

Partial Least Squares: Regression & Structural Equation Models

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Partial Least Squares

Overview

Partial least squares (PLS) analysis is an alternative to OLS regression, canonical correlation, or covariance-based structural equation modeling (SEM) of systems of independent and response variables. In fact, PLS is sometimes called “composite-based SEM”, “component-based SEM”, or “variance-based SEM”, in contrast to “covariance-based SEM,” which is the usual type (e.g., implemented by Amos, SAS, Stata, MPlus, LISREL, EQS and other major software packages).

On the response side, PLS can relate the set of independent variables to multiple dependent (response) variables. On the predictor side, PLS can handle many independent variables, even when predictors display multicollinearity. PLS may be implemented as a regression model, predicting one or more dependents from a set of one or more independents; or it can be implemented as a path model, handling causal paths relating predictors as well as paths relating the predictors to the response variable(s). PLS is implemented as a regression model by SPSS and by SAS's PROC PLS. SmartPLS is the most prevalent implementation as a path model.

PLS is characterized as a technique most suitable where the research purpose is prediction or exploratory modeling. In general, covariance-based SEM is preferred when the research purpose is confirmatory modeling. PLS is less than satisfactory as an explanatory technique because it is low in power to filter out variables of minor causal importance (Tobias, 1997: 1).

The advantages of PLS include ability to model multiple dependents as well as multiple independents; ability to handle multicollinearity among the independents; robustness in the face of data noise and missing data; and creating independent latent variables directly on the basis of cross-products involving the response variable(s), making for stronger predictions. Disadvantages of PLS include greater difficulty of interpreting the loadings of the independent latent variables (which are based on cross-product relations with the response variables, not based as in common factor analysis on covariances among the manifest independents) and because the distributional properties of estimates are not

known, the researcher cannot assess significance except through bootstrap induction.

Overall, the mix of advantages and disadvantages means PLS is favored as a predictive technique and not as an interpretive technique, except for exploratory analysis as a prelude to an interpretive technique such as multiple linear regression or covariance-based structural equation modeling. Hinseler, Ringle, and Sinkovics (2009: 282) thus state, "PLS path modeling is recommended in an early stage of theoretical development in order to test and validate exploratory models."

Developed by Herman Wold (Wold, 1975, 1981, 1985) for econometrics and chemometrics and extended by Jan-Bernd Lohmöller (1989), PLS has since spread to research in education (ex., Campbell & Yates, 2011), marketing (ex., Albers, 2009, cites PLS as the method of choice in success factors marketing research), and the social sciences (ex., Jacobs et al., 2011). See Lohmöller (1989) for a mathematical presentation of the path modeling variant of PLS, which compares PLS with OLS regression, principal components factor analysis, canonical correlation, and structural equation modeling with LISREL.

Data

Data for the section on PLS-SEM with SmartPLS uses the file jobsat.csv, a comma-delimited file which may also be read by many other statistical packages. For the jobsat file, sample size is 932. All variables are metric. Data are fictional and used for instructional purposes only. Variables in the jobsat.* file included these:

- StdEduc: respondent's educational level, standardized
- OccStat: respondent's occupational status
- Motive1: Score on the Motive1 motivational scale
- Motive2: Score on the Motive2 motivational scale
- Incent1: Score on the Incent1 incentives scale
- Incent2: Score on the Incent2 incentives scale
- Gender: Coded 0=Male, 1=Female. Used for PLS-MGA (multigroup analysis)

SPSS, SAS, and Stata versions of jobsat.* are available below.

- Click [here](#) for jobsat.csv, for SmartPLS

- Click [here](#) for jobsat4.csv, for PLS-CTA in SmartPLS
- Click [here](#) for jobsat.sav, for SPSS
- Click [here](#) for jobsat.sas7bdat, for SAS
- Click [here](#) for jobsat.dta, for Stata

The section of PLS regression modeling in SmartPLS uses the “HappyLife” data file.

