited text file with it, if it is originally a spreadsheet file. If you

try to do either of these things, and the data looks "messed up" (e.g., corrupted, or missing column names), then it is likely that the original file has problems, which may be hidden from view. For example, a spreadsheet file may be corrupted, but that may not be evident based on a simple visual inspection of the contents of the file using spreadsheet software.

F. Step 4: Define the variables and links in the SEM model

In Step 4 you will define the latent variables and links in the SEM model. The sub-steps that make up this step are discussed in more detail in the subsections below. This software employs a graphical interface that allows users to create and edit model elements visually and directly; i.e., without the need of a scripting language.

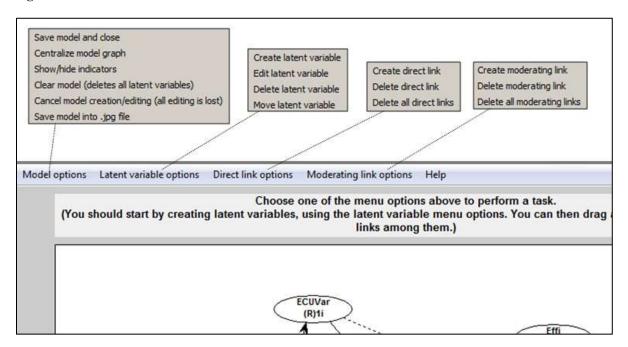
You will define the latent variables by selecting the indicators that are associated with them, and the measurement method used – either formative or reflective. The process of defining the latent variables in a SEM model in this fashion is often called "defining the outer model", in SEM lingo.

Model links can be of two types, direct and moderating links. Direct links connect pairs of latent variables. Moderating links connect latent variables and direct links; that is, they refer to effects in which a latent variable moderates the relationship between a pair of latent variables. The process of defining model links is often referred to as "defining the inner model".

F.1. Create or edit SEM model

The window used to create or edit a model is shown in Figure F.1. A model can be edited if it has been created and saved before as part of a project. While editing or creating a model you can choose from a number of menu options related to overall model functions, latent variable functions, direct link functions, and moderating link functions. As with other windows in this software, there is a help menu option that provides access to this manual, displayed as a PDF file. The help menu option also provides links to Web resources.

Figure F.1. Create or edit the SEM model window



A guiding text box is shown at the top of the model editing and creation window. The content of this guiding text box changes depending on the menu option you choose, guiding you through the sub-steps related to each option. For example, if you choose the option "Create latent variable", the guiding text box will change color, and tell you to select a location for the latent variable on the model graph.

Direct links are displayed as full arrows in the model graph, and **moderating links as dashed arrows**. Each latent variable is displayed in the model graph within an oval symbol, where its name is shown above a combination of alphanumerical characters with this general format: "(F)16i". The "F" refers to the measurement model; where "F" means formative, and "R" reflective. The "16i" reflects the number of indicators of the latent variable, which in this case is 16.

Save model and close. This option saves the model within the project, and closes the model editing and creation window. This option does not, however, save the project file. That is, the project file has to be saved for a model to be saved as part of it. This allows you to open a project file, change its model, run a SEM analysis, and discard all that you have done, if you wish to do so, reverting back to the previous project file.

Centralize model graph. This option centralizes the model graph, and is useful when you are building complex models and, in the process of doing so, end up making the model visually

unbalanced. For example, you may move variables around so that they are all accidentally concentrated on the left part of the screen. This option corrects that by automatically redrawing all symbols in the model graph so that the center of the model graph coincides with the center of the model screen.

Show/hide indicators. This option shows or hides the list of indicators for each latent variable. The indicators are shown on a vertical list next to each latent variable, and without the little boxes that are usually shown in other SEM software. This display option is used to give the model graph a cleaner look. It also has the advantage that it saves space in the model graph for latent variables. Normally you will want to keep the indicators hidden, except when you are checking whether the right indicators were selected for the right latent variables. That is, normally you will show the indicators to perform a check, and then hide them during most of the model building process.

Clear model (deletes all latent variables). This option deletes all latent variables, essentially "clearing" the model. Given that choosing this option by mistake can potentially cause some serious loss of work (not to mention some major user aggravation), the software shows a dialog box asking you to confirm that you want to clear the model before it goes ahead and deletes all latent variables. Even if you choose this option by mistake, and confirm your choice also by mistake (a double mistake), you can still undo it by choosing the option "Cancel model creation/editing (all editing is lost)" immediately after clearing the model.

Cancel model creation/editing (all editing is lost). This option cancels the model creation or editing, essentially undoing all of the model changes you have made.

Save model into .jpg file. This option allows you to save the model graph into a .jpg file. You will be asked to select the file name and the folder where the file will be saved. After saved, this file can then be viewed and edited with standard picture viewers, as well as included as a picture into reports in other files (e.g., a Word file). Users can also generate model graph files by copying the model screen into a picture-editing application (e.g., Paint), cropping it to leave out unnecessary or unneeded areas, saving it into a picture file (e.g., .jpg or .png), and then importing that file into reports.

Create latent variable. This option allows you to create a latent variable, and is discussed in more detail below. Once a latent variable is created it can be dragged and dropped anywhere within the window that contains the model.

Edit latent variable. This option allows you to edit a latent variable that has already been created, and thus that is visible on the model graph.

Delete latent variable. This option allows you to delete an existing latent variable. All links associated with the latent variable are also deleted.

Move latent variable. This option is rarely used since, once a latent variable is created, it can be easily dragged and dropped with the pointing device (e.g., mouse) anywhere within the window that contains the model. This option is a carryover from a previous version, maintained for consistency and for those users who still want to use it. It allows a user to move a latent variable across the model by first clicking on the variable and then on the destination position.

Create direct link. This option allows you to create a direct link between one latent variable and another. The arrow representing the link points from the predictor latent variable to the criterion latent variable. Direct links are usually associated with direct cause-effect hypotheses; testing a direct link's strength (through the calculation of a path coefficient) and statistical significance (through the calculation of a P value) is equivalent to testing a direct cause-effect hypothesis.

Delete direct link. This option allows you to delete an existing direct link. You will click on the direct link that you want to delete, after which the link will be deleted.

Delete all direct links. This option deletes all direct links. Given that choosing this option by mistake is a possibility, the software shows a dialog box asking you to confirm that you want to execute it before it proceeds. Even if you choose this option by mistake, and confirm your choice also by mistake, you can still undo it by choosing the option "Cancel model creation/editing (all editing is lost)".

Create moderating link. This option allows you to create a link between a latent variable and a direct link. With some exceptions, both formative and reflective latent variables can be part of moderating links. Arguably this is not possible with the PLS modes M, A and B (see Lohmöller, 1989; Kock & Mayfield, 2015), which are usually the ones implemented through other PLS-based SEM software tools. Moderating links are typically associated with moderating cause-effect hypotheses, or interaction effect hypotheses. Testing a moderating link's strength (through the calculation of a path coefficient) and statistical significance (through the calculation of a P value) is equivalent to testing a moderating cause-effect or interaction effect hypothesis.

Moderating links should be used with moderation (no pun intended), because they may introduce multicollinearity into the model, and also because they tend to add nonlinearity to the model. By introducing multicollinearity into the model they may make some model parameter estimates unstable and biased.

By using the menu option "Explore full latent growth" users can completely avoid the above problems. This menu option is available from the main software window, and allows you to estimate the effects of a latent variable or indicator on all of the links in a model (all at once), without actually including any links between the variable and other variables in the model. A full latent growth analysis could be seen as a comprehensive analysis of moderating effects where the moderating variable is "latent", in the sense that it does not "disrupt" the model in any way (Hubona & Belkhamza, 2021; Kock, 2020a).

Delete moderating link. This option allows you to delete an existing moderating link. You will click on the moderating link that you want to delete, after which the link will be deleted.

Delete all moderating links. This option deletes all moderating links. Given that choosing this option by mistake is a possibility, the software shows a dialog box asking you to confirm that you want to execute it before it proceeds. Even if you choose this option by mistake, and confirm your choice also by mistake, you can still undo it by choosing the option "Cancel model creation/editing (all editing is lost)".

After you create a model and choose the option "Save model and close" a wait bar will be displayed on the screen telling you that the SEM model structure is being created. This is an important sub-step where a number of checks are made. In this sub-step, if there are any moderating links in the model, new latent variables are created to store information about those moderating effects. You can choose among three options for moderating effects calculation (via a different menu option): Two Stages, Variable Orthogonalization, and Indicator Products. The default moderating effects calculation option is Two Stages, whereby latent variable scores are calculated first and then used in a second stage for the creation of the interaction (or product) latent variable that implements the moderating effect.

The Indicator Products option uses a product-indicator procedure described and validated by Chin et al. (2003). If this option is employed, the more moderating links a model has, the longer the model structure creation sub-step will take. In models where only reflective variables are involved in a moderating link, typically this sub-step will not take longer than a few seconds.

Moderating links with formative variables may lead to longer wait times, because formative variables are usually more complex, frequently with significantly more indicators than reflective variables.

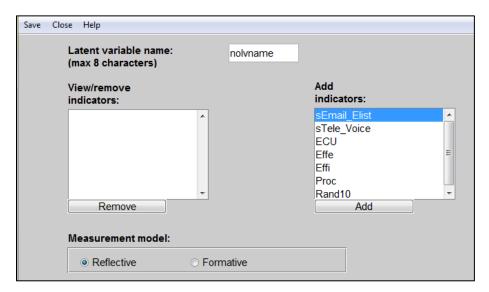
As noted above, instead of the product-indicator approach described by Chin et al. (2003), one can use an alternative approach (via the Two Stages option). This two-stage approach can also be implemented manually, which might be time-consuming. In the first stage of the manual implementation of this alternative approach, the latent variables that are part of a moderating relationship will be added to the model as new indicators. This can be done via the options "Add one or more latent variable (a.k.a. factor) scores as new standardized indicators" or "Add all latent variable (a.k.a. factor) scores as new standardized indicators", which are available under the "Modify" menu options. In the second stage, the new one-indicator latent variables will be used in the definition of a moderating relationship.

Yet another alternative is to conduct a full latent growth analysis (Hubona & Belkhamza, 2021; Kock, 2020a). As noted above, users can do this by using the menu option "**Explore full latent growth**". The "Explore full latent growth" menu option is available from the main software window, and allows you to estimate the effects of a latent variable or indicator on all of the links in a model (**all at once**), without actually including any links between the variable and other variables in the model. A full latent growth analysis could be seen as a comprehensive analysis of moderating effects where the moderating variable is "latent", in the sense that it does not "disrupt" the model in any way (Hubona & Belkhamza, 2021; Kock, 2020a).

F.2. Create or edit latent variable

The latent variable creation window is show in Figure F.2, and it is virtually identical to the latent variable editing window. The latent variable will appear in the model graph as soon as you click on the menu option under "Save", which saves the latent variable and closes the latent variable creation or editing window. A latent variable is not saved as part of a project until the model is saved as part of the project and the project file is saved.

Figure F.2. Create latent variable window



You create a latent variable by entering a name for it, which must have no more than 8 characters, but to which not many other restrictions apply. The latent variable name may contain letters, numbers, and even special characters such as "@" or "\$". It cannot contain the special symbols "*" or ":", however, because these symbols are used later by this software in selected outputs to indicate certain conditions (e.g., that a latent variable is associated with a moderating effect). After entering a name for a latent variable, you then select the indicators that make up the latent variable, and define the measurement model as reflective or formative.

A **reflective latent variable** is one in which all the indicators are expected to be highly correlated with one another, and with the latent variable itself (Kock & Mayfield, 2015). For example, the answers to certain question-statements by a group of people, measured on a 1 to 7 scale (1=strongly disagree; 7=strongly agree) and answered after a meal, are expected to be highly correlated with the latent variable "satisfaction with a meal". Among question-statements that would arguably fit this definition are the following two: "I am satisfied with this meal", and "After this meal, I feel full". Therefore, the latent variable "satisfaction with a meal", can be said to be reflectively measured through two indicators. Those indicators store answers to the two question-statements. This latent variable could be represented in a model graph as "Satisf", and the indicators as "Satisf1" and "Satisf2". Notwithstanding this simplified example, users should strive to have more than two indicators per latent variable; the more indicators, the better, since the number of indicators is inversely related to the amount of measurement error (Kock, 2015b; Nunnally, 1978; Nunnally & Bernstein, 1994).

A **formative latent variable** is one in which the indicators are expected to measure certain attributes of the latent variable, but the indicators are not expected to be highly correlated with

the latent variable itself, because they (i.e., the indicators) are not expected to be highly correlated with one another (Kock & Mayfield, 2015). For example, let us assume that the latent variable "Satisf" ("satisfaction with a meal") is now measured using the two following question-statements: "I am satisfied with the main course" and "I am satisfied with the dessert". Here, the meal comprises the main course, say, filet mignon; and a dessert, such as a fruit salad. Both main course and dessert make up the meal (i.e., they are part of the same meal) but their satisfaction indicators are not expected to be highly correlated with each other. The reason is that some people may like the main course very much, and not like the dessert. Conversely, other people may be vegetarians and hate the main course, but may like the dessert very much.

If the indicators are not expected to be highly correlated with one another, they cannot be expected to be highly correlated with their latent variable's score. Here is a general rule of thumb that can be used to decide if a latent variable is reflectively or formatively measured. If the indicators are expected to be highly correlated, and are redundant in their meaning, then the measurement model should be set as reflective. If the indicators are not expected to be highly correlated, and are clearly not redundant in meaning (they measure different facets of the same construct), even though they clearly refer to the same latent variable, then the measurement model should be set as formative.

Setting a latent variable as formative or reflective affects the calculation of model parameters only with the PLS Mode B algorithm, or with algorithms that employ the PLS Mode B algorithm or variations of it (e.g., PLS Mode B Basic, PLS Mode M). With other algorithms, setting a latent variable as formative or reflective is still recommended, as it helps the user interpret outputs and conduct certain assessments (e.g., validity assessments, discussed later in this manual).

Formative measurement has been facing increasing criticism, particularly since the late 1990s (Kock & Mayfield, 2015). See Edwards (2011) for a particularly critical and cogent discussion. Given this growing criticism, it is recommended that the Cronbach's alpha coefficients associated with formative latent variables be equal to or greater than 0.6, for reasons related to measurement error theory (Kock, 2015b; Nunnally, 1978; Nunnally & Bernstein, 1994). Since loadings tend to be relatively low with formative latent variables (and weights relatively high), reliability measures (such as the Cronbach's alpha coefficient) tend to also be relatively low. Nevertheless, Cronbach's alpha coefficients equal to or greater than 0.6 can be achieved by increasing the number of indicators used in formative measurement (Kock & Mayfield, 2015).

G. Step 5: Perform the SEM analysis and view the results

Step 5 performs the SEM analysis based on the model created in Step 4. After you click on the button to perform the SEM analysis, the software will show a wait bar. This wait bar will update you on the progress of the SEM analysis, which usually will take only a few seconds or less for simple to moderately complex models. As soon as the SEM analysis is completed, the software will show the results in graphical format on a window. That window also has menu options that allow you to view more details about the results, including some that are not shown on the graph (e.g., reliability measures), and also save the results into tab-delimited text files.

Collinearity is estimated before the SEM analysis is run. If collinearity appears to be too high, users are warned about it. A table with estimated latent variable correlations is shown, allowing users to identify the possible offending latent variables. If users so choose, they can proceed with the analysis anyway, but in most (not all) cases the full collinearity (a.k.a. multicollinearity) measures will confirm that collinearity is too high in their models for the analysis results to be considered credible.

Measurement error and composite weights are estimated before the SEM analysis is run, whenever factor-based PLS algorithms are used. Measurement error and composite weights play a key role in these algorithms. If at least one measurement error weight is greater than the corresponding composite weight, the user is warned about possible unreliability of results. This happens usually when at least one of the Cronbach's alpha coefficients associated with the latent variables is lower than 0.5. Foundational aspects of the factor-based PLS algorithms are discussed by Kock (2015b; 2019a; 2019c), and demonstrated empirically by Kock (2017; 2019a; 2019b; 2019c). Kock (2015b; 2019b) briefly lays out the mathematical basis of these algorithms, from which the importance of measurement error and composite weights can be gleaned.

New options become available from the main window after Step 5 is completed, under the "Modify" menu option. These options allow users to add one or more latent variable scores to the model as new standardized indicators, and also to add all latent variable scores as new indicators. Adding one or more latent variable scores at a time may be advisable in certain cases, such as in hierarchical analyses using selected latent variable scores as indicators at each level. In these cases, adding all latent variable scores at once may soon clutter the set of indicators available to be used in the SEM model.

The option of adding latent variable scores to the model as new standardized indicators is useful in the removal of outliers, through the use of restricted ranges for latent variable scores, particularly for outliers that are clearly visible on the plots depicting associations among latent variables. As briefly mentioned earlier, this option is also useful in hierarchical analyses, where users define second-order (and higher order) latent variables, and then conduct analyses with different models including latent variables of different orders.

New options become available from the main window after Step 5 is completed, under the "Explore" menu option, in addition to the option allowing users to estimate statistical power and minimum sample size requirements (available before Step 5). These options allow users to view T ratios and confidence intervals for various coefficients, estimate complex probabilities via conditional probabilistic queries, conduct full latent growth analyses (Kock, 2020a), conduct multi-group and measurement invariance analyses, create analytic composites (Kock, 2021a; Kock et al., 2018) and instrumental variables (which can be used to address endogeneity and analyze reciprocal relationships), perform numeric-to-categorical and categorical-to-numeric

conversions, view Dijkstra's consistent PLS outputs, view fit indices comparing indicator correlation matrices (shown together with other classic model fit and quality indices), and view new reliability measures generated in the context of factor-based PLS analyses (Kock, 2017; 2019a; 2019b; 2019c; 2020c). These menu options are discussed individually below.

This software uses algorithms that are fairly computing intensive, in some cases employing multiple checks and optimization sub-algorithms in each sub-step. Therefore the speed with which the analysis is conducted may be a little slower than that of some other publicly available SEM software. The differences in speed are not significant though, and normally the results generated by this software are more complete, and in many cases more reliable. For example, this software calculates model fit and quality indices, as well as P values for most of its parameter estimates. Publicly available PLS-based SEM software usually do not provide those measures.