- Click [here](#) for HappyLife.csv, for SmartPLS

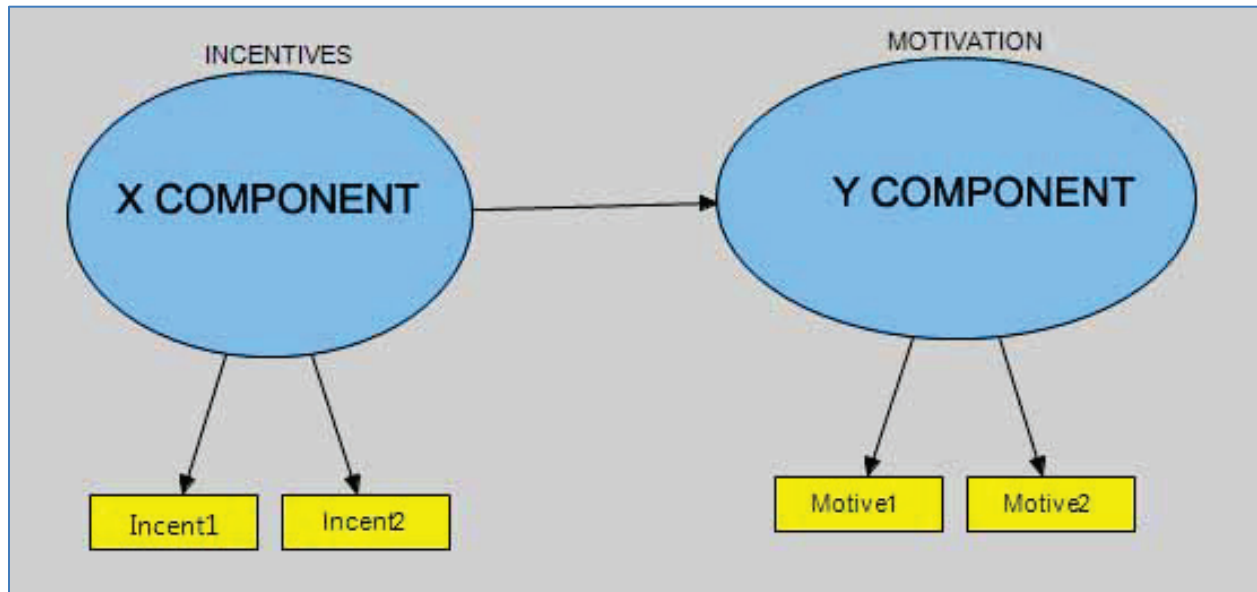
The section on PLS regression modeling in SPSS uses the SPSS sample file, 1991 U.S. General Social Survey.sav. The USGSS1991.sas7bdat file is a different format of the same variables used for the SAS example.

- Click [here](#) for 1991 U.S. General Social Survey.sav, for SPSS
- Click [here](#) for USGSS1991.sas7bdat, for SAS

Key Concepts and Terms

Background

Partial least squares (PLS) is sometimes called "Projection to Latent Structures" because of its general strategy, which is illustrated below. Note, however, that there may be more than one X component and more than one Y component and the arrows connecting the components to their indicators may be reflective as shown or may be reversed (reflective vs. formative modeling is discussed [below](#)).



The steps in the PLS-SEM algorithm, as described by Henseler, Ringle, & Sarstedt (2012), are summarized below.

1. Preliminary to applying the PLS algorithm, the measured indicator variables are normalized to have a mean of 0 and a standard deviation of 1. In this context, normalized means standardized. PLS requires standardized latent variable scores, and since latent variables in PLS are linear combinations of the indicator variables, it is necessary that the indicator variables be standardized. A consequence is that both measurement (outer model) and structural (inner model) path coefficients vary from 0 to plus or minus 1, with paths closest to absolute 1 being the strongest
2. In the first stage of the PLS algorithm, the measured indicator variables are used to create the X and Y component scores. To do this, an iterative process is used, looping repeatedly through four steps:
 - i. Latent variable scores are given initial approximations based on equally weighted indicator scores.
 - ii. Initial weights are assigned to the structural (inner) paths connecting the latent variables using a path weighting scheme based on regression, to maximize the R-squared of each endogenous latent variable. That is, component scores as estimated in a given iteration are used to calculate structural path weights. Put a third way, using

regression, successive iterations adjust the structural weights to maximize the strength of the relation of successive pairs of X and Y component scores by maximizing the covariance of each X-score with the Y variables. This maximizes the explained variance of the dependent component.

* Note that alternative to this path weighting scheme, factor-based and centroid-based weighting schemes may be used by different algorithms. PLS-regression in SPSS and SAS, for instance, uses a factor-based weighting scheme. See [below](#).