Some model elements may reduce the speed of the SEM analysis more than others. These are: formative latent variables with many indicators and, more generally, latent variables with many indicators (even if they are reflective); moderating effects, particularly if they are associated with latent variables aggregating many indicators; setting the number of resamples for Bootstrapping or Blindfolding as 200 or higher; and using Jackknifing as the resampling method, if the sample size is larger than 200.

In Jackknifing, the number of resamples equals the sample size, which is why using Jackknifing as the resample method may reduce the speed of the SEM analysis with relatively large samples. Generating resamples and running calculations on them is one of the most computing intensive sub-steps of the SEM analysis. However, Jackknifing often produces more stable parameter estimates with warped analysis. So there is a tradeoff between speed and reliability when warping algorithms are being used. This tradeoff may tip the balance in favor of using Jackknifing, alone or in addition to Bootstrapping or Blindfolding, even if the user has to wait longer for the results.

An alternative is the use of the "stable" quasi-parametric methods: Stable 1, Stable 2, and Stable 3. This alternative is highly recommended, particularly with the Stable 3 method, the software's default. As their name implies, these methods yield stable coefficients. They also provide fairly accurate estimates of standard errors, which are used in the calculation of P values. These methods do not actually generates resamples, so calling them resampling methods is done here for simplicity in the grouping of settings options. Because no resamples are generated, these are rather efficient methods from a computing load perspective. These methods can be particularly useful in the analysis of large datasets, as in these cases creating resamples can be computationally very taxing. With the emergence of the concept of "big data", the need to analyze large datasets is becoming increasingly common.

H. View and save results

As soon as the SEM analysis is completed, the software shows the results in graphical format on a window, which also contains a number of menu options that allow you to view and save more detailed results (see Figure H.1.1). The graph with the results shows path coefficients, respective P values, and R-squared coefficients.

The "Save" menu options allow users to save most of the results that they can view, with the majority of those results saved under the option to save all classic model estimates into a tab-delimited text file. Additionally, users can save the factor scores calculated for each latent variable. These can be useful in some specialized applications; e.g., users may want to generate customized graphs based on those scores.

Save Close Help SEM analysis completed. The main results are shown in the graph below. You can now view and save other, more detailed, Choose one of the View or Save menu options above to do so. Save Close Help Save all classic model estimates into a tab-delimited .txt file View Save Close Help Save correlations among indicators into a tab-delimited .bxt file Save latent variable (a.k.a. factor) scores into a tab-delimited .bxt file View general results View path coefficients and P values View standard errors and effect sizes for path coefficients Effi View indicator loadings and cross-loadings (R)5i View indicator weights R2=0.22 -0.411 View latent variable coefficients View correlations among latent variables and errors p=-0.19 View block variance inflation factors View correlations among indicators p=0.29 (P<.01) View/plot linear and nonlinear relationships among latent variables (R)3 (R)71 View indirect and total effects R²=0.05 View causality assessment coefficients

Figure H.1.1. View and save results window

Just to be clear, the "factor" scores are the latent variable scores; even though classic PLS algorithms approximate latent variables though composites, not factors. This is generally perceived as a limitation of classic PLS algorithms (Kock, 2015a; 2015b; 2017; 2019a; 2019b; 2019c), which is addressed through the factor-based PLS algorithms offered by this software (Kock, 2017; 2019a; 2019b; 2019c). The latter, factor-based PLS algorithms, estimate latent variables through the estimation of the true factors. The term "factor" is often used when we refer to latent variables, in the broader context of SEM analyses in general. The reason is that factor analysis, from which the term "factor" originates, can be seen as a special case of SEM analysis.

The path coefficients are noted as beta coefficients. "Beta coefficient" is another term often used to refer to path coefficients in PLS-based SEM analyses; this term is commonly used in multiple regression analyses as well. The P values are displayed below the path coefficients, within parentheses. The R-squared coefficients are shown below each endogenous latent variable (i.e., a latent variable that is hypothesized to be affected by one or more other latent variables), and reflect the percentage of the variance in the latent variable that is explained by the latent variables that are hypothesized to affect it. To facilitate the visualization of the results, the path

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coefficients and P values for moderating effects are shown in a way similar to the corresponding values for direct effects, namely next to the arrows representing the effects.

H.1. View general results

General SEM analysis results include: the version of WarpPLS used in the SEM analysis; project file details, such as the project file name and when the file was last saved; model fit and quality indices (shown in Figure H.1.2), which are discussed in more detail below; and general model elements, such as the algorithm and resampling method used in the SEM analysis.

Figure H.1.2. General results window

Model fit and quality indices

Average path coefficient (APC)=0.196, P<0.001

Average R-squared (ARS)=0.169, P<0.001

Average adjusted R-squared (AARS)=0.164, P<0.001

Average block VIF (AVIF)=1.361, acceptable if <= 5, ideally <= 3.3

Average full collinearity VIF (AFVIF)=1.571, acceptable if <= 5, ideally <= 3.3

Tenenhaus GoF (GoF)=0.292, small >= 0.1, medium >= 0.25, large >= 0.36

Sympson's paradox ratio (SPR)=1.000, acceptable if >= 0.7, ideally = 1

R-squared contribution ratio (RSCR)=1.000, acceptable if >= 0.9, ideally = 1

Statistical suppression ratio (SSR)=1.000, acceptable if >= 0.7

Nonlinear bivariate causality direction ratio (NLBCDR)=0.861, acceptable if >= 0.7

Under the project file details, both the raw data path and file are provided. Those are provided for completeness, because once the raw data is imported into a project file, it is no longer needed for the analysis. Once a raw data file is read, it can even be deleted without any effect on the project file, or the SEM analysis.

Ten global model fit and quality indices are provided (Kock, 2010; 2014a; 2015d): average path coefficient (APC), average R-squared (ARS), average adjusted R-squared (AARS), average block variance inflation factor (AVIF), average full collinearity VIF (AFVIF), Tenenhaus GoF (GoF), Simpson's paradox ratio (SPR), R-squared contribution ratio (RSCR), statistical suppression ratio (SSR), and nonlinear bivariate causality direction ratio (NLBCDR).

Additional model fit and quality indices are available under the menu option "**Explore** additional coefficients and indices", which is itself under the "Explore" menu option that is available from the main software window. These additional indices allow investigators to assess the fit between the model-implied and empirical indicator correlation matrices (Kock, 2020c).

For the APC, ARS, and AARS, P values are also provided. These P values are calculated through a process that involves resampling estimations coupled with corrections to counter the standard error compression effect associated with adding random variables, in a way analogous to Bonferroni corrections (Kock, 2011c; 2014a; Rosenthal & Rosnow, 1991). This is necessary since the model fit and quality indices are calculated as averages of other parameters.

The interpretation of the model fit and quality indices depends on the goal of the SEM analysis. If the goal is to only test hypotheses, where each arrow represents a hypothesis, then the model fit and quality indices are, as a whole, of less importance. However, if the goal is to find out whether one model has a better fit with the original data than another, then the model fit and quality indices are a useful set of measures related to model quality. **When assessing the model fit with the data**, several criteria are recommended. These criteria are discussed below, together with the discussion of the model fit and quality indices.

APC, ARS and **AARS**. Typically the addition of new latent variables into a model will increase the ARS, even if those latent variables are weakly associated with the existing latent

variables in the model. However, that will generally lead to a decrease in the APC, since the path coefficients associated with the new latent variables will be low. (Here it is important to note that the APC is calculated based on the absolute values of the path coefficients.) Thus, the APC and ARS will counterbalance each other (Kock, 2010; 2011c), and will only increase together if the latent variables that are added to the model enhance the overall predictive and explanatory quality of the model. The AARS is generally lower than the ARS for a given model (see, e.g., Kock, 2015d). The reason is that it averages adjusted R-squared coefficients (Theil, 1958; Wooldridge, 1991), which themselves correct for spurious increases in R-squared coefficients due to predictors that add no explanatory value in each latent variable block. It is recommended that the P values for the APC, ARS and AARS all be equal to or lower than 0.05; that is, significant at the 0.05 level (Kock, 2011c). A more relaxed rule would be that the P values for the APC and ARS only be equal to or lower than 0.05.

AVIF and AFVIF. The AVIF index will increase if new latent variables are added to the model in such a way as to add vertical collinearity in the model's latent variable blocks. The AFVIF index will increase if new latent variables are added to the model in such a way as to add full collinearity into the model (i.e., either vertical or lateral collinearity; see Kock & Lynn, 2012). Full collinearity is often referred to as "muticollinearity". High AVIF and AFVIF values may result from the inclusion of new latent variables that overlap in meaning with existing latent variables (Kock, 2021a). It is generally undesirable to have different latent variables in the same model that measure the same underlying construct; those should be combined into one single latent variable. Thus, the AVIF and AFVIF indices bring in new dimensions that add to a comprehensive assessment of a model's overall predictive and explanatory quality. Because of the way in which these indices are calculated (for more details, see: Kock & Lynn, 2012), the AFVIF is not sensitive to variations in collinearity due to the use of nonlinear algorithms. The AVIF, on the other hand, is sensitive to the use of nonlinear algorithms. Therefore it is recommended that both indices, AVIF and AFVIF, be reported in studies, as they are not redundant indices. It is recommended (ideally) that both the AVIF and AFVIF be equal to or lower than 3.3, particularly in models where most of the variables are measured through two or more indicators. A more relaxed (acceptable) criterion is that both indices be equal to or lower than 5, particularly in models where most variables are single-indicator variables (and thus not "true" latent variables). The reason for these differences in criteria in different contexts is that PLS-based SEM algorithms in general tend to be particularly effective at reducing collinearity (Kock, 2021a; Kock & Lynn, 2012), but only if multiple indicators are available to be aggregated in the calculation of latent variable scores.

GoF. Similarly to the ARS, the GoF index, referred to as "Tenenhaus GoF" in honor of Michel Tenenhaus, is a measure of a model's explanatory power (see, e.g., Kock, 2015d). Tenenhaus et al. (2005) defined the GoF as the square root of the product between what they refer to as the average communality index and the ARS. The communality index for a given latent variable is defined as the sum of the squared loadings for that latent variable, each loading associated with an indicator, divided by the number of indicators. The average communality index for a model is defined similarly, and takes all latent variables into account in its calculation. The loadings referred to here are the unrotated loadings, which are available from the structure loadings and cross-loadings table. It is also worth noting that the definition of the communality index used by Tenenhaus et al. (2005) does not match the typical definition of communality, at least as it is normally stated in the context of factor analysis. As noted by Wetzels et al. (2009), the average variance extracted (AVE) for each latent variable equals the

corresponding communality index. Wetzels et al. (2009) also proposed the **following thresholds for the GoF: small if equal to or greater than 0.1, medium if equal to or greater than 0.25, and large if equal to or greater than 0.36**. They did so by assuming a minimum acceptable average AVE of 0.5, and using Cohen's (1988) thresholds for small, medium, and large effect sizes. A value lower than 0.1 for the GoF suggests that the explanatory power of a model may be too low to be considered acceptable.

SPR. The SPR index is a measure of the extent to which a model is free from Simpson's paradox instances (Kock, 2015e; Kock & Gaskins, 2016; Pearl, 2009; Wagner, 1982). An instance of Simpson's paradox occurs when a path coefficient and a correlation associated with a pair of linked variables have different signs (Kock, 2015e; Kock & Gaskins, 2016). A Simpson's paradox instance is a possible indication of a causality problem, suggesting that a hypothesized path is either implausible or reversed. The SPR index is calculated by dividing the number of paths in a model that are not associated with Simpson's paradox instances by the total number of paths in the model. At the time of this writing the SPR was an experimental index, and thus the following recommendations should also be treated as experimental. Ideally the SPR should equal 1, meaning that there are no instances of Simpson's paradox in a model; acceptable values of SPR are equal to or greater than 0.7, meaning that at least 70 percent of the paths in a model are free from Simpson's paradox.

RSCR. The RSCR index is a measure of the extent to which a model is free from negative Rsquared contributions, which occur together with Simpson's paradox instances (Kock, 2015e; Kock & Gaskins, 2016; Pearl, 2009; Wagner, 1982). When a predictor latent variable makes a negative contribution to the R-squared of a criterion latent variable (note: the predictor points at the criterion), this means that the predictor is actually reducing the percentage of variance explained in the criterion. Such a reduction takes into consideration the contributions of all predictors plus that of the residual. This index is similar to the SPR. The key difference is that it is calculated based on the actual values of the R-squared contributions, not on the number of paths where these contributions have specific signs. The RSCR index is calculated by dividing the sum of positive R-squared contributions in a model by the sum of the absolute R-squared contributions (be they negative or positive) in the model. At the time of this writing the RSCR was an experimental index, and thus the following recommendations should also be treated as experimental. Ideally the RSCR should equal 1, meaning that there are no negative R-squared contributions in a model; acceptable values of RSCR are equal to or greater than 0.9, meaning that the sum of positive R-squared contributions in a model makes up at least 90 percent of the total sum of the absolute R-squared contributions in the model.

SSR. The SSR index is a measure of the extent to which a model is free from statistical suppression instances (Kock & Gaskins, 2016; MacKinnon et al., 2000). An instance of statistical suppression occurs when a path coefficient is greater, in absolute terms, than the corresponding correlation associated with a pair of linked variables. Like a Simpson's paradox instance, a statistical suppression instance is a possible indication of a causality problem (Kock, 2015e; Kock & Gaskins, 2016; Spirtes et al., 1993), suggesting that a hypothesized path may be either implausible or reversed. The SSR index is calculated by dividing the number of paths in a model that are not associated with medium or greater statistical suppression instances by the total number of paths in the model. A medium or greater statistical suppression instance is characterized by an absolute path-correlation ratio that is greater than 1.3. At the time of this writing the SSR was an experimental index, and thus the following recommendation should also

be treated as experimental. Acceptable values of SSR are equal to or greater than 0.7, meaning that at least 70 percent of the paths in a model are free from statistical suppression.

NLBCDR. One interesting property of nonlinear algorithms is that bivariate nonlinear coefficients of association vary depending on the hypothesized direction of causality. That is, they tend to be stronger in one direction than the other, which means that the residual (or error) is greater when the hypothesized direction of causality is in one way or another. As such, they can be used, together with other coefficients, as partial evidence in support or against hypothesized causal links. The NLBCDR index is a measure of the extent to which bivariate nonlinear coefficients of association provide support for the hypothesized directions of the causal links in a model. The NLBCDR index is calculated by dividing the number of path-related instances in a model where the support for the reversed hypothesized direction of causality is more than weak by the total number of path-related instances involved in this test (this is discussed in more detail later). All of the available nonlinear algorithms are used in this test. Therefore the total number of path-related instances involved in this test is greater than the total number of paths. At the time of this writing the NLBCDR was an experimental index, and thus the following recommendation should also be treated as experimental. Acceptable values of NLBCDR are equal to or greater than 0.7, meaning that in at least 70 percent of path-related instances in a model the support for the reversed hypothesized direction of causality is weak or less. Here "less" may mean that the support for reversed hypothesized direction of causality is less than weak (e.g., neutral), or that the hypothesized direction of causality is supported.

H.2. View path coefficients and P values

Path coefficients and respective P values are shown together, as can be seen in Figure H.2. Each path coefficient is displayed in one cell, where the column refers to the predictor latent variable and the row to the criterion. For example, let us consider the case in which the cell shows 0.225, the column refers to the latent variable "ECUVar", and the row to the latent variable "Proc". This means that the path coefficient associated with the arrow that points from "ECUVar" to "Proc" is 0.225.

Close Help Path coefficients **ECUVar** Proc Effi Effe Effi*Proc **ECUVar** 0.225 Proc 0.059 0.459 Effi 0.291 -0.186 Effe Effi*Proc P values **ECUVar** Proc Effi Effe Effi*Proc **ECUVar** < 0.001 0.406 < 0.001 Effi <0.001 0.016 Effe Effi*Proc

Figure H.2. Path coefficients and P values window

Since the results refer to standardized variables, a path coefficient of 0.225 means that, in a linear analysis, a 1 standard deviation variation in "ECUVar" leads to a 0.225 standard deviation variation in "Proc". In a nonlinear analysis, the meaning is generally the same, except that it applies to the overall linear trend of the transformed (or warped) relationship (Kock, 2010; 2016c). However, it is important to note that in nonlinear relationships the path coefficient at each point of a curve varies (Kock, 2016c). In nonlinear relationships, the path coefficient at each point is given by the first derivative of the nonlinear function that describes the relationship (Kock, 2016c; Kock & Gaskins, 2016).

The P values shown are calculated through one of several methods available, and are thus method-specific; i.e., they change based on the P value calculation method chosen. In the calculation of P values, a one-tailed test is generally recommended if the coefficient is assumed to have a sign (positive or negative), which should be reflected in the hypothesis that refers to the corresponding association (Kock, 2015a). Hence this software reports one-tailed P values for path coefficients; from which two-tailed P values can be easily obtained if needed (Kock, 2015a).

One puzzling aspect of many publicly available PLS-based SEM software systems is that they have historically avoided providing P values, instead providing standard errors and T values, and leaving the users to figure out what the corresponding P values are. Often users have to resort to

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tables relating T to P values, or other software (e.g., Excel), to calculate P values based on T values.

This is puzzling because typically research reports will provide P values associated with path coefficients, which are more meaningful than T values for hypothesis testing purposes (Kock, 2015a; 2016b). This is due to the fact that P values reflect not only the strength of the relationship (which is already provided by the path coefficient itself) but also the power of the test, which increases with sample size. The larger the sample size, the lower a path coefficient has to be to yield a statistically significant P value.

H.3. View standard errors and effect sizes for path coefficients

Standard errors and effect sizes for path coefficients are provided in two tables where one standard error and effect size is provided for each path coefficient (see Figure H.3). The effect sizes provided are similar to Cohen's (1988) *f*-squared coefficients, but calculated through a different procedure to avoid a distortion inherent in the use of classic PLS-based SEM algorithms (Kock, 2014a). Standard errors and effect sizes are provided in the same order as the path coefficients, so that users can easily visualize them; and, in certain cases, use them to perform additional analyses.

Close Help Standard errors for path coefficients **ECU** Effe Proc Proc*Effi **ECU** 0.109 Effi 0.043 0.056 0.055 Effe Proc Proc*Effi Effect sizes for path coefficients **ECU** Effe Proc Proc*Effi **ECU** Effi 0.030 0.015 0.284 0.001 Effe Proc Proc*Effi

Figure H.3. Standard errors and effect sizes for path coefficients window

As noted earlier, even though the effect sizes provided are similar to Cohen's (1988) *f*-squared coefficients, and have a similar interpretation, they are calculated using a different procedure. The reason for this is that the stepwise regression procedure proposed by Cohen (1988) for the calculation of *f*-squared coefficients is generally not compatible with classic PLS-based SEM algorithms. The removal of predictor latent variables in latent variable blocks, used in the stepwise regression procedure proposed by Cohen (1988), tends to cause changes in the weights linking latent variable scores and indicators, thus biasing the effect size measures.

The effect sizes are calculated by this software as the absolute values of the individual contributions of the corresponding predictor latent variables to the R-squared coefficients of the criterion latent variable in each latent variable block. With the effect sizes users can ascertain whether the effects indicated by path coefficients are small, medium, or large. The values usually recommended are 0.02, 0.15, and 0.35; respectively (Cohen, 1988). Values below 0.02 suggest effects that are too weak to be considered relevant from a practical point of view, even when the corresponding P values are statistically significant; a situation that may occur with large sample sizes (Kock, 2014a).

Additional types of analyses that may be conducted with standard errors are tests of the significance of any mediating effects using the approach discussed by Kock (2014a). This

approach consolidates the approaches discussed by Preacher & Hayes (2004), for linear relationships; and Hayes & Preacher (2010), for nonlinear relationships. The latter, discussed by Hayes & Preacher (2010), assumes that nonlinear relationships are force-modeled as linear; which means that the equivalent test using this software would use warped coefficients with the earlier linear approach discussed by Preacher & Hayes (2004). Again, for the consolidated version of these approaches, see Kock (2014a). The classic approach used for testing mediating effects is discussed by Kock (2011b). This approach is a concise version of Baron & Kenny's (1986) classic approach, which does not rely on standard errors.

An alternative approach to the analysis of mediating effects, which is arguably much less time-consuming and prone to error than the approaches mentioned above, would be to rely on the estimation of indirect effects. These indirect effects and related P values are automatically calculated by the software, and allow for the test of multiple mediating effects at once, including effects with more than one mediating variable. Kock & Gaskins (2014) provide an empirical illustration of the use of this approach. Indirect and total effects are discussed in more detail later.

Another type of analysis that can employ standard errors for path coefficients is what is often referred to as a multi-group analysis, where path and measurement model coefficients (usually weights) can be compared. One of the main goals of this type of analysis is to compare pairs of path coefficients for identical models but based on different samples. An example would be the analysis of the same model but with data collected in two different countries. See Kock (2014a) for a more detailed discussion on the use of effect sizes and other coefficients generated by this software on advanced mediating effects tests, comprehensive multi-group analyses, and measurement model assessments.

The above steps are significantly simplified by the features available through the menu options "Explore multi-group analyses" and "Explore measurement invariance". These menu options allow you to conduct analyses where the data is segmented in various groups, all possible combinations of pairs of groups are automatically generated, and each pair of groups is compared. The grouping variables can be unstandardized indicators, standardized indicators, and labels. The sub-options available for group pair comparison refer to the following methods: constrained latent growth, Satterthwaite, and pooled standard error (Kock, 2014a).

H.4. View indicator loadings and cross-loadings

The "View indicator loadings and cross-loadings" menu options (see Figure H.4.1) allow users to view various variations of loadings and cross-loadings (Kock, 2014a): combined loadings and cross-loadings, normalized combined loadings and cross-loadings, pattern loadings and cross-loadings, normalized pattern loadings and cross-loadings, structure loadings and cross-loadings, and normalized structure loadings and cross-loadings.

Figure H.4.1. Indicator loadings and cross-loadings options



Combined loadings and cross-loadings are shown in a window, as illustrated in Figure H.4.2. The same is true for other combinations of loadings and cross-loadings, which are shown in similar windows. Combined loadings and cross-loadings are provided in a table with each cell referring to an indicator-latent variable link. Latent variable names are listed at the top of each column, and indicator names at the beginning of each row. In this table, the loadings are from a structure matrix (i.e., unrotated), and the cross-loadings from a pattern matrix (i.e., rotated). Indicator types, as defined, are also provided – reflective or formative.

Figure H.4.2. Combined loadings and cross-loadings window

	ECUVar	Proc	Effi	Effe	Type (as defined)	SE	P value
ECUVari	(1.000)	0.000	0.000	0.000	Reflective	0.050	<0.001
Proc1	0.000	(0.844)	0.039	-0.030	Reflective	0.051	<0.001
Proc2	-0.040	(0.885)	-0.081	0.130	Reflective	0.051	<0.001
Proc3	0.044	(0.814)	0.047	-0.111	Reflective	0.052	<0.001
Effi1	-0.006	-0.014	(0.896)	-0.019	Reflective	0.051	<0.001
Effi2	-0.065	0.035	(0.884)	-0.126	Reflective	0.051	<0.001
Effi3	0.005	0.052	(0.821)	-0.026	Reflective	0.052	<0.001
Effi4	0.079	-0.117	(0.813)	-0.011	Reflective	0.052	< 0.001
Effi5	-0.008	0.043	(0.796)	0.200	Reflective	0.052	<0.001
Effe1	-0.041	0.060	-0.050	(0.931)	Reflective	0.051	<0.001
Effe2	0.032	-0.007	-0.051	(0.947)	Reflective	0.050	<0.001
Effe3	0.006	0.024	0.080	(0.831)	Reflective	0.051	<0.001
Effe4	0.007	0.018	-0.038	(0.952)	Reflective	0.050	<0.001
Effe5	0.036	-0.075	0.006	(0.917)	Reflective	0.051	<0.001
Effe6	0.032	-0.026	-0.066	(0.906)	Reflective	0.051	<0.001
Effe7	-0.074	0.007	0.132	(0.894)	Reflective	0.051	<0.001

In the combined loadings and cross-loadings window, since loadings are from a structure matrix, and unrotated, they are always within the -1 to 1 range. With some exceptions, which are discussed below, this obviates the need for a normalization procedure to avoid the presence of loadings whose absolute values are greater than 1. The expectation here is that for

reflective latent variables loadings, which are shown within parentheses, will be high; and cross-loadings will be low. **The type of the latent variable as defined** by the user, namely **reflective or formative**, **is also provided** in this window to facilitate the application of validity and reliability tests. The criteria used in these tests are typically different for formative and reflective latent variables.

P values are provided for indicators associated with all latent variables. These P values are often referred to as validation parameters of a confirmatory factor analysis (Kline, 1998; Kock, 2014a; Schumacker & Lomax, 2004), since they result from a test of a model where the relationships between indicators and latent variables are defined beforehand. Conversely, in an exploratory factor analysis (Ehremberg & Goodhart, 1976), relationships between indicators and latent variables are not defined beforehand, but inferred based on the results of a factor extraction algorithm. The principal components analysis algorithm is one of the most popular of these algorithms, even though it is often classified as outside the scope of classic factor analysis. Confirmatory factor analyses, instead of exploratory factor analyses, are usually conducted in conjunction with SEM analyses.

For research reports, users will typically use the table of combined loadings and cross-loadings provided by this software when describing the convergent validity of their measurement instrument. A measurement instrument has good convergent validity if the question-statements (or other measures) associated with each latent variable are understood by the respondents in the same way as they were intended by the designers of the question-statements. In this respect, two criteria are recommended as the basis for concluding that a measurement model has acceptable convergent validity: that the **P values associated with the loadings be equal to or lower than 0.05**; and that the **loadings be equal to or greater than 0.5** (Amora, 2021; Hair et al., 1987; 2009; Kock, 2014a).

Indicators for which these criteria are not satisfied may be removed. This does not apply to formative latent variable indicators, which are assessed in part based on P values associated with indicator weights (Kock, 2014a). If the offending indicators are part of a moderating effect, then you should consider removing the moderating effect if it does not meet the requirements for formative measurement (Kock, 2014a; Kock & Lynn, 2012). Moderating effect latent variable names are displayed on the table as product latent variables (e.g., Effi*Proc).

Moderating effect indicator names are displayed on the table as product indicators (e.g., "Effi1*Proc1"). Long names are reduced to avoid a "crowded" look. High P values for moderating effects, to the point of being non-significant at the 0.05 level, may suggest multicollinearity problems; which can be further checked based on the latent variable coefficients generated by the software, more specifically, the full collinearity VIFs (Kock, 2021a). Some degree of collinearity is to be expected with moderating effects, since the corresponding product variables are likely to be correlated with at least their component latent variables. Moreover, moderating effects add nonlinearity to models, which can in some cases compound multicollinearity problems. Because of these and other related issues, moderating effects should be included in models with caution.

Standard errors are also provided for the loadings, in the column indicated as "SE", for indicators associated with all latent variables. They can be used in specialized tests. Among other purposes, these standard errors can be used in multi-group analyses, with the same model but different subsamples. In these cases, users may want to compare the measurement models to ascertain equivalence based on loadings and weights, using a multi-group comparison technique

such as the one documented by Kock (2014a) and Keil et al. (2000), and thus ensure that any observed between-group differences in structural model coefficients are not due to measurement model differences. Keil et al.'s (2000) discussion on multi-group analyses includes an equation that contains an error; the correct form of the equation is used in Kock's (2014a) discussion. The equation in question is for the calculation of a pooled standard error, and is one of the two equations discussed by Kock (2014a) in the context of multi-group analyses; the other implements the alternative Satterthwaite method. According to Keil et al. (2000), the original proponent of the pooled standard error equation is Wynne Chin, one of the world's foremost authorities on PLS-based SEM.

Normalized loadings and cross-loadings. Normalized versions of the combined, pattern, and structure loadings and cross-loadings tables are also provided. In windows showing normalized loadings and cross-loadings, a Kaiser normalization is employed to calculate them (Ferguson, 1981; Kaiser, 1958; Kock, 2014a; Ogasawara, 1999). Through a Kaiser normalization, each row of a table of loadings and cross-loadings is divided by the square root of its communality (Kock, 2014a). This has the effect of making the sum of squared values in each row add up to 1.

Using a Kaiser normalization is reasonably standard practice (Ferguson, 1981; Kock, 2014a; Ogasawara, 1999). Sometimes the normalization is followed by a de-normalization, which is not the case with this software. The normalized values are useful in situations where the PLS Regression algorithm is used and some of the latent variables have only 2 indicators, particularly with respect to options displaying unrotated loadings. In such cases the unrotated loadings in the combined loadings and cross-loadings window that are associated with each of the 2 indicators are the same, because with the PLS Regression algorithm the inner model does not influence the outer model (Kock & Moqbel, 2016). A Kaiser normalization will usually make indicator loadings diverge in value in these cases, in a way that is consistent with standard practice and that, some researchers argue, frequently leads to more conservative estimates of loadings and cross-loadings (Kock, 2014a). For a more detailed discussion, and a review of different perspectives on this topic, see Kock (2014a) and Ogasawara (1999).

Pattern loadings and cross-loadings are provided in a table with each cell referring to an indicator-latent variable link. Latent variable names are listed at the top of each column, and indicator names at the beginning of each row. In this table, both the loadings and cross-loadings are from a pattern matrix (i.e., rotated). Since these loadings and cross-loadings are from a pattern matrix, they are obtained after the transformation of a structure matrix through a widely used oblique rotation frequently referred to as Promax (Kock, 2014a).

The structure matrix contains the Pearson correlations between indicators and latent variables, which are not particularly meaningful prior to rotation in the context of measurement instrument validation. **Because an oblique rotation is employed, in some cases loadings may be higher than 1** (Kock, 2014a; Rencher, 1998). This could be a hint that two or more latent variables are collinear, although this may not necessarily be the case; better measures of collinearity among latent variables are the full collinearity VIFs reported with other latent variable coefficients (Kock, 2021a; Kock & Lynn, 2012). **In the normalized version of this table, typically there will be no loadings higher than 1**.

The main difference between oblique and orthogonal rotation methods is that the former assume that there are correlations, some of which may be strong, among latent variables (Kock, 2014a). Arguably **oblique rotation methods are the most appropriate in a SEM analysis**, because by definition latent variables are expected to be correlated (Kock, 2011b; 2015c). Otherwise, no path coefficient would be significant. Technically speaking, it is possible that a

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research study will hypothesize only neutral relationships between latent variables, which could call for an orthogonal rotation. However, this is rarely, if ever, the case.

are provided in a table with each cell referring to an indicator-latent variable link. Latent variable names are listed at the top of each column, and indicator names at the beginning of each row. In this table, both the loadings and cross-loadings are from a structure matrix (i.e., unrotated). Often these are the only loadings and cross-loadings provided by other PLS-based SEM software systems.

As the structure matrix contains the Pearson correlations between indicators and latent variables, this matrix is not particularly meaningful or useful prior to rotation in the context of collinearity or measurement instrument validation. Here the unrotated cross-loadings tend to be fairly high, even when the measurement instrument passes widely used validity and reliability tests. This is generally true for the normalized version of this matrix.

Still, some researchers recommend using the structure loadings and cross-loadings table as well to assess convergent validity, by following two criteria: that the **cross-loadings be lower than 0.5**; and that the **loadings be equal to or greater than 0.5** (Amora, 2021; Hair et al., 1987; 2009; Kock, 2014a). Note that the loadings here are the same as those provided in the combined loadings and cross-loadings table. The cross-loadings, however, are different. Also, these two criteria generally apply to the version of this table that is *not* normalized.

H.5. View indicator weights

Indicator weights are provided in a table, much in the same way as indicator loadings are (see Figure H.5). All cross-weights are zero, because indicators are expected to fully explain the variance in the latent variable to which they are associated, either by themselves or together with the measurement error associated with the latent variable (Kock, 2015b; Kock & Moqbel, 2016). Each latent variable score is calculated as an exactly linear combination of its indicators (Kock & Moqbel, 2016), or of its indicators and measurement error (Kock, 2015b), where the weights are multiple regression coefficients linking the indicators to the latent variable.

P value VTE WLS Proc Effe **ECU** Type (as defined) SE ES (0.393)0.000 0.000 0.000 Reflective 0.031 < 0.001 1 781 0.333 Proc1 (0.421)0.000 0.000 0.000 Reflective 0.030 < 0.001 2.051 0.375 Proc2 (0.362)0.000 0.000 0.000 Reflective 0.035 < 0.001 1 593 0.292 Proc3 0.000 (0.245)0.000 0.000 Reflective 0.014 <0.001 3.800 0.218 1 Fffi1 0.000 (0.222)0.000 0.000 Reflective 0.016 < 0.001 4.036 0.194 Effi2 Effi3 0.000 (0.238)0.000 0.000 Reflective 0.019 <0.001 2.414 1 0.194 0.000 0.000 0.019 2 522 0.168 Effi4 (0.206)0.000 Reflective < 0.001 0.000 (0.278)0.000 0.000 0.020 2.494 0.227 Reflective < 0.001 1 Effi5 0.000 0.013 7.843 0.000 (0.157)0.000 Reflective < 0.001 0.147 Effe1 0.000 0.000 (0.152)0.000 Reflective 0.012 < 0.001 9.430 0.143 Effe2 0.000 0.000 (0.160)0.000 0.013 < 0.001 2.628 0.134 Effe3 Reflective 0.000 0.000 (0.158)0.000 Reflective 0.012 < 0.001 8.708 0.150 Effe4 1 0.000 0.011 6.612 Effe5 0.000 (0.149)0.000 Reflective < 0.001 0.136 0.000 0.000 (0.139)0.000 Reflective 0.010 < 0.001 5.548 0.125 0 000 0.000 (0.183) 0.013 < 0.001 4 209 0.165 0.000 Reflective Effe7 0.000 0.000 0.000 (-0.321)Formative 0.266 0.114 4.434 -1 0.068 **FCUFmail** (0.405)FCLIFmaillist 0.000 0.000 0.000 (0.405)

Notes: P values < 0.05 and VIFs < 2.5 are desirable for formative indicators: Formative 0.297 0.087
VIF = indicator variance inflation factor: Simpson's paradox in I.v.); ES = indicator effect size.

Figure H.5. Indicator weights window

As with indicator loadings, **standard errors are also provided** here for the weights, in the column indicated as "SE", for indicators associated with all latent variables. These standard errors can be used in specialized tests. Among other purposes, they can be used in multi-group analyses, with the same model but different subsamples. Here users may want to compare the measurement models to ascertain equivalence, using a multi-group comparison technique such as the one documented by Kock (2014a), and thus ensure that any observed between-group differences in structural model coefficients, particularly in path coefficients, are not due to measurement model differences.

P values are provided for weights associated with all latent variables. These values can also be seen, together with the P values for loadings, as the result of a confirmatory factor analysis (Kock, 2014a). In research reports, users may want to report these P values as an indication that formative latent variable measurement items were properly constructed. This also applies to moderating latent variables that pass criteria for formative measurement, when those variables do not pass criteria for reflective measurement.

As in multiple regression analysis (Miller & Wichern, 1977; Mueller, 1996), it is recommended that **weights with P values that are equal to or lower than 0.05** be considered valid items in a formative latent variable measurement item subset (Kock, 2014a). Formative latent variable indicators whose weights do not satisfy this criterion may be considered for removal.

With these P values, users can also check whether moderating latent variables satisfy validity and reliability criteria for formative measurement, if they do not satisfy criteria for reflective measurement. This can help users demonstrate validity and reliability in hierarchical analyses involving moderating effects, where double, triple etc. moderating effects are tested (Kock, 2011b). For instance, moderating latent variables can be created, added to the model as standardized indicators, and then their effects modeled as being moderated by other latent variables; an example of double moderation.

In addition to P values, **variance inflation factors (VIFs) are provided** for the indicators of all latent variables, including moderating latent variables. These can be used for indicator redundancy assessment. In reflective latent variables indicators are expected to be redundant (Kock, 2015c). This is not the case with formative latent variables (Kock & Mayfield, 2015). In formative latent variables indicators are expected to measure *different* facets of the same construct, which means that they should *not* be redundant.

The **VIF threshold of 3.3 has been recommended** in the context of PLS-based SEM in discussions of formative latent variable measurement (Cenfetelli & Bassellier, 2009; Kock, 2014a; Petter et al., 2007). A rule of thumb rooted in the use of this software for many SEM analyses in the past suggests an even more conservative approach: that **capping VIFs to 2.5 for indicators used in formative measurement leads to improved stability** of estimates (Kock, 2014a). The multivariate analysis literature, however, tends to gravitate toward higher thresholds. Also, capping VIFs at 2.5 or 3.3 may in some cases severely limit the number of possible indicators available. Given this, it is recommended that VIFs be capped at 2.5 or 3.3 if this does not lead to a major reduction in the number of indicators available to measure formative latent variables, and if the Cronbach's alpha coefficient associated with the formative latent variable does not fall below 0.6 (Kock, 2014a). One example would be the removal of only 2 indicators out of 16 by the use of this rule of thumb, with the Cronbach's alpha coefficient remaining equal to or greater than 0.6. Otherwise, the criteria below should be employed.