- iii. The structural (inner) weights are used to adjust the estimates of the latent variable scores.
- iv. The measurement (outer) weights connecting the latent variables to their indicator variables are estimated differently, depending on whether the model is reflective or formative (that is, which way the measurement arrows go, discussed [below](#)). For the usual reflective model, with arrows going from the latent variable to the indicator variables, measurement path weights are based on the covariances between the estimate of the latent variable and the indicator variable. If the model is formative, with arrows going from the indicators to the latent variable, measurement path weights are based on regression of the latent variable on its indicator.

Iterations of these four steps stop when there is no significant change in the measurement (outer) weights of the indicator variables. The weights of the indicator variables in the final iteration are the basis for computing the final estimates of latent variable scores. The final latent variable scores, in turn, are used as the basis of OLS regressions to calculate the final structural (inner) weights in the model.

The overall result of the PLS algorithm is that the components of X are used to predict the scores of the Y components, and the predicted Y component scores are used to predict the actual values of the measured Y variables. This strategy means that while the original X variables may be multicollinear, the X components used to predict Y will be orthogonal. Also, the X variables may have missing values, but there will be a computed score for every case on every X component. Finally, since only a few components (often two or three) will be used in predictions, PLS coefficients may be computed even when there may have been

more original X variables than observations (though results are more reliable with more cases). In contrast, any of these three conditions (multicollinearity, missing values, and too few cases in relation to number of variables) may well render traditional OLS regression estimates unreliable or impossible. The same is true of estimates by other procedures in the general and generalized linear model families.

Models

Overview

Partial least squares as originally developed in the 1960s by Wold was a general method which supported modeling causal paths among any number of "blocks" of variables (latent variables), somewhat akin to covariance-based structural equation modeling, the subject of the separate Statistical Associates "Blue Book" volume, "Structural Equation Modeling." PLS-regression models are a subset of PLS-SEM models, where there are only two blocks of variables: the independent block and the dependent block. SPSS and SAS implement PLS-regression models. For more complex path models it is necessary to employ specialized PLS software. SmartPLS is perhaps the most popular and is the software used in illustrations below, but there are alternatives discussed [below](#).

PLS-regression vs. PLS-SEM models

PLS-regression models are an alternative to OLS regression or canonical correlation. PLS regression has been used, for instance, for econometric growth modeling (Korkmazoglu & Kemalbay, 2012). Comparing OLS and PLS regression, one simulation study (Temme, Kreis, & Lutz, 2006: 20) found "In our study, results for simulated data, however, are very similar to those resulting from OLS regression."

PLS-SEM models, in contrast, are path models in which some variables may be effects of others while still be causes for variables later in the hypothesized causal sequence. PLS-SEM models are an alternative to covariance-based structural equation modeling (traditional SEM).

For an extended critique of PLS-SEM as not being suitable as a structural equation modeling (SEM) approach, see Rönkkö & Evermann (2013). For critique of Rönkkö

& Evermann, see Henseler, Dijkstra, Sarstedt et. al. (2014). To summarize this complex exchange in simple terms, Rönkkö & Evermann took the view that PLS yields inconsistent and biased estimates compared to traditional SEM, and in addition PLS-SEM lacks a test for over-identification. Defending PLS, Henseler, Dijkstra, Sarstedt et. al. took the view that Rönkkö & Evermann wrongly assumed SEM must revolve around common factors and failed to recognize that “structural equation models allow more general measurement models than traditional factor analytic structures” on which traditional SEM is based (Bollen & Long, 1993: 1). That is, these authors argued that PLS should be seen as a more general form of SEM, supportive of composite as well as common factor models (for an opposing view, see McIntosh, Edwards, & Antonakis, 2014). Henseler et al. wrote “scholars have started questioning the reflex-like application of common factor models (Rigdon, 2013). A key reason for this skepticism is the overwhelming empirical evidence indicating that the common factor model rarely holds in applied research (as noted very early by Schönemann & Wang, 1972). For example, among 72 articles published during 2012 in what Atinc, Simmering, and Kroll (2012) consider the four leading management journals that tested one or more common factor model(s), fewer than 10% contained a common factor model that did not have to be rejected.”

The critical bottom line for the researcher, agreed upon by both sides of the composite vs. common factors debate, is that factors do not have the same meaning in PLS-SEM models as they do in traditional SEM models. Coefficients from the former therefore do not necessarily correspond closely to those from the latter. As in all statistical approaches, it is not a matter of a technique being “right” or “wrong” but rather it is a matter of properly understanding what the technique is.