Two criteria, one more conservative and one more relaxed, are recommended by the multivariate analysis literature in connection with VIFs; criteria that can arguably also be used in this type of context. More conservatively, it is recommended that VIFs be lower than 5; a more relaxed criterion is that they be lower than 10 (Hair et al., 1987; 2009; Kline, 1998; Kock, 2014a). High VIFs usually occur for pairs of indicators in formative latent variables, and suggest that the indicators measure the same facet of a formative construct. This calls for the removal of one of the indicators from the set of indicators used for the formative latent variable measurement (Kock & Lynn, 2012).

These criteria are generally consistent with formative latent variable theory (see, e.g., Diamantopoulos, 1999; Diamantopoulos & Winklhofer, 2001; Diamantopoulos & Siguaw, 2006; Kock, 2014a). Among other characteristics, formative latent variables are expected, often by design, to have many indicators. Yet, given the nature of multiple regression, indicator weights will normally go down as the number of indicators go up, as long as those indicators are somewhat correlated (Kock & Gaskins, 2016), and thus P values will normally go up as well. Moreover, as more indicators are used to measure a formative latent variable, the likelihood that one or more will be redundant increases. This will be reflected in high VIFs (Kock & Lynn, 2012).

Indicator weight-loading signs (WLS) are provided for the indicators of all latent variables. A negative WLS (i.e., -1) for an indicator means that the indicator in question is making a negative contribution to the R-squared of its latent variable. That is, a negative WLS suggests the

existence of a Simpson's paradox instance (Kock, 2015e; Kock & Gaskins, 2016; Pearl, 2009; Wagner, 1982) in the outer model, associated with a specific indicator assigned to a latent variable. A Simpson's paradox instance in this context is a possible indication of a causality problem, suggesting that a hypothesized link between an indicator and a latent variable is either implausible or reversed (Kock, 2015e; Kock & Gaskins, 2016). Therefore, **it is recommended that all indicator WLS values be positive**, for both formative and reflective latent variables (Kock, 2014a). Indicators associated with negative WLS values may be considered for removal.

Effect sizes are provided in the column indicated as "ES" for the indicators of all latent variables. As with the effect sizes for paths, the effect sizes for indicators are calculated as the absolute values of the individual contributions of the corresponding indicators to the R-squared coefficients of the latent variable to which each indicator is associated. Similarly to the effect sizes for paths, with the indicator effect sizes users of this software can ascertain whether the indicator effects are small, medium, or large. The values usually recommended are 0.02, 0.15, and 0.35; respectively (Cohen, 1988; Kock, 2014a). Values below 0.02 suggest effects that are too weak to be considered relevant from a practical point of view, even when the corresponding P values are statistically significant. It is recommended that all indicator effect sizes be equal to or greater than 0.02, for both formative and reflective latent variables (Kock, 2014a). Indicators with effect sizes that do not meet this criterion may be considered for removal.

H.6. View latent variable coefficients

Several estimates are provided for each latent variable; these can be used in research reports for discussions on the measurement instrument's reliability, discriminant and predictive validity, as well as overall collinearity (see Figure H.6). R-squared, adjusted R-squared, and Q-squared coefficients are provided only for endogenous latent variables; and reflect the percentages of explained variance and predictive validity associated with each of those latent variables, respectively. Composite reliability and Cronbach's alpha coefficients are provided for all latent variables. Also provided for all latent variables are: minimum and maximum values, medians, modes, skewness and excess kurtosis coefficients, results of unimodality and normality tests, and histograms. Means and standard deviations are not shown because latent variables are standardized; i.e., they all have a mean of 0 and a standard deviation of 1.

Figure H.6. Latent variable coefficients window

	Commor	Easgen	Easund	Complet
R-squared		0.009	0.453	0.003
Adj. R-squared		0.002	0.446	-0.003
Composite reliab.	1.000	0.926	0.897	0.860
Cronbach's alpha	1.000	0.881	0.828	0.755
Avg. var. extrac.	1.000	0.807	0.744	0.672
Full collin. VIF	1.430	1.761	2.291	1.178
Q-squared		0.010	0.454	0.006
Min	-0.997	-2.871	-2.982	-2.329
Max	0.997	1.850	1.931	2.815
Median	0.000	-0.039	-0.034	-0.033
Mode	-0.997	-0.039	-0.034	-0.614
Skewness	-0.000	-0.765	-0.537	0.111
Exc. kurtosis	-2.000	0.561	-0.002	-0.206
Unimodal-RS	No	Yes	Yes	Yes
Unimodal-KMV	No	Yes	Yes	Yes
Normal-JB	No	No	No	Yes
Normal-RJB	No	No	No	Yes
Histogram	View	View	View	View

Composite reliability and Cronbach's alpha coefficients are measures of reliability. Serious questions have been raised regarding Cronbach's alpha's (Cronbach, 1951; Kline, 2010; Kock, 2015b) psychometric properties (Sijtsma, 2009). However, while the Cronbach's alpha coefficient is reported by this software, and the some of the factor-based PLS algorithms employ it as a basis for the estimation of measurement error and composite weights, no assumptions are made about the coefficient's main purported psychometric properties that have been the target of criticism (Kock, 2015b; 2017). This is an important caveat in light of measurement error theory (Kock, 2015b; Nunnally & Bernstein, 1994). Users should also keep in mind that an alternative and generally more acceptable reliability measure is available, the composite reliability coefficient (Dillon & Goldstein, 1984; Peterson & Yeolib, 2013). Composite reliability coefficients are also known as Dillon–Goldstein rho (Tenenhaus et al., 2005) and congeneric reliability (a.k.a. rho_C) coefficients (Raykov, 1997).

Average variances extracted (AVEs) and full collinearity variance inflation factors (VIFs) are also provided for all latent variables; and are used in the assessment of discriminant validity and overall collinearity, respectively (Kock, 2021a; Kock & Lynn, 2012).

Adjusted R-squared coefficients (Theil, 1958; Wooldridge, 1991) are equivalent to R-squared coefficients, with the key difference that they correct for spurious increases in R-squared coefficients due to predictors that add no explanatory value in each latent variable block. Consistently with general recommendations made by Cohen (1988; see, also, Kock, 2014a), values of R-squared coefficients and adjusted R-squared coefficients below 0.02 suggest combined effects of predictors in latent variable blocks that are too weak to be considered relevant from a practical point of view. Therefore, **models where R-squared coefficients or adjusted R-squared coefficients are below 0.02 should be considered for revision**, as the explanatory power in sub-models (i.e., latent variable blocks) is below reasonable expectations. Revisions in these models could involve inner and outer model changes, such as removal or change in location of mediating latent variables as well as removal or reassignment of indicators.

The following criteria, one more conservative and the other two more relaxed, are suggested in the assessment of the reliability of a measurement instrument. **These criteria apply only to reflective latent variable indicators**. Reliability is a measure of the quality of a measurement instrument; the instrument itself is typically a set of question-statements. A measurement instrument has good reliability if the question-statements (or other measures) associated with each latent variable are understood in the same way by different respondents.

More conservatively, both the **composite reliability and the Cronbach's alpha coefficients should be equal to or greater than 0.7** (Fornell & Larcker, 1981; Nunnaly, 1978; Nunnally & Bernstein, 1994; Kock, 2014a; Kock & Lynn, 2012). The more relaxed version of this criterion, which is widely used, is that one of the two coefficients should be equal to or greater than 0.7 (Kock & Lynn, 2012). This typically applies to the composite reliability coefficient, which is usually the higher of the two (Fornell & Larcker, 1981; Kock & Lynn, 2012). An even more relaxed version sets this threshold at 0.6 (Nunnally & Bernstein, 1994; Kock & Lynn, 2012). If a latent variable does not satisfy any of these criteria, the reason will often be one or a few indicators that load weakly on the latent variable. These indicators should be considered for removal (Kock & Lynn, 2012).

AVEs are normally used for discriminant validity assessment and, less commonly, for convergent validity assessment. For discriminant validity assessment, AVEs are used in conjunction with latent variable correlations. This is discussed in more detail later, together with the discussion of the table of correlations among latent variables that includes square roots of AVEs. For convergent validity assessment, the AVE threshold frequently recommended for acceptable validity is 0.5 (Amora, 2021; Fornell & Larcker, 1981; Kock & Lynn, 2012), and applies only to reflective latent variables.

Full collinearity VIFs are shown for all latent variables, separately from the VIFs calculated for predictor latent variables in individual latent variable blocks. These VIFs are calculated based on a full collinearity test (Kock & Lynn, 2012), which enables the identification of not only vertical but also lateral collinearity, and allows for a test of collinearity involving all latent variables in a model (Kock, 2021a). Vertical, or classic, collinearity is predictor-predictor latent variable collinearity in individual latent variable blocks. Lateral collinearity is a term coined by Kock & Lynn (2012) that refers to predictor-criterion latent variable collinearity; a type of collinearity that can lead to particularly misleading results. Full collinearity VIFs can also be used for common method bias tests (Kock, 2015c; 2021a; Kock & Lynn, 2012; Lindell &

Whitney, 2001) that are more conservative than, and arguably superior to, the traditionally used tests relying on exploratory and confirmatory factor analyses. One traditionally used check is Harman's single factor test, which can also be easily done using the software (Kock, 2021b).

A rule of thumb rooted in the use of this software for many SEM analyses in the past suggests that **full collinearity VIFs of 3.3 or lower suggest** the existence of **no multicollinearity** in the model **and no common method bias** (Kock, 2015c; Kock & Lynn, 2012). This is also the recommended threshold for VIFs for latent variables in PLS-based SEM (Kock & Lynn, 2012) and also in slightly different contexts (Cenfetelli & Bassellier, 2009; Kock, 2014a; Petter et al., 2007). On the other hand, two criteria, one more conservative and one more relaxed, are recommended by the multivariate analysis literature in connection with VIFs. They may apply in this type of context as well; although they may be more adequate in path analyses, where all latent variables are measured through single indicators. More conservatively, **it is recommended that VIFs be lower than 5; a more relaxed criterion is that they be lower than 10** (Hair et al., 1987; 2009; Kline, 1998; Kock, 2014a; 2021a).

Q-squared coefficients are also known as Stone-Geisser Q-squared coefficients (Kock, 2015d; Kock & Gaskins, 2014), so named after their principal original proponents (Geisser, 1974; Stone, 1974). The Q-squared coefficient is a nonparametric measure traditionally calculated via blindfolding. It is used for the assessment of the predictive validity (or relevance) associated with each latent variable block in the model, through the endogenous latent variable that is the criterion variable in the block (Kock, 2015d; Kock & Gaskins, 2014). The Q-squared coefficient is sometimes referred to as a resampling analog of the R-squared coefficient. It is often similar in value to that measure; even though the Q-squared coefficient can more easily assume negative values. **Acceptable predictive validity in connection with an endogenous latent variable is suggested by a Q-squared coefficient greater than zero**.

The unimodality tests for which results are provided are the Rohatgi- Székely test (Rohatgi & Székely, 1989) and the Klaassen-Mokveld-van Es test (Klaassen et al., 2000). The normality tests for which results are provided are the classic Jarque-Bera test (Jarque & Bera, 1980; Bera & Jarque, 1981) and Gel & Gastwirth's (2008) robust modification of this test. Since these tests are applied to latent variables, which are combinations either of indicators or of indicators and measurement errors, the outcomes of these tests can be seen as "multivariate" unimodality and normality test results.

Both unimodality and normality test results take the form of a "Yes" or "No", meaning that the latent variable distributions are or are not, respectively, unimodal or normal. No unimodality or normality for at least one latent variable (or indicator) is usually seen as a sign that the nonparametric methods used in this software are particularly appropriate. That is, users of this software can justify employing it by noting that not all latent variables are unimodal and normal. It is noteworthy that **the non-normality justification for the use of** non-parametric **PLS-based SEM** methods **has been widely employed** in the past, arguably correctly since these methods seems to be fairly robust to univariate and multivariate deviations from normality (Kock, 2016a), but typically **without any accompanying test of normality!**

H.7. View correlations among latent variables and errors

The "View correlations among latent variables and errors" menu options (see Figure H.7.1) allow users to view tables containing correlations among latent variables, the P values associated with those correlations, square roots of AVEs, correlations among latent variable error terms (or residuals), and the VIFs associated with latent variable error terms (see figures H.7.2 and H.7.3).

Figure H.7.1. Correlations among latent variables and errors options

View correlations among latent variables and errors	•	View correlations among latent variables with sq. rts. of AVEs
View block variance inflation factors		View correlations among latent variable error terms with VIFs

Figure H.7.2. Correlations among latent variables with square roots of AVEs

Correlations among I.vs. with sq. rts. of AVEs						
	Proc	Effi	Effe	ECU		
Proc	(0.848)	0.460	0.348	0.371		
Effi	0.460	(0.842)	0.540	0.101		
Effe	0.348	0.540	(0.912)	0.157		
ECU	0.371	0.101	0.157	(0.335)		

Figure H.7.3. Correlations among latent variable error terms with VIFs

Correlations among I.v. error terms with VIFs						
	(e)Proc	(e)Effi	(e)Effe			
(e)Proc	(1.001)	0.025	-0.028			
(e)Effi	0.025	(1.001)	-0.002			
(e)Effe	-0.028	-0.002	(1.001)			

In most research reports, users will typically show the table of correlations among latent variables, with the square roots of the average variances extracted on the diagonal, to demonstrate that their measurement instruments pass widely accepted criteria for discriminant validity assessment. A measurement instrument has good discriminant validity if the question-statements (or other measures) associated with each latent variable are not confused by the respondents answering the questionnaire with the question-statements associated with other latent variables, particularly in terms of the meaning of the question-statements.

The following criterion is recommended for discriminant validity assessment: for each latent variable, the square root of the average variance extracted should be higher than any of the correlations involving that latent variable (Fornell & Larcker, 1981; Kock, 2015c; Kock & Lynn, 2012). That is, the values on the diagonal of the table containing correlations among latent variables, which are the square roots of the average variances extracted for each latent variable, should be higher than any of the values above or below them, in the same column. Or, the values on the diagonal should be higher than any of the values to their left or right, in the same row; which means the same as the previous statement, given the repeated values of the latent variable correlations table.

The above criterion applies to reflective and formative latent variables, as well as product latent variables representing moderating effects. If it is not satisfied, the culprit is usually an indicator that loads strongly on more than one latent variable. Also, the problem may involve

more than one indicator. You should check the loadings and cross-loadings tables to see if you can identify the offending indicator or indicators, and consider removing them.

Second to latent variables involved in moderating effects, formative latent variables are the most likely to lead to discriminant validity problems. This is one of the reasons why formative latent variables are not used as often as reflective latent variables in empirical research. In fact, it is wise to use formative variables sparingly in models that will serve as the basis for SEM analysis. Formative variables can in many cases be decomposed into reflective latent variables, which themselves can then be added to the model. Often this provides a better understanding of the empirical phenomena under investigation (Edwards, 2011), in addition to helping avoid discriminant validity problems.

A table with correlations among latent variable error terms containing VIFs associated with the error terms on the diagonal is also provided. This table may be useful in identifying error terms that are highly correlated, which suggest the existence of confounders. More specifically, if a latent variable A points at a latent variable B, and the error terms (e)A and (e)B are strongly correlated, then this may be an indication of the existence of a hidden confounder. This hidden confounder may be the real cause behind a significant association between A and B, suggesting a causality problem; namely one in which a link may in fact not be a "true" causal link but rather be due to a third variable, the confounder. Particularly problematic are situations in which error terms are so highly correlated that they can be considered redundant, which are indicated by high VIFs in the diagonal of this table. To rule out these situations, and consistently with recommendations by Kock & Lynn (2012), it is recommended that the VIFs associated with the error terms be equal to or lower than 3.3.

H.8. View block variance inflation factors

Block variance inflation factors (VIFs) are provided in table format (see Figure H.8) for each latent variable that has two or more predictors in a latent variable block. Block VIFs cannot be calculated for latent variables with only one predictor or no predictor. Here each VIF is associated with one of the two or more predictors, and relates to the link between that predictor and its latent variable criterion. (When one predictor latent variable points at two or more different latent variables in the model, then that latent variable is said to have multiple criteria associated with it.)

Figure H.8. Block variance inflation factors window

In this context, a VIF is a measure of the degree of "vertical" collinearity (Kock & Lynn, 2012), or redundancy, among the latent variables that are hypothesized to affect another latent variable. This classic type of collinearity refers to predictor-predictor collinearity in a latent variable block containing one or more latent variable predictors and one latent variable criterion (Kock & Lynn, 2012). For example, let us assume that there is a block of latent variables in a model, with three latent variables A, B, and C (predictors) pointing at latent variable D. In this case, VIFs are calculated for A, B, and C, and are estimates of the multicollinearity among these predictor latent variables.

A rule of thumb rooted in the use of this software for many SEM analyses in the past, as well as past methodological research, suggests that block VIFs of 3.3 or lower suggest the existence of no vertical multicollinearity in a latent variable block (Kock & Lynn, 2012). This is also the recommended threshold for VIFs in slightly different contexts (Cenfetelli & Bassellier, 2009; Kock, 2015c; Petter et al., 2007). On the other hand, two criteria, one more conservative and one more relaxed, are also recommended by the multivariate analysis literature, and can also be seen as applicable in connection with VIFs in this context.

More conservatively, it is recommended that block VIFs be lower than 5; a more relaxed criterion is that they be lower than 10 (Hair et al., 1987; 2009; Kline, 1998; Kock & Lynn, 2012). These criteria may be particularly relevant in the context of classic path analyses (Kock & Lynn, 2012), where all latent variables are measured through single indicators (technically, these are not "true" latent variables). The reason why these criteria may be particularly relevant in the context of path analyses is that, without multiple indicators per latent variable, the PLS-based SEM algorithms do not have the "raw material" that they need to reduce collinearity (Kock & Lynn, 2012). PLS-based SEM algorithms are particularly effective at reducing collinearity, but chiefly when "true" latent variables are present; that is, when latent variables are measured through multiple indicators.

High block VIFs usually occur for pairs of predictor latent variables, and suggest that the latent variables measure the same construct. If this is not due to indicator assignment problems, it

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would arguably call for the removal of one of the latent variables from the block, or from the model (Kock & Lynn, 2012).

H.9. View correlations among indicators

The software allows users to view the correlations among all indicators included in the model, in table format. Only the correlations for indicators included in the model are shown through the menu option "View correlations among indicators", available from the "View and save results" window. The term "indicator" is frequently used as synonymous with that of "manifest variable", a convention that is used in this document. More technically, however, indicators are manifest variables that are actually used in the measurement model as direct measures of latent variables. Thus there can be manifest variables in the dataset that are not indicators, if the manifest variables are not included in the measurement model.

This option is useful for users who want to run a quick check on the correlations among indicators while they are trying to identify possible sources of multicollinearity. This option may also be useful in the identification of candidate indicators for latent variables through the anchor variable procedure developed by Kock & Verville (2012).

The table of correlations among indicators used in the model is usually much larger, with many more columns and rows, than that of the correlations among latent variables. For this reason, the P values for the correlations are not shown in the screen view option together with the correlations, but are saved in the related tab-delimited text file.

To save correlations among all indicators and respective P values, including those indicators not included in the model, use the menu option "Data", and the appropriate sub-options therein. As noted above, indicators that are not included in the model are not technically "true" indicators. Nevertheless, they do fall under the more general term "manifest variables"; as they are directly measured, and thus not "latent", variables. They refer to the columns of the original dataset.

The menu option for saving correlations among all manifest variables, which refer to all columns of the original dataset, is available from the main software window under "Data", after Step 3 is completed. This option is generally more meaningful for users who want to include the correlations among manifest variables in their research reports, as part of a descriptive statistics table, and for users employing the anchor variable procedure developed by Kock & Verville (2012). This option also generates means, standard deviations, and other descriptive statistics for each of the manifest variables. Manifest variables that are not used in the model, and that thus are not "true" indicators, may simply be deleted prior to the inclusion in a research report.

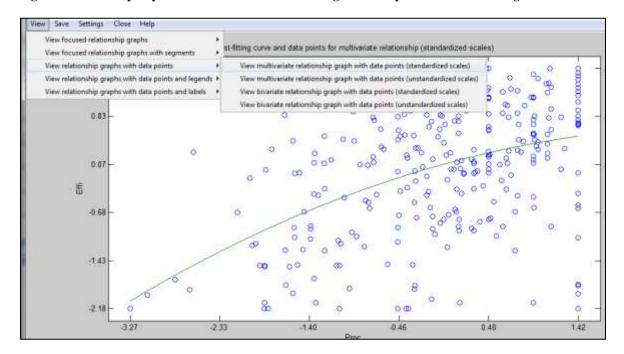
H.10. View/plot linear and nonlinear relationships among latent variables

Choosing the menu option "View/plot linear and nonlinear relationships among latent variables" causes the software to show a table with the types of relationships, warped or linear, between latent variables that are linked in the model (see Figure H.10.1). The term "warped" is used for relationships that are clearly nonlinear, and the term "linear" for linear or quasi-linear relationships. Quasi-linear relationships are slightly nonlinear relationships, which look linear upon visual inspection on plots of the regression curves that best approximate the relationships.

Figure H.10.1. Linear and nonlinear ("warped") relationships among latent variables window

Close	Help					
	Click on a "Lir	near" or "V	/arped" rela	ationship c	ell to view	plot
		ECUVar	Proc	Effi	Effe	Effi*Proc
	ECUVar					
	Proc	Warped				
	Effi	Warped	Warped			
	Effe		Warped			Warped
	Effi*Proc					

Figure H.10.2. Graph options for direct effects including one with points and best-fitting curve



Several graphs (a.k.a. plots) for direct effects can be viewed by clicking on a cell containing a relationship type description. These cells are the same as those that contain path coefficients, in the path coefficients table that was shown earlier. Among the options available are graphs showing the points as well as the curves that best approximate the relationships (see Figure H.10.2).

H.10.1. Graphs for direct effects

The "View focused relationship graphs" options allow users to view graphs that focus on the best-fitting line or curve and that exclude data points to provide the effect of zooming in on the best-fitting line or curve area. The options available are: "View focused multivariate relationship graph (standardized scales)", "View focused multivariate relationship graph (unstandardized scales)", "View focused bivariate relationship graph (standardized scales)", and "View focused bivariate relationship graph (unstandardized scales)".

The options above, like other direct effects graph options discussed here, combine variations in terms of two main aspects: whether the scales are **standardized or unstandardized**, and whether the graphs refer to **multivariate or bivariate** relationships.

By default, **latent variable scores are standardized aggregations of indicators**. The latter, namely the indicators, are originally in unstandardized format. Therefore, to obtain the unstandardized equivalents of the latent variable scores, some decisions must be made and extra calculations performed. The unstandardized equivalents of latent variable scores are always approximations.

Unstandardization of scales for latent variable scores, whereby standardized scales are converted to their unstandardized equivalents, is based on the unstandardization option chosen by the user using the "Settings" menu option. Three unstandardization options are available: "Highest loading indicator", the default option, whereby the mean and standard deviation of the highest loading indicator is used in the unstandardization; "Average of indicators", whereby the mean and standard deviation of the average of indicators is used; and "Weighted average of indicators", whereby the mean and standard deviation of the weighted average of indicators is used.

Through the "Settings" menu option the user can also set the graph title, the X axis label, and the Y axis label. The graph title is the text shown at the top of the graph. The X axis label is the text shown next to the X axis, or the horizontal axis. The Y axis label is the text shown next to the Y axis, or the vertical axis.

Multivariate and bivariate relationship graphs usually differ only when two or more predictor latent variables point at one criterion latent variable in a latent variable block. The addition of predictors will normally reduce the path coefficients in a latent variable block. Because of this, typically a multivariate relationship graph will have a lower overall inclination (or steepness) than its corresponding bivariate relationship graph. However, this is not always the case. In statistical suppression instances (Kock & Gaskins, 2016; MacKinnon et al., 2000), a multivariate relationship graph will have a greater overall inclination than its corresponding bivariate relationship graph. In Simpson's paradox instances (Kock, 2015e; Kock & Gaskins, 2016; Pearl, 2009; Wagner, 1982), multivariate and bivariate relationship graphs will have reversed overall inclinations – e.g., one will be positive and the other negative.

This software is arguably the first and only, at the time of this writing, to provide both multivariate and bivariate representations of nonlinear relationships. The mathematics underlying the rendering of these representations is complex and somewhat novel. Therefore, these representations should be treated as experimental by users of this software, and any conclusions derived from visual inspection of these representations should be treated with caution.

The "View focused relationship graphs with segments" options allow users to view graphs that focus on the best-fitting line or curve, that exclude data points to provide the effect of zooming in on the best-fitting line or curve area, and that show curves as linear segments (Kock,

2016c). The segments are shown with their respective beta coefficients and with or without P values. The options available are: "View focused multivariate relationship graph with segments (standardized scales)", "View focused multivariate relationship graph with segments (standardized scales)", "View focused multivariate relationship graph with segments (unstandardized scales)", "View focused bivariate relationship graph with segments (standardized scales)", "View focused bivariate relationship graph with segments (standardized scales, P values)", and "View focused bivariate relationship graph with segments (unstandardized scales)".

The number of segments shown in the graphs above depends on the **absolute effect segmentation delta** chosen by the user through the "**Settings**" menu option. This absolute effect segmentation delta is the change (or delta) threshold in the first derivative of the nonlinear function depicting the relationship before a new segment is started (Kock, 2016c). For example, a delta of 0.1 means that in each segment the first derivative of the nonlinear function depicting the relationship does not vary more than 0.1. Since the first derivative does not change in linear relationships, segmentation only occurs in nonlinear relationships. This graph segmentation option allows for the identification of unobserved heterogeneity (Kock, 2016c; Sarstedt & Ringle, 2010) without a corresponding reduction in sample size, providing an alternative to data segmentation approaches such as FIMIX-PLS (Hahn et al., 2002; Kock, 2016c).

The "View relationship graphs with data points" options allow users to view graphs with the best-fitting lines or curves and the data points used to produce the best-fitting lines or curves. These options show all the data points, and thus do not provide the effect of zooming in on the best-fitting line or curve area. The options available are: "View multivariate relationship graph with data points (standardized scales)", "View multivariate relationship graph with data points (unstandardized scales)", "View bivariate relationship graph with data points (standardized scales)", and "View bivariate relationship graph with data points (unstandardized scales)".

The "View relationship graphs with data points and legends" options allow users to view graphs with the best-fitting lines or curves, the data points used to produce the best-fitting lines or curves, and legends associated with data labels. These options show all the data points, and thus do not provide the effect of zooming in on the best-fitting line or curve area. They are useful in cases where many data points are available, because in these cases showing legends instead of data labels next to points avoids graph crowding (Kock, 2014d). The options available are: "View multivariate relationship graph with data points and legends (standardized scales)", "View bivariate relationship graph with data points and legends (standardized scales)", and "View bivariate relationship graphs with data points and legends (standardized scales)", and "View bivariate relationship graphs with data points and legends (unstandardized scales)".

The "View relationship graphs with data points and labels" options allow users to view graphs with the best-fitting lines or curves, the data points used to produce the best-fitting lines or curves, and data labels next to the data points to which they refer. These options show all the data points, and thus do not provide the effect of zooming in on the best-fitting line or curve area. They are useful in cases where **few data points** are available, because in these cases showing data labels next to points provides a clear picture of what each data point refers to without graph crowding (Kock, 2014d). The options available are: "View multivariate relationship graph with data points and labels (standardized scales)", "View multivariate relationship graphs with data points and labels (unstandardized scales)", "View bivariate relationship graph

with data points and labels (standardized scales)", and "View bivariate relationship graphs with data points and labels (unstandardized scales)".

As mentioned earlier in this manual, the Warp2 and the Warp2 Basic algorithms try to identify a U-curve relationship between each pair of predictor-criterion latent variables, and, if that relationship exists, the algorithm used transforms (or "warps") the scores of the predictor latent variables so as to better reflect the U-curve relationship in the estimated path coefficients in the model. The Warp3 and the Warp3 Basic algorithms, the former being the default algorithm used by this software, try to identify a relationship defined by a function whose first derivative is a U-curve. This type of relationship follows a pattern that is more similar to an S-curve (or a somewhat distorted S-curve), and can be seen as a combination of two connected U-curves, one of which is inverted.

Sometimes a Warp3-based analysis will lead to results that tell you that a relationship between two latent variables has the form of a U-curve or a line, as opposed to an S-curve. Similarly, sometimes a Warp2-based analysis will tell you that a relationship has the form of a line. This is because the underlying algorithms find the type of relationship that best fits the distribution of points associated with a pair of latent variables, and sometimes those types are not S-curves or U-curves (Kock, 2010; 2011b).

H.10.2. Graphs for moderating effects

As with direct effects, several graphs (a.k.a. plots) for moderating effects can be viewed by clicking on a cell containing a relationship type description. These cells are the same as those that contain path coefficients, in the path coefficients table that was shown earlier. Their column labels are displayed on the table as product latent variables (e.g., Effi*Proc). In this example, namely Effi*Proc, the latent variable Effi is hypothesized to moderate the relationship between Proc and another latent variable, where Proc points at the third latent variable. The third latent variable is listed in the corresponding row label. Among the options available are 3-dimensional (3D) graphs showing the points as well as the surfaces that best approximate the relationships (see Figure H.10.2.1).

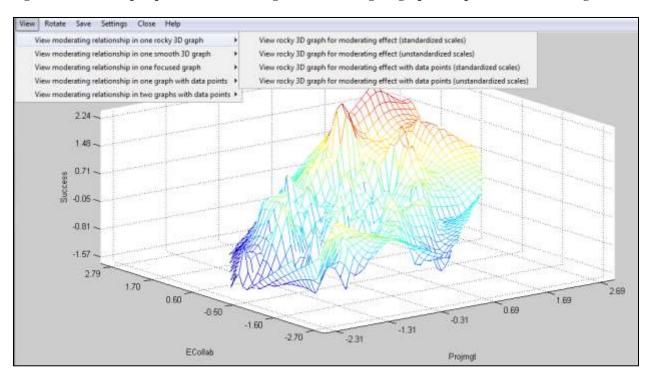


Figure H.10.2.1. Graph options for moderating effects including 3D graph with points and best-fitting surface

Moderating relationships involve three latent variables, the moderating variable and the pair of variables that are connected through a direct link. The **sign and strength of a path coefficient for a moderating relationship** refer to the **effect of the moderating variable on the sign and strength of the path for the direct relationship** that it moderates (Kock, 2016d). For example, if the path for the direct relationship has its sign going from negative to positive and becomes significantly stronger in that direction as one moves from the low to the high range of the moderating variable, then the sign of the path coefficient for the corresponding moderating relationship will be positive and the path coefficient will be relatively high; possibly high enough to yield a statistically significant effect.

No moderating relationship graph currently available from this software accurately represents the true nature of a moderating relationship. This comment seems to apply to all other publicly available SEM software tools; to the best of our knowledge, and at the time of this writing. Therefore various graphs are provided so that users can choose the one that in their view best

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illustrates the relationship. An accurate representation of a moderating relationship would be that of a multivariate distortion in the surface representing the relationship. The distortion refers to a "twisting" of the surface around the moderating variable axis, with a multivariate adjustment, and with corresponding changes in the overall inclinations of the sections of the surface representing the direct effect being moderated. The mathematical underpinnings of such representation were still under development at the time of this writing, and may be available for implementation in future versions of this software.

H.10.2.1. Graphs in 3D for moderating effects

The "View moderating relationship in one rocky 3D graph" options allow users to view 3D graphs where the surfaces are generated through Delaunay triangulations (Chew, 1989; Lee & Schachter, 1980; Kock, 2016d) without smoothing. Surfaces can be viewed with data points excluded or included. The displays with data points excluded are analogous to those used in the focused 2D graphs (discussed later). The options to view surfaces with data points excluded are: "View rocky 3D graph for moderating effect (standardized scales)" and "View rocky 3D graph for moderating effect with data points included are: "View rocky 3D graph for moderating effect with data points (standardized scales)", and "View rocky 3D graph for moderating effect with data points (unstandardized scales)".

The "Rotate" menu option allows the user to rotate a 3D graph up, down, left, and right. Through the "Settings" menu option the user can set the following 3D graph options: the graph title, the moderating variable (M) axis label, the X axis label, and the Y axis label. The graph title is the text shown at the top of the graph. The M axis label is the text shown next to the moderating variable axis. The X axis label is the text shown next to the X axis, or the predictor variable axis. The Y axis label is the text shown next to the Y axis, or the criterion variable axis.

The "View moderating relationship in one smooth 3D graph with data points" options allow users to view 3D graphs where the surfaces are generated through Delaunay triangulations (Chew, 1989; Lee & Schachter, 1980; Kock, 2016d) with smoothing. Because the surfaces are generated with smoothing, they sometimes resemble more bed sheets than rocky mountain formations. Surfaces can be viewed with data points excluded or included. The options to view surfaces with data points excluded are: "View smooth 3D graph for moderating effect (unstandardized scales)" and "View smooth 3D graph for moderating effect with data points (standardized scales)", and "View smooth 3D graph for moderating effect with data points (unstandardized scales)".

In addition to 3D graphs, this software also provides various 2-dimensional (2D) graphs of moderating relationships. The 2D graphs shown for moderating relationships refer to low and high values of the moderating variable, and display the relationships of the variables connected through the moderated direct links in those ranges (Kock, 2016d).

H.10.2.2. Graphs in 2D for moderating effects

The "View moderating relationship in one focused graph" options allow users to view 2D moderating effect graphs that focus on the best-fitting lines or curves for high and low values of the moderating variable, and that exclude data points to provide the effect of zooming in on the area comprising the best-fitting lines or curves. The options available are: "View focused graph with low-high values of moderating variable (standardized scales)", and "View focused graph with low-high values of moderating variable (unstandardized scales)". Figure H.10.2.2 illustrates the former option, with standardized scales.

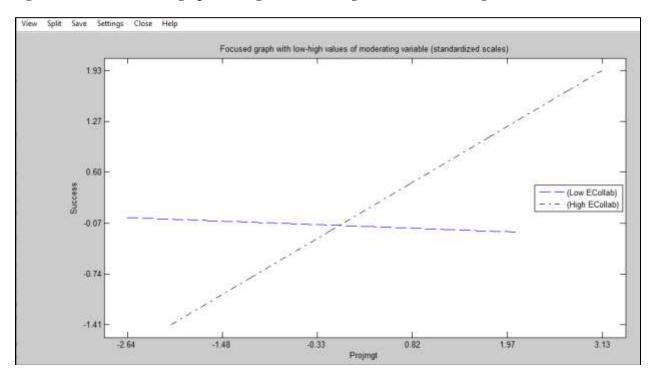


Figure H.10.2.2. Focused 2D graph showing lines for low-high values of moderating variable

Users can set "**fractional splits**" for 2D moderating effects graphs, through the "**Split**" menu option. The default is 0.5, which splits the sample right in the middle when drawing the lines for the effects and the "low" and "high" values of the moderating variable. For instance, if you set the fractional split to 0.1, the software splits the sample in 10% (of the sample) to the left and 90% to the right, respectively for the "low" and "high" values of the moderating variable. This new and powerful fractional split feature enables users to significantly expand their options for illustrating moderating effects in 2D graphs.

In most software tools that perform moderating effects analyses, typically the split is set at 0.5 (i.e., in the middle), with no way to modify it. The problem with this is that a split of 0.5 may yield a graph that gives the impression that there is no actual moderating effect, even when the corresponding coefficient is strong and statistically significant. In cases like this, changing the split to 0.1 or 0.9 may yield graphs that clearly show the nature of the moderation. Users also have the option of creating multiple graphs with different splits, and include all of the graphs in research reports to illustrate a moderating effect in a more "dynamic" way. This is better aligned with the notion of moderation, where the path coefficient for a direct link changes for different

values of the moderating variable. For example, users may create three graphs with splits 0.1, 0.5, and 0.9; and use all three graphs to illustrate a moderating effect in a research report.

Through the "Settings" menu option the user can also set the following 2D moderating effect graph options: the graph title, the labels associated with high and low values of the moderating variable, and the location of the legend box containing these labels. These options allow users to create more informative 2D moderating relationship graphs. For example, instead of "Low Exp" and "High Exp", more informative labels such as "Novices" and "Veterans" could be used. Setting the location of the legend box (e.g., from "East" to "Northwest") allows users to move the legend box from more to less crowded areas of the graph, giving the graph a more balanced and "cleaner" appearance.