Components vs. common factors

As mentioned above, traditional variance-based PLS-SEM is a component-based approach using a type of principle components analysis to construct latent variables. This contrasts with traditional covariance-based SEM, which uses a type of common factor analysis to create latent variables. While latent variables are traditionally conceptualized as common factors, a construct might also be a component, which is what they are in PLS-SEM.

Common factors models assume that all the covariation among the set of its indicator variables is explained by the common factor. In a pure common factor model in SEM, in graphical/path terms, arrows are drawn from the factor to the indicators, and neither direct arrows nor covariance arrows connect the indicators.

Component factors, also called composite factors, have a more general model of the relationship of indicators to factors. Specifically, it is not assumed that all covariation among the set of indicator variables is explained by the factor. Rather, covariation may also be explained by relationships among the indicators. In graphical/path terms, covariance arrows may connect each indicator with each other indicator in its set. Henseler, Dijkstra, Sarstedt, et al. (2014: 185) note, “the composite factor model does not impose any restrictions on the covariances between indicators of the same construct.”

Traditional common factor based SEM seeks to explain the covariance matrix, including covariances among the indicators. Specifically, in the pure common factor model, the model-implied covariance matrix assumes covariances relating indicators within its own set or with those in other sets is 0 (as reflected by the absence of connecting arrows in the path diagram). Goodness of fit is typically assessed in terms of the closeness of the actual and model-implied covariance matrices.

Traditional component based PLS-SEM does not attempt to explain the covariances connecting indicators. Henseler, Dijkstra, Sarstedt, et al. (2014: 186) write, “The composite factor model leaves the covariation between indicators of the same block unexplained, which means that the implied covariances between these indicators equal the empirical covariances”.

In summary, latent variables in traditional PLS-SEM are components whereas in traditional SEM they are common factors. Because of this, PLS-SEM can be said to be more general than traditional SEM. Traditional SEM can be said to be more parsimonious than traditional PLS-SEM (fewer arrows in its model). Whether the researcher’s data fits a common factor model or fits a component model better is an empirical question, the answer to which is conditional on the particular data at hand. Advocates of composite factor models are likely to assert that component (composite) models are more prevalent in the “real world” ([Bentler & Huang, in press](#)). In practice, researchers using traditional SEM may add covariance arrows

connecting indicators precisely because good fit cannot be achieved without moving toward a composite factor model (Bentler, 1976).

This discussion applies to the traditional PLS algorithm. The “consistent PLS” (PLSc) algorithm discussed further [below](#) is employed in conjunction with common factor models and not with composite models. For a discussion of components vs. common factors in modeling, see Henseler, Dijkstra, Sarstedt, et al. (2014). For criticism, see McIntosh, Edwards, & Antonakis, 2014).

Components vs. summation scales

It is common in social science to create scales, which are a type of latent variable, simply by making the scale an additive (or otherwise weighted) sum of the indicators. In the PLS world, this is called the “sum score approach”. Typically, the sum score approach weights each indicator equally. The PLS-SEM approach, in contrast, gives more weight to indicators with higher predictive validity.

As noted by Henseler, Dijkstra, Sarstedt, et al. (2014: 192), “PLS construct scores can only be better than sum scores if the indicators vary in terms of the strength of relationship with their underlying construct. If they do not vary, any method that assumes equally weighted indicators will outperform PLS.” That is, PLS-SEM assumes that indicators vary in the degree that each is related to the measured latent variable. If not, summation scales are preferable. SmartPLS 3 will use the sum scores approach if, as discussed [below](#), maximum iterations are set to 0.

PLS-DA models

PLS-DA models are PLS discriminant analysis models. These are an alternative to discriminant function analysis, for PLS regression models where the dependent/response variable is binary variable or a dummy variable rather than a block of continuous variables.

Mixed methods

Note that researchers may combine both PLS regression modeling with PLS-SEM modeling. For instance, Tenenhaus et al. (2004), in a marketing study, used PLS regression to obtain a graphical display of products and their characteristics, with a mapping of consumer preferences. Then PLS-SEM was used to obtain a detailed

analysis of each consumer group by building a causal model involving consumer preference, physico-chemical, and sensory blocks of variables.

Bootstrap estimates of significance

As the distribution of PLS is unknown, conventional significance testing is impossible. However, testing may be accomplished by resampling methods such as the bootstrap or the jackknife, as illustrated by Davies (2001). Resampling methods do not have specific sample size requirements but the smaller the sample, the more likely that fitted confidence limits will be fitted to noise in the data rather than to a true underlying distribution. Wakeling & Morris (2005), based on Monte Carlo simulation studies, have created tables of critical values of r^2_{cv} . Since resampling estimates are data-driven, results may not hold up for other datasets and therefore cross-validation is recommended (ex., developing the PLS model for even-numbered observations and validating it for odd-numbered observations, after randomizing the order of observations).

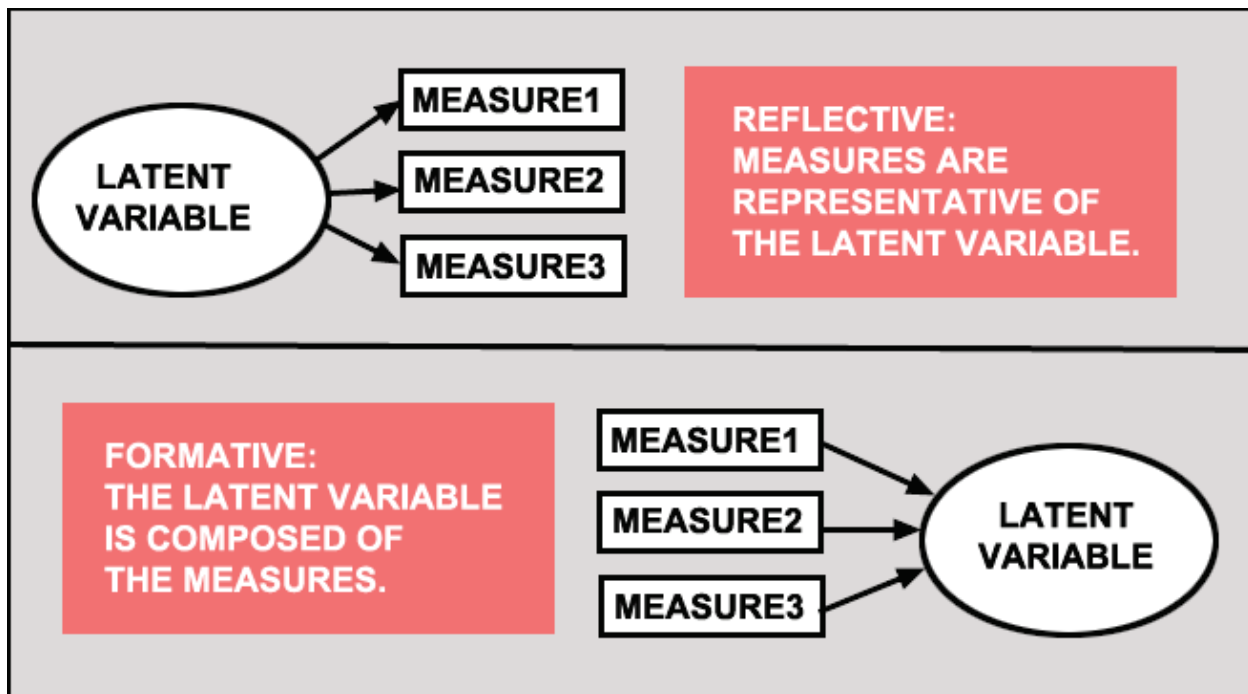
Some PLS packages use bootstrapping (e.g., SmartPLS) while others use jackknifing (e.g., PLS-GUI). Both result in estimates of the standard error of regression paths and other model parameters. The estimates are usually very similar. Bootstrapping, which involves taking random samples and randomly replacing dropped values, will give slightly different standard error estimates on each run. Jackknifing, which involves a leave-one-out approach for $n - 1$ samples, will always give the same standard error estimates. Where jackknifing estimates the point variance, bootstrapping estimates the point variance and the entire distribution and thus bootstrapping is required when the research purpose is distribution estimation. As the research purpose is much more commonly variance estimation, jackknifing is often preferred on grounds of replicability and being less computationally intensive.

Reflective vs. formative models

A path model is reflective if in the path diagram causal arrows go from the latent variable (factor) to the measured indicator variables. A path model is formative if the arrows go from the observed measures to the latent variables. Sometimes reflective models are called “Mode A” models and formative models are called “Mode B” models. SmartPLS allows both types of models (choose Selection, Invert measurement model from the menu).

Both traditional SEM and PLS-SEM support both reflective and formative models. By historical tradition, reflective models have been the norm in structural equation modeling and formative models have been the norm in partial least squares modeling. This is changing as researchers become aware that the choice between reflective and formative models should depend on the nature of the indicators.