The "View moderating relationship in one graph with data points" options allow users to view 2D moderating effect graphs with the best-fitting lines or curves for high and low values of the moderating variable, and the data points used to produce the best-fitting lines or curves. These options show all the data points, and thus do not provide the effect of zooming in on the area comprising the best-fitting lines or curves. The options available are: "View graph with low-high values of moderating variable and data points (standardized scales)", and "View graph with low-high values of moderating variable and data points (unstandardized scales)".

The "View moderating relationship in two graphs with data points" options allow users to view 2D moderating effect graphs with the best-fitting lines or curves for high and low values of the moderating variable, and the data points used to produce the best-fitting lines or curves, in two graphs shown side-by-side. These options show all the data points, and thus do not provide the effect of zooming in on the areas comprising the best-fitting lines or curves. The options available are: "View two graphs with low-high values of moderating variable and data points (standardized scales)", and "View two graphs with low-high values of moderating variable and data points (unstandardized scales)".

The graphs of relationships between pairs of latent variables, and between latent variables and links (moderating relationships), provide a much more nuanced view of how latent variables are related than most of the graphs available through other publicly available multivariate statistics data analysis tools. These latter graphs tend to restrict themselves to linear relationship depictions. However, caution must be taken in the interpretation of these graphs, especially when the distribution of data points is very uneven.

An extreme example would be a warped graph in which all of the data points would be concentrated on the right part of the graph, with only one data point on the far left part of the graph. That single data point, called an outlier, could strongly influence the shape of the nonlinear relationship. In cases such as this, the researcher must decide whether the outlier is "good" data that should be allowed to shape the relationship, or is simply "bad" data resulting from a data collection error.

If the outlier is found to be "bad" data, it can be removed from the analysis, even as it remains in the dataset, by a simple procedure. The user should first add the latent variable score to the set of standardized indicators used in a SEM analysis, using the appropriate menu option under the option "Modify", from the main software window, after Step 5 is completed. The user can then remove the outlier by restricting the values assumed by the latent variable, using the appropriate selections under the "Settings" options, to a range that excludes the outlier. This allows for the exclusion of the outlier without the user having to modify and re-read a dataset. This procedure

may lead to a visible change in the shape of the nonlinear relationship, and significantly affect the results.

An outlier that is found to be "bad" data can also be removed from the dataset, and thus from the analysis, by a more time-consuming procedure. The user should first save the latent variable scores into a file, using the appropriate Save" menu option in the results window, after Step 5 is completed. Then the user should add those scores to the original dataset; the rows will be in the same order. Next the user should open the modified dataset with a spreadsheet software tool (e.g., Excel). The outlier should be easy to identify on the dataset (e.g., a value greater than 4), and should be eliminated. Then the user should re-read this modified file as if it was the original data file, and run all of the SEM analysis steps again.

H.11. View indirect and total effects

Through the "View indirect and total effects" options the software allows users to view outputs for indirect and total effects (Bollen, 1987; Kock & Gaskins, 2014) associated with all latent variables that are linked via one or more paths with more than one segment. These can be used in mediation tests of various levels of complexity (Hubona & Belkhamza, 2021; Moqbel et al., 2020). The options available are "View indirect and total effects (table view)" and "View indirect and total effects (classic view)". The difference between these two options is that the former shows indirect and total effects outputs in extendable table format, and the latter in wrapped text format. The former option, corresponding to the table view, is recommended in complex models with many links among latent variables. Figure H.11 illustrates the latter option, the classic view, which is so named because it was the option used in previous versions of the software.

Total effects ECU Effi Effe Proc Proc"Ef ECU 0.173 Effi Effe 0.180 0.526 0.004 Proc Proc'Ef Number of paths for total effects ECU Effi Proc Effe Proc°Ef ECU Effi Effe Proc Proc*Ef P values for total effects ECU Effi Effe Proc Proc'Ef ECU 0.057 Effi Effe 0.025 < 0.001 0.459 Proc Proc"Ef

Figure H.11. Indirect and total effects window

For each set of indirect and total effects, the following values are provided: the path coefficients associated with the effects, the number of paths that make up the effects, the P values associated with effects (calculated via resampling, using the selected resampling method), the standard errors associated with the effects, and effect sizes associated with the effects.

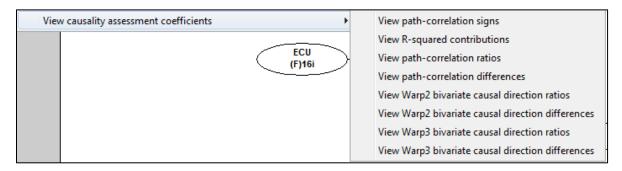
Indirect effects are aggregated for paths with a certain number of segments. As such, the software provides separate reports, within the same output window, for paths with 2, 3 etc. segments (Kock, 2014a; Kock & Gaskins, 2014; Moqbel et al., 2020). The software also provides a separate report for sums of indirect effects, as well as for total effects. All of these reports include P values, standard errors, and effect sizes.

Having access to indirect and total effects can be critical in the evaluation of downstream effects of latent variables that are mediated by other latent variables, especially in complex models with multiple mediating effects along concurrent paths (Kock, 2014a; Kock & Gaskins, 2014; Moqbel et al., 2020). Indirect effects also allow for direct estimations, via resampling, of the P values associated with mediating effects that have traditionally relied on non-automated and thus time-consuming calculations (Kock, 2014a; Kock & Gaskins, 2014; Moqbel et al., 2020) based on linear (Preacher & Hayes, 2004) and nonlinear (Hayes & Preacher, 2010) assumptions.

H.12. View causality assessment coefficients

The "View causality assessment coefficients" options allow users to view a number of coefficients associated with individual paths that can be used in causality assessment. The options available are: "View path-correlation signs", "View R-squared contributions", "View path-correlation differences", "View Warp2 bivariate causal direction ratios", "View Warp2 bivariate causal direction differences", "View Warp3 bivariate causal direction ratios", and "View Warp3 bivariate causal direction differences". Figure H.12 illustrates these options. The topic of causality assessment in the context of SEM is controversial (Kock & Gaskins, 2016; Pearl, 2009). Therefore, these causality assessment coefficients should be treated as experimental by users of this software, and any conclusions derived from them should be treated with caution.

Figure H.12: Causality assessment coefficients options



The "View path-correlation signs" option allows users to identify path-specific Simpson's paradox instances (Kock, 2015e; Kock & Gaskins, 2016; Pearl, 2009; Wagner, 1982), by inspecting a table with the path-correlation signs (shown in the table as the values 1 and -1). A negative path-correlation sign, or the value -1, is indicative of a Simpson's paradox instance (Kock, 2015e; Kock & Gaskins, 2016). A Simpson's paradox instance is a possible indication of a causality problem, suggesting that a hypothesized path is either implausible or reversed (Kock & Gaskins, 2016).

The interpretation of individual Simpson's paradox instances can be difficult. This may be especially the case with demographic variables when these are included in the model as control variables, suggesting what may appear to be unlikely or impossible reverse directions of causality. For example, let us say that a negative path-correlation sign occurs when we include the control variable "Age" (time from birth, measured in years) into a model pointing at the variable "Job performance" (self-assessed, measured through multiple indicators on Likert-type scales). This may be interpreted as suggesting that "Job performance" causes "Age" in the sense that increased job performance causes someone to age, or causes time to pass faster.

Alternative explanations frequently exist for Simpson's paradox instances, as well as for other "red flags" suggested by causality assessment coefficients. Taking the example above, one possible alternative explanation is that increased job performance causes employment to be maintained at more advanced ages, supporting the direction of causality from "Job performance" to "Age" instead of the reverse path. It can also mean that, because of sampling problems, those with greater job performance included in the sample tended to be older. Yet another alternative explanation is that there is no link between "Job performance" and "Age", and that the inclusion of another control variable artificially induces that link; which tends to happen when path

coefficients are associated with negligible R-squared contributions (i.e., lower than 0.02). Whatever the case may be, ideally models should be free from Simpson's paradox instances, because, as noted below, these instances generally detract from the explanatory power of the model.

Because an instance of Simpson's paradox occurs when a path coefficient and a correlation associated with a pair of linked variables have different signs, the corresponding contribution to the R-squared of the criterion variable in the latent variable block where it occurs is negative (see Kock & Gaskins, 2016; Mueller, 1996). For a discussion of this effect in the context of evolutionary biology, see: Kock (2011a). The "View R-squared contributions" option allows users to view the values of the individual contributions to the R-squared of the criterion variable in each latent variable block by each of the predictor latent variables in the block.

The "View path-correlation ratios" option allows users to identify statistical suppression instances (Kock & Gaskins, 2016; MacKinnon et al., 2000), by inspecting a table with the absolute path-correlation ratios. These ratios are calculated by dividing path coefficients by their respective correlation coefficients and taking the absolute values of those divisions. An instance of statistical suppression occurs when a path coefficient is greater, in absolute terms, than the corresponding correlation associated with a pair of linked variables. This leads to a path-correlation ratio that is greater than 1. Like a Simpson's paradox instance, a statistical suppression instance is a possible indication of a causality problem (Kock, 2015e; Kock & Gaskins, 2016; Spirtes et al., 1993), suggesting that a hypothesized path is either implausible or reversed. The following interpretations are suggested for absolute path-correlation ratios: ratio > 1 indicates statistical suppression; 1 < ratio <= 1.3: weak suppression; 1.3 < ratio <= 1.7: medium; 1.7 < ratio: strong.

In the same way that one can distinguish between a statistically significant and non-significant direct association, one can also distinguish between statistically significant and non-significant suppression instances. The "View path-correlation differences" option allows users to do just that, by inspecting a table with the absolute path-correlation differences and their respective P values. The absolute path-correlation differences can be used together with the absolute path-correlation ratios to identify paths that need special attention, because path-correlation ratios alone can sometimes provide an inflated perception of problems, especially when paths and correlations are both very small. Generally speaking, a path that meets the following criteria should be seen as referring to a link that needs special attention in terms of possible elimination or careful interpretation: absolute path-correlation ratio greater than 1.3, and P value for absolute path-correlation difference equal to a lower than 0.05. However, a path that meets these criteria will not necessarily be associated with causality problems; it may in fact suggest a particularly interesting and unique finding (see, e.g., Kock & Gaskins, 2016; MacKinnon et al., 2000).

One useful and interesting property of nonlinear algorithms, such as the Warp2 and Warp3 algorithms, is that often bivariate nonlinear coefficients of association calculated using those algorithms vary depending on the hypothesized direction of causality. That is, they tend to be stronger in one direction than the other, which means that the residual (or error) is greater when the hypothesized direction of causality is in one way or the other. As such, they can be used, together with other coefficients, as partial evidence in support or against hypothesized causal links.

The "View Warp2 bivariate causal direction ratios" option allows users to identify instances in which the Warp2 algorithm suggests that causality may be reversed, by inspecting a

table with the Warp2 bivariate causal direction ratios. These ratios are calculated by dividing the path coefficient obtained for the reversed link by the path coefficient obtained for the link with the hypothesized direction. The following interpretations are suggested for Warp2 bivariate causal direction ratios: ratio > 1 supports reversed link; 1 < ratio <= 1.3: weak support; 1.3 < ratio <= 1.7: medium; 1.7 < ratio: strong.

In the same way that one can distinguish between a statistically significant and non-significant direct association, one can also distinguish between a statistically significant and non-significant Warp2 bivariate causal direction reversal instance. The "View Warp2 bivariate causal direction differences" option allows users to do just that, by inspecting a table with the absolute Warp2 bivariate causal direction differences and their respective P values. The absolute Warp2 bivariate causal direction differences can be used together with the Warp2 bivariate causal direction ratios to identify paths that need special attention, because Warp2 bivariate causal direction ratios alone can sometimes provide an inflated perception of problems, especially when paths in one direction and the other are both very small. Generally speaking, a path that meets the following criteria should be seen as referring to a link that needs special attention in terms of possible direction reversal: Warp2 bivariate causal direction ratio greater than 1.3, and P value for absolute Warp2 bivariate causal direction difference equal to a lower than 0.05.

Since the Warp3 and Warp2 algorithms are different, a similar set of outputs exists in connection with Warp3 bivariate causal direction inferences to those available for Warp2. Often these different sets outputs will be fairly consistent, but sometimes they will not.

The "**View Warp3 bivariate causal direction ratios**" option allows users to identify instances in which the Warp3 algorithm suggests that causality may be reversed, by inspecting a table with the Warp3 bivariate causal direction ratios. These ratios are calculated by dividing the path coefficient obtained for the reversed link by the path coefficient obtained for the link with the hypothesized direction. The following interpretations are suggested for Warp3 bivariate causal direction ratios: ratio > 1 supports reversed link; 1 < ratio <= 1.3: weak support; 1.3 < ratio <= 1.7: medium; 1.7 < ratio: strong.

The "View Warp3 bivariate causal direction differences" option allows users to distinguish between a statistically significant and non-significant Warp3 bivariate causal direction reversal instance. Users can do that by inspecting a table with the absolute Warp3 bivariate causal direction differences and their respective P values. The absolute Warp3 bivariate causal direction differences can be used together with the Warp3 bivariate causal direction ratios to identify paths that need special attention, because Warp3 bivariate causal direction ratios alone can sometimes provide an inflated perception of problems, especially when paths in one direction and the other are both very small. Generally speaking, a path that meets the following criteria should be seen as referring to a link that needs special attention in terms of possible direction reversal: Warp3 bivariate causal direction ratio greater than 1.3, and P value for absolute Warp3 bivariate causal direction difference equal to a lower than 0.05.

Since ratios and P values are generated for the Warp2 and Warp3 algorithms, a more relaxed approach would be to consider for special attention in terms of possible direction reversal only links that meet both the criteria for Warp2 and Warp3 above. Another approach, also somewhat relaxed, would be to consider for special attention only links that meet the criteria that refer to the nonlinear algorithm used for the calculation of the path coefficient associated with the link, either Warp2 or Warp3 (this includes the "basic" options). Having said that, the above criteria arguably apply to paths calculated using the Linear algorithm.

The extent to which using more or less relaxed approaches would lead to "false positives" and "false negatives" in terms of support and lack of support for hypothesized directions of causality is an issue that will require future research, particularly research employing Monte Carlo simulations (Kock, 2016a; Robert & Casella, 2010) where the true directions of causality are known.

A path meeting the above criteria for both Warp2 and Warp3 algorithms, in terms of support for causal direction reversal, may in some cases appear to lead to an absurd conclusion. Upon further consideration, however, reversing the path may not sound as absurd. For example, let us say that a path from the variable "Age" (time from birth, measured in years) pointing at the variable "Job performance" (self-assessed, measured through multiple indicators on Likert-type scales) meets the above criteria, suggesting that it should be reversed. This may be interpreted as suggesting that "Job performance" causes "Age" in the sense that increased job performance causes someone to age, or causes time to pass faster. These could be seen as absurd conclusions, even if we consider work as a possible cause of oxidative stress, and thus accelerated decrepitude (note that "Age" is defined as time from birth, measured in years). However, a different interpretation is that increased job performance causes employment to be maintained at more advanced ages, supporting the direction of causality from "Job performance" to "Age" in a more reasonable and intuitively appealing way.

I. Concluding remarks and additional issues

This software provides users with a wide range of features, including experimental features and also other features that are not available from competing SEM software. For example, this software is the first and only (at the time of this writing) to explicitly identify nonlinear functions connecting pairs of latent variables in SEM models and calculate coefficients of association accordingly.

A wide range of features means that there are many coefficients, graphs and other elements that users can choose to include in research reports, and many possible interpretations of those elements. This user manual does not cover all possible interpretations. Users are strongly advised to keep abreast of the latest developments on methodological issues employing this software, particularly those from research published in academic outlets (e.g., academic journals).

Multivariate statistical analysis software systems, like this software, are inherently complex; sometimes yielding results that are biased and disconnected with the reality of the phenomena being modeled. Users are strongly cautioned against accepting the results provided by this software as a completely unbiased representation of the underlying reality that the software attempts to unveil.

No multivariate statistical analysis software yields completely unbiased results. If one such "perfect" software tool existed, the percentages of false positives and false negatives based on a number of trials with the software using simulated data would all be zero. That is, no false positives or false negatives of any kind (e.g., association strength, direction of causality) would occur.

Achieving this level of perfection is the driving force behind the development of this software, even though this level of perfection will never be achieved – simply because it is not achievable. Some additional issues regarding this quest for perfection are discussed in the following subsections.

I.1. Warping from a conceptual perspective

What this software does when it "warps" relationships is relatively simple at a conceptual level. It identifies a set of functions F1(LVp1), F2(LVp2) ... that relate blocks of latent variable predictors (LVp1, LVp2 ...) to a criterion latent variable (LVc) in this way (Kock, 2010; 2011b; 2016c):

$$LVc = p1*F1(LVp1) + p2*F2(LVp2) + ... + E$$

In the equation above, p1, p2 ... are path coefficients, and E is the error term of the equation. All variables are standardized. Any model can be decomposed into a set of blocks relating latent variable predictors and criteria in this way.

Typically, the more the functions F1(LVp1), F2(LVp2) ... look like curves, and unlike lines, the greater is the difference between the path coefficients p1, p2 ... and those that would have been obtained through a strictly linear analysis.

What this software does is not unlike what a researcher would do if he or she modified predictor latent variable scores prior to the calculation of path coefficients using a function like the logarithmic function. An example is provided in the equation below, where a logarithmic transformation is applied to LVp1.

$$LVc = p1*log(LVp1) + p2*LVp2 + ... + E$$

This software, however, does that automatically and for a much wider range of functions, with modification constants included. For example, in the term A*log(B*LVp1) the constants A and B are modification constants; using simply log(LVp1) as a modifier function in an equation like the one above assumes that A=1 and B=1, which may be incorrect assumptions that will lead to distorted results and mistaken conclusions.

As mentioned above, often the path coefficients p1, p2 ... will go up in value due to warped analysis, but that may not always be the case. Given the nature of multivariate analysis, an increase in a path coefficient may lead to a decrease in a different path coefficient, for predictor latent variables associated with the same criterion latent variable, because each path coefficient in a block is calculated in a way that controls for the effects of the other predictor latent variables. That is, in any given block of latent variables, the predictor latent variables "compete" for the explained variance in the criterion latent variable.