It should be noted there is a controversy in the literature with regard to the proper statistical modeling procedure for reflective and formative models. Adherents to the PLS approach, such as Christian Ringle, Oliver Götz, et al. (2009). (2014) and Jörg Henseler, Theo Dijkstra, Marko Sarstedt, et al. (2014), see PLS being applicable to both reflective and formative models. Critics such as McIntosh, Edwards, & Antonakis (2014: 215) express the view that PLS should be applied only to formative composite models (see discussion [above](#)), not to common factors models, since traditional SEM (covariance-based SEM) has superior statistical properties for reflective latent variable models.



In reflective models, indicators are a representative set of items which all reflect the latent variable they are measuring. Reflective models assume the factor is the "reality" and measured variables are a sample of all possible indicators of that reality. This implies that dropping one indicator may not matter much since the

other indicators are representative also. The latent variable will still have the same meaning after dropping one indicator.

In formative models, each indicator represents a dimension of meaning of the latent variable. The set of indicators collectively represent all dimensions of the latent variable. Formative models assume the indicators are "reality" and are all the dimensions of the factor. Dropping an indicator in a formative model is equivalent to dropping a dimension of meaning, causing the meaning of the latent variable to change. To the extent that a dimension dropped is important, the meaning of the latent variable will change. The researcher may retain the same label for the latent variable (ex., "motivation") even though the dimensions change, misleading readers into thinking "motivation" means the same thing across models.

Albers and Hildebrandt (2006; sourced in Albers, 2010: 412) give an example for a latent variable dealing with satisfaction with hotel accommodations. A reflective model might have the representative measures "I feel well in this hotel", "This hotel belongs to my favorites", "I recommend this hotel to others", and "I am always happy to stay overnight in this hotel." A formative model, in contrast, might have the constituent measures, "The room is well equipped", "I can find silence here", "The fitness area is good", "The personnel are friendly", and "The service is good".

Suppression is another possible problem in formative models. Because the indicator items in a formative model represent different dimensions, there is the possibility one item may be negatively correlated with another. If a first item is negatively related to a second indicator but positively related to the latent variable, the positive correlation of the second indicator with the latent variable may be suppressed due push-pull effect of the co-occurrence of positive and negative weights (see Henseler, Ringle, & Sarstedt, 2012: 270).

SmartPLS outputs a table of "Indicator Data (Correlations)", shown below. Output for reflective and formative models is identical. Coefficients are the raw bivariate correlations. For a reflective model, one would expect the correlations of indicators for the same construct would be high since indicators should be representative measures of the same phenomenon. For instance, the correlation of Incent1 with Incent2 for the construct Incentives is .656. For a formative model, indicators should represent different dimensions of the phenomenon and

would not be expected to necessarily correlate highly unless there are multiple measures for the same dimension. Examination of this table provides one type of evidence of whether the data should be modeled reflectively or formatively.

Indicator Data (Correlations)

	Incent1	Incent2	Motive1	Motive2	OccStat	?StdEduc
Incent1	1.000	0.656	0.582	0.483	-0.343	-0.354
Incent2	0.656	1.000	0.446	0.529	-0.330	-0.364
Motive1	0.582	0.446	1.000	0.647	-0.343	-0.388
Motive2	0.483	0.529	0.647	1.000	-0.323	-0.421
OccStat	-0.343	-0.330	-0.343	-0.323	1.000	0.536
?StdEduc	-0.354	-0.364	-0.388	-0.421	0.536	1.000

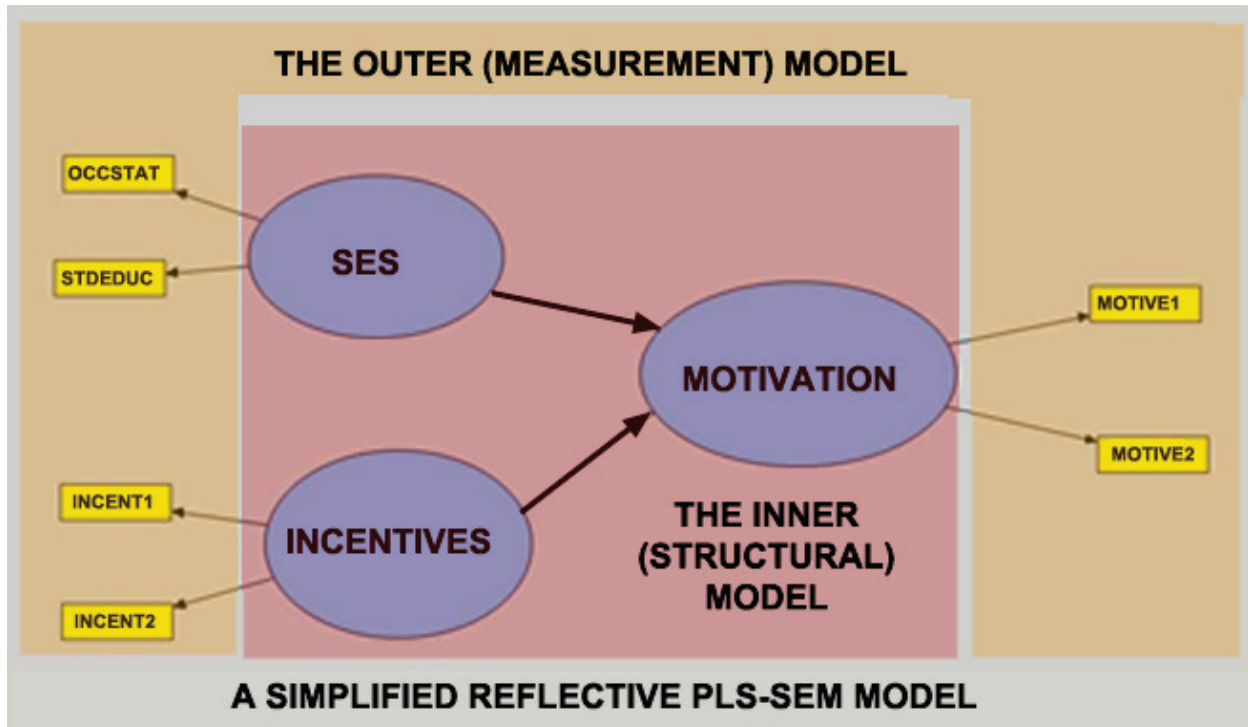
In terms of estimation methods discussed further below, the traditional PLS algorithm is well suited for formative and composite models. In early applications of PLS, formative modeling was more prevalent than reflective modeling, quite in contrast to the tradition of covariance-based structural equation modeling, where reflective modeling has always been dominant. Some, such as Rigdon (2013), have even argued that the use of PLS should be restricted to formative and composite measurement models (see response to Rigdon by Dijkstra, 2014). The “consistent PLS” algorithm (PLSc), discussed [below](#), is designed to produce consistent estimated for reflective models and may be preferred in reflective applications.

Confirmatory vs. exploratory models

Most statisticians see PLS is seen as an exploratory procedure. Wold himself (1981) advised against using PLS for confirmatory models since PLS lacks goodness-of-fit tests, which in turn means absence of criteria for selecting the optimum model. The literature, however, reveals more confirmatory than exploratory uses of PLS modeling by a large margin.

Inner (structural) model vs. outer (measurement) model

When a model is created, factors are represented by ellipses and indicator (measured) variables by rectangles. The factor ellipses and arrow creating them are called the inner or structural model. The indicator rectangles and arrows connecting them are called the outer or measurement model. This is illustrated below.



Endogenous vs. exogenous latent variables

These are terms pertaining to the inner or structural model. A latent variable is exogenous if it is not an effect of any other latent variable in the model (there are no incoming arrows from other latent variables). A latent variable is endogenous if it is an effect of at least one other latent variable (there is at least one incoming arrow from another latent variable). In the diagram above, SES and INCENTIVES are exogenous while MOTIVATION is endogenous.