There is no guarantee that the functions F1(LVp1), F2(LVp2) ... discovered by this software will match perfectly that "true" underlying functions. As mentioned earlier, this level of perfection is one that should be strived for, but that is essentially impossible to achieve due to one key factor – measurement error.

The more measurement error exists (i.e., the greater is its magnitude), the more likely it is that the functions F1(LVp1), F2(LVp2) ... discovered by this software will be distorted by error. In fact, the existence of significant measurement error may lead this software to model relationships that are actually linear as nonlinear.

With the above caveats in mind, users can check, through simple visual inspection tests, whether the functions discovered by this software are at least good approximations of the true underlying functions.

To do so, users can divide the dataset into a number of quantiles (e.g., 3), and then build graphs containing the mean values of each criteria latent variable for each of the quantiles. These graphs can be simple bar charts or scatter plots.

This allows users to check whether the shapes of the plots are similar to the shapes of the best-fitting curves generated by this software. The best-fitting curves are representations of the functions F1(LVp1), F2(LVp2) ... discovered by this software.

I.2. Interpreting warped relationships

Linear relationships between pairs of latent variables, that is, those relationships best described by a line, are relatively easy to interpret. They suggest that an increase in one variable either leads to an increase (if the slope of the line is positive) or decrease (if the slope is negative) in the other variable.

Nonlinear relationships provide a much more nuanced view of the data, but at the same time are much more difficult to interpret (Kock, 2010; 2011b; 2016c; Kock et al., 2017). Figure I.2 shows what could be seen as a distorted S curve that is fitted to the data points. The latent variables are "Proc", the extent to which various teams charged with developing new products kept track of their work and costs (i.e., engaged in procedural structuring); and "Effe", the effectiveness of the teams, measured as the market success in terms of sales and profits of the new products that the teams developed.

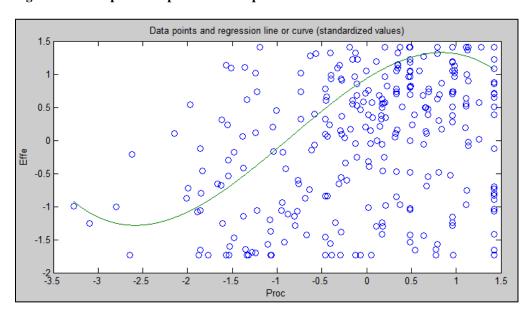


Figure I.2. Example of warped relationship

The distorted S can in turn be seen as a combination of two distorted U curves (or J curves), one straight and the other inverted, connected at an inflection point. The inflection point is the point at the curve where the curvature changes direction; i.e., the second derivative of the S curve changes sign. The inflection point is located at around minus 1 standard deviations from the "Proc" mean. That mean is at the zero mark on the horizontal axis, since the data shown is standardized.

Because an S curve is a combination of two distorted U curves, we can interpret each U curve section separately. A straight U curve, like the one shown on the left side of the graph, before the inflection point, can be interpreted as follows.

The first half of the U curve goes from approximately minus 3.4 to minus 2.5 standard deviations from the mean, at which point the lowest team effectiveness value is reached for the U curve. In that first half of the U curve, an increase in team procedural structuring leads to a decrease in team effectiveness. After that first half, an increase in team procedural structuring leads to an increase in team effectiveness.

One interpretation is that the first half of the U curve refers to novice users of procedural structuring techniques. That is, the process of novice users struggling to use procedural structuring techniques more and more intensely, which they may not be familiar with, ends up leading to effectiveness losses for their teams. At a certain point, around minus 2.5 standard deviations, that situation changes, and the teams start to really benefit from procedural structuring, possibly because the second half of the U curve refers to users with more experience using procedural structuring techniques.

The interpretation of the second U curve on the right, this one an inverted U curve, should be done in a similar fashion. Usually there are multiple interpretations that can be plausible depending on context and other data. Other data may include qualitative data, which can be very useful when combined with quantitative data.

As can be inferred from this example, it is not easy to interpret nonlinear relationships. But the apparent simplicity of strictly linear modeling, or linear estimations of possibly nonlinear relationships, is nothing but a mirage.

I.3. Correlation versus collinearity

Let us consider a theoretical case in which two predictor variables point at a criterion variable, and the predictor variables are uncorrelated. In this case, the value of the R for the criterion variable (the positive square root of the R-squared) will be a function of two other correlation values, R_1 and R_2 , which are the correlations between each of the predictor variables and the criterion. The value of the VIF, which is itself a function of R, will consequently be a function of R_1 and R_2 .

The values of the VIF for the scenario above are plotted in Figure I.3, generated based on a simulation with MATLAB. Three dimensions are needed because three variables are involved. As it can be seen, the variable VIF can reach unacceptably high values, clearly suggestive of collinearity, and for much lower values of R_1 and R_2 than in the case when only two variables are present. Let us assume that we were to set the threshold of VIF for collinearity at 3.3. In this case, a correlation of 0.835 or higher would suggest collinearity in a situation involving only two variables (Kock & Lynn, 2012).

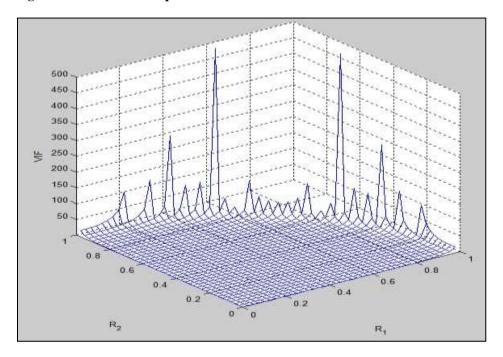


Figure I.3. The relationship between the VIF and the Rs for three variables

The points at which the VIF values increase steeply are indicated as peaks (including small peaks) on the three-dimensional plot. Here a combination of values of R_1 and R_2 in the range of 0.6 to 0.8 lead to VIF values that are suggestive of collinearity for a threshold level of 3.3. For example, if R_1 and R_2 are both equal to 0.625, the corresponding VIF will be 4.57.

As models become more complex from a structural perspective, with more variables in them, the absolute values of the correlations that can lead to significant multicollinearity goes progressively down. Even if not in the same block, latent variables may still be redundant and cause interpretation problems when correlations are relatively low. This is why it is important that users of this software take the various VIFs that are reported into consideration when assessing their models.

The example above also illustrates the fact that the concepts of collinearity and correlation are distinct concepts, even though they are often confused. Collinearity is a multivariate notion, whereas correlation refers to a pair of variables (Kock & Lynn, 2012). Two or more variables are said to be collinear when they measure the same attribute of an object; the latter is also called a construct. In this sense, the variables "satisfaction with a technology" and "excitement about the technology" may be collinear, if the question-statements related to these two variables are seen as referring to the same object attribute "affective response to the technology" by the respondents of a questionnaire. Two variables are said to be correlated if they vary in concert with each other, even though the variables may measure totally different object attributes; e.g., a person's weight from 1 to 20 years of age, and the price of gasoline during those years.

I.4. Stable P value calculation methods

A Monte Carlo simulation was conducted to assess the performance of three P value calculation methods implemented through this software: Bootstrapping, Stable2, and Stable3. Performance was assessed in terms of statistical power and closeness to the actual standard errors obtained through the analyses of simulated samples. Standard errors are used, together with path coefficients, to obtain P values. Table I.4, adapted from Kock (2014b) and Kock (2018b), summarizes the results of this simulation.

Table I.4. Summarized Monte Carlo experiment results for P value calculation methods

Method	BOOT	STBL2	STBL3	ВООТ	STBL2	STBL3
Sample size	50	50	50	300	300	300
CO>GT(TruePath)	0.450	0.450	0.450	0.450	0.450	0.450
CO>GT(AvgPath)	0.383	0.383	0.383	0.388	0.388	0.388
CO>GT(Power)	0.905	0.954	0.946	1	1	1
CO>GT(SEPath)	0.125	0.125	0.125	0.076	0.076	0.076
CO>GT(EstSEPath)	0.120	0.115	0.122	0.047	0.053	0.054
CO>EU(TruePath)	0.400	0.400	0.400	0.400	0.400	0.400
CO>EU(AvgPath)	0.347	0.347	0.347	0.347	0.347	0.347
CO>EU(Power)	0.781	0.900	0.867	1	1	1
CO>EU(SEPath)	0.131	0.131	0.131	0.072	0.072	0.072
CO>EU(EstSEPath)	0.133	0.116	0.124	0.049	0.053	0.055
CO>AC(TruePath)	0.250	0.250	0.250	0.250	0.250	0.250
CO>AC(AvgPath)	0.224	0.224	0.224	0.218	0.218	0.218
CO>AC(Power)	0.419	0.611	0.559	0.985	0.995	0.994
CO>AC(SEPath)	0.141	0.141	0.141	0.061	0.061	0.061
CO>AC(EstSEPath)	0.166	0.118	0.129	0.054	0.054	0.056
GT>SU(TruePath)	0.500	0.500	0.500	0.500	0.500	0.500
GT>SU(AvgPath)	0.333	0.333	0.333	0.347	0.347	0.347
GT>SU(Power)	0.711	0.863	0.823	1	1	1
GT>SU(SEPath)	0.206	0.206	0.206	0.160	0.160	0.160
GT>SU(EstSEPath)	0.146	0.116	0.125	0.052	0.053	0.055
EU>SU(TruePath)	0.230	0.230	0.230	0.230	0.230	0.230
EU>SU(AvgPath)	0.175	0.175	0.175	0.163	0.163	0.163
EU>SU(Power)	0.254	0.410	0.356	0.917	0.921	0.906
EU>SU(SEPath)	0.131	0.131	0.131	0.085	0.085	0.085
EU>SU(EstSEPath)	0.157	0.119	0.132	0.054	0.054	0.056
AC>SU(TruePath)	0.200	0.200	0.200	0.200	0.200	0.200
AC>SU(AvgPath)	0.159	0.159	0.159	0.147	0.147	0.147
AC>SU(Power)	0.240	0.405	0.335	0.866	0.868	0.849
AC>SU(SEPath)	0.137	0.137	0.137	0.073	0.073	0.073
AC>SU(EstSEPath)	0.165	0.119	0.132	0.053	0.054	0.056

The column labels BOOT, STBL2 and STBL3 respectively refer to the Bootstrapping, Stable2, and Stable3 methods. The latent variables in the model used as a basis for the simulation are: CO = communication flow orientation; GT = usefulness in the development of IT solutions; EU = ease of understanding; AC = accuracy; and SU = impact on redesign success (for more details, see: Kock, 2014b and Kock, 2018b). The meanings of the acronyms within parentheses are the following: TruePath = true path coefficient; AvgPath = mean path coefficient estimate; Power = statistical power; SEPath = standard error of path coefficient estimate; and EstSEPath = method-specific standard error of path coefficient estimate.

To conduct the simulation, we created an analyzed 1,000 samples for each of the following sample sizes: 50, 100, 200, 300, and 500. The PLS Mode A algorithm was used in the analyses. In this summarized set of results, we restrict ourselves to sample sizes 50 and 300. Full results, for all sample sizes included in the simulation, are available from Kock (2014b) and Kock (2018b).

As we can see, the mean path coefficient estimates differ from the true path coefficients across different sample sizes, and generally underestimate the true path coefficients. This underestimation stems from the use of composites in PLS Mode A, which in turn leads to the known composite *correlation* attenuation (Kock, 2015b; Nunnally & Bernstein, 1994). This attenuation "propagates" to the path coefficients (Kock, 2015b; 2016a). This problem is addressed in this software through the availability of factor-based PLS algorithms (Kock, 2017; 2019a; 2019b; 2019c).

Generally, the method-specific standard errors of path coefficient estimates obtained via Stable3 were the closest to the actual (or true) standard errors of path coefficient estimates. This suggests that standard errors estimated via Stable3 are not only stable when compared with those estimated via Bootstrapping, but also more accurate. Moreover, both Stable2 and Stable3 led to greater statistical power than Bootstrapping at small sample sizes. This is noteworthy, because power tends to be compromised the most with small sample sizes, and to invariably increase as sample sizes go up regardless of the standard error and P value calculation method used.

I.5. Missing data imputation methods

A Monte Carlo simulation was conducted to assess the performance of five missing data imputation methods implemented through this software: Arithmetic Mean Imputation, Multiple Regression Imputation, Hierarchical Regression Imputation, Stochastic Multiple Regression Imputation, and Stochastic Hierarchical Regression Imputation. Table I.5, adapted from Kock (2014c) and Kock (2018a), summarizes the results of this simulation.

Table I.5. Summarized Monte (Carlo experimen	t results for missing	data imputation methods

Missing data imputation scheme	NMD	MEAN	MREGR	HREGR	MSREG	HSREG
CO>GT(TruePath)	0.450	0.450	0.450	0.450	0.450	0.450
CO>GT(AvgPath)	0.390	0.348	0.367	0.354	0.333	0.300
CO>GT(SEPath)	0.075	0.113	0.110	0.113	0.138	0.162
CO>EU(TruePath)	0.400	0.400	0.400	0.400	0.400	0.400
CO>EU(AvgPath)	0.349	0.312	0.321	0.313	0.289	0.262
CO>EU(SEPath)	0.069	0.101	0.108	0.106	0.133	0.151
CO>AC(TruePath)	0.250	0.250	0.250	0.250	0.250	0.250
CO>AC(AvgPath)	0.219	0.198	0.206	0.195	0.188	0.161
CO>AC(SEPath)	0.062	0.078	0.090	0.083	0.100	0.108
GT>SU(TruePath)	0.500	0.500	0.500	0.500	0.500	0.500
GT>SU(AvgPath)	0.381	0.357	0.359	0.352	0.334	0.312
GT>SU(SEPath)	0.127	0.152	0.156	0.158	0.179	0.195
EU>SU(TruePath)	0.230	0.230	0.230	0.230	0.230	0.230
EU>SU(AvgPath)	0.192	0.183	0.199	0.178	0.188	0.163
EU>SU(SEPath)	0.062	0.072	0.077	0.078	0.082	0.089
AC>SU(TruePath)	0.200	0.200	0.200	0.200	0.200	0.200
AC>SU(AvgPath)	<u>0.165</u>	0.157	0.176	0.154	0.166	0.141
AC>SU(SEPath)	0.058	0.067	0.073	0.072	0.077	0.081
GT3 <gt(trueload)< th=""><th>0.700</th><th>0.700</th><th>0.700</th><th>0.700</th><th>0.700</th><th>0.700</th></gt(trueload)<>	0.700	0.700	0.700	0.700	0.700	0.700
GT3 <gt(avgload)< th=""><th>0.811</th><th>0.691</th><th>0.606</th><th>0.649</th><th>0.623</th><th>0.652</th></gt(avgload)<>	0.811	0.691	0.606	0.649	0.623	0.652
GT3 <gt(seload)< th=""><th>0.113</th><th>0.042</th><th>0.120</th><th>0.076</th><th>0.115</th><th>0.090</th></gt(seload)<>	0.113	0.042	0.120	0.076	0.115	0.090

The column labels NMD, MEAN, MREGR, HREGR, MSREG and HSREG respectively refer to no missing data, Arithmetic Mean Imputation, Multiple Regression Imputation, Hierarchical Regression Imputation, Stochastic Multiple Regression Imputation, and Stochastic Hierarchical Regression Imputation. The latent variables in the model used as a basis for the simulation are: CO = communication flow orientation; GT = usefulness in the development of IT solutions; EU = ease of understanding; AC = accuracy; and SU = impact on redesign success (for more details, see: Kock, 2014c; 2018a). The meanings of the acronyms within parentheses are the following: TruePath = true path coefficient; AvgPath = mean path coefficient estimate; SEPath = standard error of path coefficient estimate; TrueLoad = true loading; AvgLoad = mean loading estimate; and SELoad = standard error of loading estimate.

When creating data for our Monte Carlo simulation we varied the following conditions: percentage of missing data (0%, 30%, 40%, and 50%), and sample size (100, 300, and 500). This led to a 4 x 3 factorial design, with 12 conditions. We created an analyzed 1,000 samples for each of these 12 conditions; a total of 12,000 samples. In this summarized set of results we restrict ourselves to 30% missing data and the sample size of 300. Full results, for all percentages of missing data and sample sizes included in the simulation, are available from Kock (2014c) and Kock (2018a). Since all loadings are the same in the true population model, loading-related

estimates for only one indicator of the composites are shown. This avoids crowding and repetition, as the same pattern of results repeats itself in connection with all loadings.

The mean path coefficient estimates that are shown underlined were obtained through the application of the PLS Mode A algorithm to datasets where no data was missing (NMD). Note that they generally underestimate the true path coefficients. This underestimation stems from the use of composites, discussed earlier, which leads to an attenuation of composite *correlations* (Nunnally & Bernstein, 1994). This correlation attenuation extends to the path coefficients (Kock, 2015a; 2015b), leading to the observed underestimation. The opposite effect is observed in connection with loadings, which tend to be overestimated in PLS-based SEM analyses employing PLS Mode A. As noted earlier, these problems are addressed in this software through the availability of factor-based PLS algorithms (Kock, 2017; 2019a; 2019b; 2019c).

Multiple Regression Imputation (MREGR) yielded the least biased mean path coefficient estimates, followed by Arithmetic Mean Imputation (MEAN). When we look at mean loading estimates, Arithmetic Mean Imputation (MEAN) yielded the least biased results, followed by Stochastic Hierarchical Regression Imputation (HSREG) and Hierarchical Regression Imputation (HREGR.

Compared with the no missing data condition (NMD), none of the methods induced a reduction in standard errors for path coefficients. This is noteworthy since prior results outside the context of PLS-based SEM have tended to show a significant downward bias in standard errors, particularly for non-stochastic missing data imputation varieties. Such downward bias in standard errors has led to concerns regarding an inflation in type I errors, and warnings against the use of single missing data imputation methods in general (Enders, 2010; Kock, 2014c; 2018a; Newman, 2014). Our results suggest that such concerns may not be warranted in the context of PLS-based SEM.

I.6. Factor-based PLS algorithms

The factor-based PLS algorithms available in this software combine the precision of covariance-based SEM algorithms, under common factor model assumptions (Kock, 2015b; 2019a; 2019b; 2019c), with the nonparametric characteristics of classic PLS algorithms. Moreover, the factor-based PLS algorithms address head-on a problem that has been discussed since the 1920s – the factor indeterminacy problem. Classic PLS algorithms yield composites, as linear combinations of indicators, which can be seen as factor approximations. The factor-based PLS algorithms, on the other hand, provide estimates of the true factors, as linear combinations of indicators and measurement errors (Kock, 2017; 2019a; 2019b; 2019c).

A Monte Carlo simulation was conducted to comparatively assess the performance of one of the factor-based PLS algorithms, namely the Factor-Based PLS Type CFM1 algorithm, against that of the PLS Mode A algorithm. Like covariance-based SEM algorithms, the Factor-Based PLS Type CFM1 algorithm is fully compatible with common factor model assumptions, including the assumption that all indicator errors are uncorrelated. Table I.6, adapted from Kock (2015b), summarizes the results of this simulation.

SEM method	PLSA	PLSF	PLSA	PLSF	PLSA	PLSF
Sample size	50	50	100	100	300	300
EU>TE(TruePath)	0.400	0.400	0.400	0.400	0.400	0.400
EU>TE(AvgPath)	0.339	0.380	0.309	0.385	0.303	0.394
EU>TE(SEPath)	0.125	0.161	0.128	0.127	0.110	0.070
EU>TP(TruePath)	0.300	0.300	0.300	0.300	0.300	0.300
EU>TP(AvgPath)	0.260	0.301	0.248	0.294	0.234	0.297
EU>TP(SEPath)	0.135	0.157	0.108	0.133	0.085	0.079
TE>TP(TruePath)	0.200	0.200	0.200	0.200	0.200	0.200
TE>TP(AvgPath)	0.201	0.234	0.189	0.225	0.174	0.203
TE>TP(SEPath)	0.144	0.163	0.098	0.132	0.061	0.079
EU3 <eu(trueload)< th=""><th>0.700</th><th>0.700</th><th>0.700</th><th>0.700</th><th>0.700</th><th>0.700</th></eu(trueload)<>	0.700	0.700	0.700	0.700	0.700	0.700
EU3 <eu(avgload)< th=""><th>0.793</th><th>0.692</th><th>0.802</th><th>0.695</th><th>0.808</th><th>0.699</th></eu(avgload)<>	0.793	0.692	0.802	0.695	0.808	0.699
EU3/EU(SELoad)	0.129	0.108	0.113	0.077	0.112	0.049

Table I.6. Summarized Monte Carlo experiment results for composite-based and factor-based algorithms

The column labels PLSA and PLSF respectively refer to the PLS Mode A and Factor-Based PLS Type CFM1 algorithms. The latent variables in the model used as a basis for the simulation are: EU = e-collaboration technology use; TE = team efficiency; and TP = team performance (for more details, see Kock, 2015b). The meanings of the acronyms within parentheses are the following: TruePath = true path coefficient; AvgPath = mean path coefficient estimate; SEPath = standard error of path coefficient estimate; TrueLoad = true loading; AvgLoad = mean loading estimate; and SELoad = standard error of loading estimate.

In the Monte Carlo simulation 300 samples were created for each of the following sample sizes: 50, 100, and 300. We show results for all of the structural paths in the model, but restrict ourselves to loadings for one indicator in one factor since all loadings are the same in the true population model used. This is also done to avoid repetition, as the same general pattern of results for loadings repeats itself for all indicators in all factors.

As we can see from the summarized results, the Factor-Based PLS Type CFM1 algorithm yielded virtually unbiased estimates at the sample size of 300, whereas the PLS Mode A algorithm yielded significantly biased estimates at that same sample size. One of the reasons for

these significantly biased estimates with PLS Mode A are the relatively low loadings in the true population model used as a basis for simulation, namely 0.7 for all indicators, which tend to be a challenge for algorithms based on Wold's original PLS design (Kock, 2015a; 2015b; 2017).

The relatively low loadings in the true population model apparently had little effect on the Factor-Based PLS Type CFM1 algorithm's asymptotic convergence to the true values of the model parameters, although those loadings probably slowed down that convergence somewhat as sample sizes increased. In other simulations we conducted with higher loadings, convergence was achieved at smaller sample sizes.

For several of the path coefficients and loadings the Factor-Based PLS Type CFM1 algorithm yielded lower standard errors, particularly as sample sizes increased. This is noteworthy because the Factor-Based PLS Type CFM1 algorithm is considerably more computationally complex than the PLS Mode A algorithm (Kock, 2015b), and thus could have been expected to have a greater "cost" in terms of standard errors.

Nevertheless, standard errors yielded at the sample size of 50 were generally higher for the Factor-Based PLS Type CFM1 algorithm. Apparently the difference was enough to have a negative effect on power, as the ratios of path coefficients to standard errors indicate. That is, at the sample size of 50 one could argue based on the results that the PLS Mode A algorithm has greater power than the Factor-Based PLS Type CFM1 algorithm for this particular model, although the ratios of path coefficients to standard errors suggest that both algorithms may struggle to avoid type II errors at this small sample size, particularly for the paths whose true coefficients were lower than 0.400 (the path with the highest strength).

J. Glossary

Adjusted R-squared coefficient. A measure equivalent to the R-squared coefficient, with the key difference that it corrects for spurious increases in the R-squared coefficient due to predictors that add no explanatory value in each latent variable block. Like R-squared coefficients, adjusted R-squared coefficients can assume negative values. These are rare occurrences that normally suggest problems with the model in which they occur; e.g., severe collinearity or model misspecification.

Analytic composites. Analytic composites (Kock, 2021a; Kock et al., 2018) are weighted aggregations of indicators where the relative weights are set by the user, usually based on an existing theory.

Average variance extracted (AVE). A measure associated with a latent variable, which is used in the assessment of the discriminant validity of a measurement instrument. Less commonly, it can also be used for convergent validity assessment.

Composite reliability coefficient. This is a measure of reliability associated with a latent variable. Another name for it is Dillon–Goldstein rho coefficient. Unlike the Cronbach's alpha coefficient, another measure of reliability, the compositive reliability coefficient takes indicator loadings into consideration in its calculation. It often is slightly higher than the Cronbach's alpha coefficient.

Construct. A conceptual entity measured through a latent variable. Sometimes it is referred to as "latent construct". The terms "construct" or "latent construct" are often used interchangeably with the term "latent variable".

Convergent validity of a measurement instrument. Convergent validity is a measure of the quality of a measurement instrument; the instrument itself is typically a set of question-statements. A measurement instrument has good convergent validity if the question-statements (or other measures) associated with each latent variable are understood by the respondents in the same way as they were intended by the designers of the question-statements.

Cronbach's alpha coefficient. This is a measure of reliability associated a latent variable. It usually increases with the number of indicators used, and is often slightly lower than the composite reliability coefficient, another measure of reliability.

Discriminant validity of a measurement instrument. Discriminant validity is a measure of the quality of a measurement instrument; the instrument itself is typically a set of question-statements. A measurement instrument has good discriminant validity if the question-statements (or other measures) associated with each latent variable are not confused by the respondents, in terms of their meaning, with the question-statements associated with other latent variables.

Effect size. The effect size is a measure of the magnitude of an effect that is independent of the size of the sample analyzed. The effect sizes are calculated by this software as the absolute values of the individual contributions of the corresponding predictor latent variables to the R-squared coefficients of the criterion latent variable in each latent variable block. With the effect sizes users can ascertain whether the effects indicated by path coefficients are small, medium, or large. The values usually recommended are 0.02, 0.15, and 0.35; respectively. Values below 0.02 suggest effects that are too weak to be considered relevant from a practical point of view, even when the corresponding P values are statistically significant; a situation that may occur with large sample sizes.

Endogeneity. The term "endogeneity" refers to a phenomenon that is characterized by the structural error term for an endogenous variable being correlated with any of the variable's

predictors. For example, let us consider a simple population model with the following links A > B and B > C. This model presents endogeneity with respect to C, because variation flows from A to C via B, leading to a biased estimation of the path for the link B > C via ordinary least squares regression. Adding a link from A to C could be argued as "solving the problem", but in fact it creates the possibility of a type I error, since the link A > C does not exist at the population level. A more desirable solution to this problem is to create an instrumental variable iC, incorporating only the variation of A that ends up in C and nothing else, and revise the model so that it has the following links: A > B, B > C and iC > C. The link iC > C can be used to test for endogeneity, via its P value and effect size. This link (i.e., iC > C) can also be used to control for endogeneity, thus removing the bias when the path coefficient for the link B > C is estimated via ordinary least squares regression. Endogeneity may also arise from multilevel effects (Kock, 2020b).

Endogenous latent variable. This is a latent variable that is hypothesized to be affected by one or more other latent variables. An endogenous latent variable has one or more arrows pointing at it in the model graph.

Exogenous latent variable. This is a latent variable that does not depend on other latent variables, from a SEM analysis perspective. An exogenous latent variable does not have any arrow pointing at it in the model graph.

Factor score. A factor score is the same as a latent variable score; see the latter for a definition.

Formative latent variable. A formative latent variable is one in which the indicators are expected to measure certain attributes of the latent variable, but the indicators are not expected to be highly correlated with the latent variable score, because they (i.e., the indicators) are not expected to be correlated with one another. For example, let us assume that the latent variable "Satisf" ("satisfaction with a meal") is measured using the two following question-statements: "I am satisfied with the main course" and "I am satisfied with the dessert". Here, the meal comprises the main course, say, filet mignon; and a dessert, a fruit salad. Both main course and dessert make up the meal (i.e., they are part of the same meal) but their satisfaction indicators are not expected to be highly correlated with each other. The reason is that some people may like the main course very much, and not like the dessert. Conversely, other people may be vegetarians and hate the main course, but may like the dessert very much.

Full collinearity VIFs. Variance inflation factors (VIFs) are measures of the degree of collinearity (or multicollinearity) among variables, including both indicators and latent variables. With latent variables, collinearity can take two main forms: vertical and lateral collinearity (Kock & Lynn, 2012). Vertical, or classic, collinearity is predictor-predictor latent variable collinearity in individual latent variable blocks. Lateral collinearity is a term coined by Kock & Lynn (2012) that refers to predictor-criterion latent variable collinearity; a type of collinearity that can lead to particularly misleading results. Full collinearity VIFs allow for the simultaneous assessment of both vertical and lateral collinearity in a SEM model. They can also be used for common method bias and discriminant validity assessment.

Heterotrait-monotrait (HTMT) ratios. These ratios have been proposed for discriminant validity assessment, particularly in the context of composite-based SEM via classic PLS algorithms; as opposed to factor-based SEM via modern algorithms that estimate factors (which have been available from this software for quite some time now). Discriminant validity is a measure of the quality of a measurement instrument; the instrument itself is typically a set of question-statements. A measurement instrument has good discriminant validity if the question-statements (or other measures) associated with each latent variable are not confused by the

respondents, in terms of their meaning, with the question-statements associated with other latent variables.

Indicator. The term indicator is frequently used as synonymous with that of manifest variable; a convention that is used here. Thus, see the latter for a definition. More technically though, indicators are manifest variables that are actually used in the measurement model as direct measures of latent variables. As such, technically speaking, there can be manifest variables that are not indicators, if the manifest variables in question are part of the original dataset but not included in the measurement model.

Inner model. In a structural equation modeling analysis, the inner model is the part of the model that describes the relationships among the latent variables that make up the model. In this sense, the path coefficients are inner model parameter estimates.

Instrumental variable. Instrumental variables are variables that selectively share variation with other variables, and only with those variables. Instrumental variables can be used to test and control for endogeneity, and also to estimate reciprocal relationships (Morrow & Conger, 2021). Endogeneity may arise from multilevel effects (Kock, 2020b).

Latent variable. A latent variable is a variable that is measured through multiple variables called indicators or manifest variables. For example, "satisfaction with a meal" may be a latent variable measured through two manifest variables that store the answers on a 1 to 7 scale (1=strongly disagree; 7 strongly agree) to the following question-statements: "I am satisfied with this meal", and "After this meal, I feel full".

Latent variable block. A latent variable block is a group of latent variables in which one or more predictor latent variables point at one criterion latent variable. In a PLS-based SEM analysis, once latent variable scores are calculated, a series of multiple least squares regressions are conducted to calculate path coefficients. Each multiple least squares regression is performed on a latent variable block, until all blocks are covered. The term "latent variable block" is also used in the PLS-based SEM literature to refer to a group of manifest variables linked to their assigned latent variable; i.e., a latent variable and its indicators.

Latent variable score. Latent variable scores are values calculated based on the indicators defined by the user as associated with the latent variable. They are calculated using one of the outer model analysis algorithms available. These scores may be understood as new columns in the data, with the same number of rows as the original data (unless a range-restricted analysis is conducted), and which generally tend to maximize the loadings and minimize the cross-loadings of a pattern matrix of loadings after an oblique rotation.

Latent variable error. An error variable that accounts for the variance in an endogenous latent variable that is not accounted for by the latent variable predictors that point at the endogenous latent variable. The terms "error" and "residual" are used interchangeably in this document. Nevertheless, they refer to subtly different entities. Technically speaking, the term "error" typically refers to the error variable in the true population model, which is assumed to be uncorrelated with latent variables other than the endogenous latent variable to which it is associated. Conversely, the term "residual" typically refers to the corresponding estimated error, the difference between the expected value of the latent variable and its point estimate, which in practice is often correlated with latent variables other than the endogenous latent variable to which it is associated. This is an example of a broader occurrence in multivariate analyses: more often than not sample-specific estimates violate assumptions about the theoretical true values, even if slightly.

Manifest variable. A manifest variable is one of several variables that are used to indirectly measure a latent variable. For example, "satisfaction with a meal" may be a latent variable measured through two manifest variables, which assume as values the answers on a 1 to 7 scale (1=strongly disagree; 7 strongly agree) to the following question-statements: "I am satisfied with this meal", and "After this meal, I feel full".

Minimum required sample size. The minimum required sample size needed for an SEM test to achieve an acceptable level of power (usually .8) depends on the effect size associated with the path coefficient under consideration and the significance level used for hypothesis testing (normally 0.05). The higher is the magnitude of a path coefficient at the population level, the higher is usually its effect size, and the greater is the probability that a true effect will be properly detected with a small sample. Therefore strong path coefficients at the population level, whether they are negative or positive, tend to require very small sample sizes for their proper identification. This software allows users to obtain estimates of the minimum required sample sizes for empirical studies based on the following model elements: the minimum absolute significant path coefficient in the model (e.g., 0.21), the significance level used for hypothesis testing (e.g., 0.05), and the power level required (e.g., 0.80).

Outer model. In a SEM analysis, the outer model is the part of the model that describes the relationships among the latent variables that make up the model and their indicators. In this sense, the weights and loadings are outer model parameter estimates.

Portable document format (PDF). This is an open standard file format created by Adobe Systems, and widely used for exchanging documents. It is the format used for this software's documentation.

Power. Statistical power, often referred to simply as "power", is a statistical test's probability of avoiding type II errors, or false negatives. Power is often estimated for a particular coefficient of association and sample size, for samples drawn from a population, at a given significance level (usually P < .05). For example, let us consider an SEM test employing PLS Mode A and bootstrapping. Let us assume that such a test is able to recognize a path coefficient as statistically significant, where the path coefficient is associated with a "real" effect at the population level of magnitude .2; which would be referred to as the "true" path coefficient. Let us also assume that the test correctly recognizes the path coefficient as significant 83 percent of the time when samples of size 150 are randomly taken from the population. Under these circumstances, we would conclude that the power of the test is 83 percent, or .83.

Q-squared coefficient. This measure is also known after its main proponents as the Stone-Geisser Q-squared coefficient (Geisser, 1974; Kock, 2015d; Kock & Gaskins, 2014; Stone, 1974). The Q-squared coefficient is a nonparametric measure traditionally calculated via blindfolding. It is used for the assessment of the predictive validity (or relevance) associated with each latent variable block in the model, through the endogenous latent variable that is the criterion variable in the block. The Q-squared coefficient is sometimes referred to as a resampling analog of the R-squared. It is often similar in value to that measure. The Q-squared coefficient can assume negative values.

Reflective latent variable. A reflective latent variable is one in which all of the indicators are expected to be highly correlated with the latent variable score, and also highly correlated with one another. For example, the answers to certain question-statements by a group of people, measured on a 1 to 7 scale (1=strongly disagree; 7 strongly agree) and answered after a meal, are expected to be highly correlated with the latent variable "satisfaction with a meal". The question-statements are: "I am satisfied with this meal", and "After this meal, I feel full". Therefore, the

latent variable "satisfaction with a meal", can be said to be reflectively measured through these two indicators. These indicators store answers to the two question-statements. This latent variable could be represented in a model graph as "Satisf", and the indicators as "Satisf1" and "Satisf2".

Reliability of a measurement instrument. Reliability is a measure of the quality of a measurement instrument; the instrument itself is typically a set of question-statements. A measurement instrument has good reliability if the question-statements (or other measures) associated with each latent variable are understood in the same way by different respondents.

R-squared coefficient. This is a measure calculated only for endogenous latent variables, and that reflects the percentage of explained variance for each of those latent variables. The higher the R-squared coefficient, the better is the explanatory power of the predictors of the latent variable in the model, especially if the number of predictors is small. Contrary to popular belief and in spite of what their name implies, R-squared coefficients are not calculated by squaring a correlation-like measure. They can assume negative values, although these are rare occurrences that normally suggest problems with the model in which they occur; e.g., severe collinearity or model misspecification.

Statistical power. Statistical power is often referred to simply as "power"; see the latter for a definition.

Structural equation modeling (SEM). A general term used to refer to a class of multivariate statistical methods where complex relationships among latent variables and indicators are estimated at once. In a SEM analysis, each latent variable is typically measured through multiple indicators, although there may be cases in which only one indicator is used to measure a latent variable. Key measures of relationships among latent variables are path coefficients (or standardized partial regression coefficients) and corresponding P values. Key measures of relationships among latent variables and their respective indicators are weights and loadings, and corresponding P values.

Variance inflation factor (VIF). This is a measure of the degree of collinearity (or multicollinearity) among variables, including both indicators and latent variables. With latent variables, collinearity can take two main forms: vertical and lateral collinearity (Kock & Lynn, 2012). Vertical, or classic, collinearity is predictor-predictor latent variable collinearity in individual latent variable blocks. Lateral collinearity is a term coined by Kock & Lynn (2012) that refers to predictor-criterion latent variable collinearity; a type of collinearity that can lead to particularly misleading results. Full collinearity VIFs allow for the simultaneous assessment of both vertical and lateral collinearity in a SEM model.

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