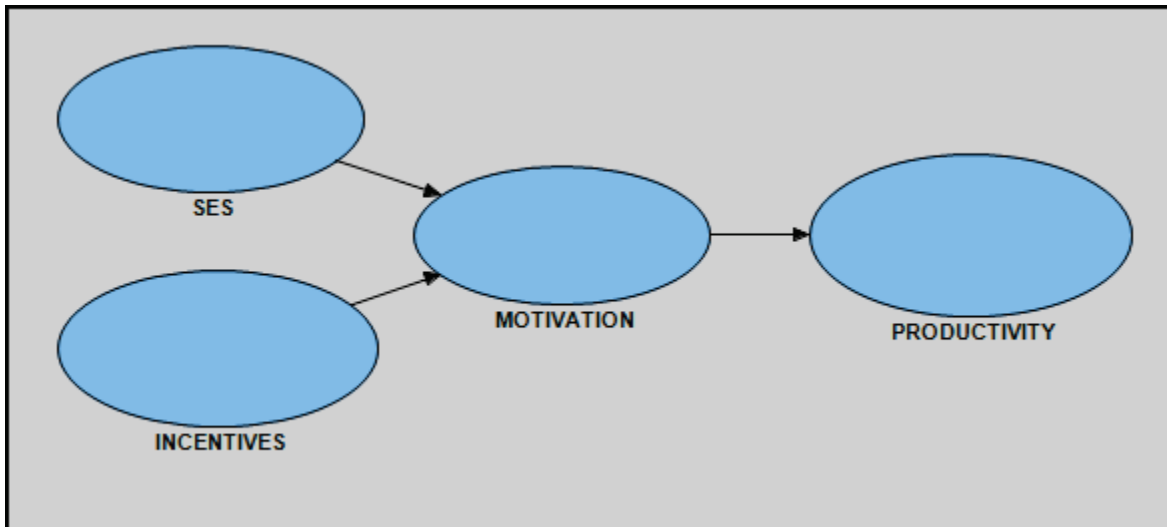
Mediating variables

A mediating variable is simply an intervening variable. In the model below, Motivation is a mediating variable between SES and Incentives on the one hand and Productivity on the other.

If there were also direct paths from SES and/or Incentives to Productivity, the SES and/or Incentives would be antecedent variables (or “moderating variables” as defined [below](#)) for both Motivation and Productivity. Motivation would still be a mediating variable.

A common type of “mediator analysis” involving just such mediating and moderating effects is to start with a direct path, say SES → Productivity, then see what the consequences are when an indirect, mediated path is added, such as SES → Motivation → Productivity. There are a number of possible findings when the mediated path is added:

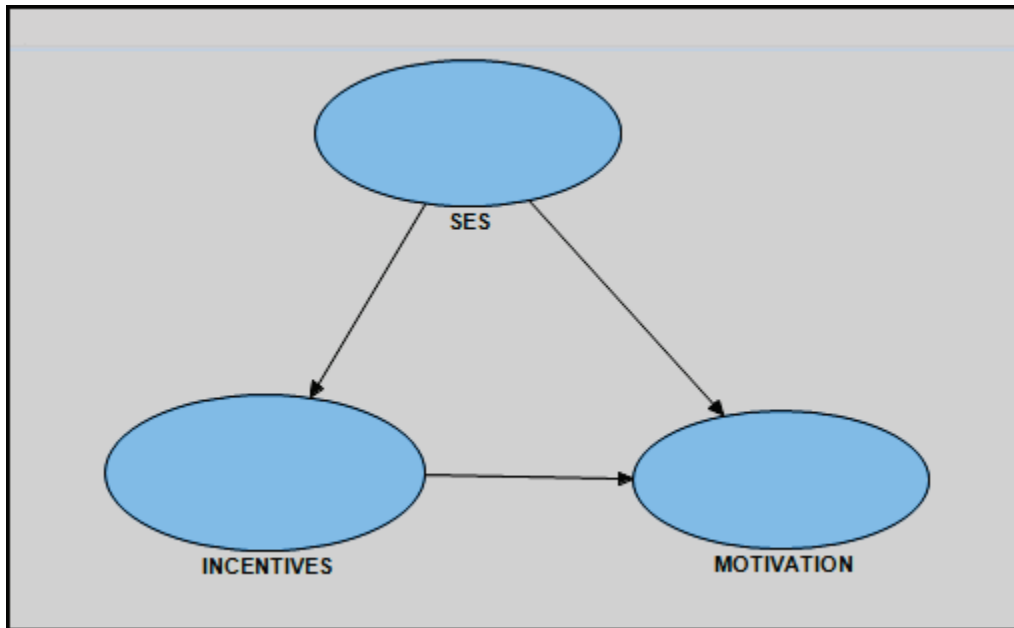
- The correlation of SES and Productivity drops to 0, meaning there is no SES → Productivity path as the entire causality is mediated by Motivation. This is called a “full control” effect of Motivation as a mediating variable.
- The correlation of SES and Productivity remains unchanged, meaning mediated path is inconsequential. This is “no effect”.
- The correlation of SES and Productivity drops only part way toward 0, meaning both the direct and indirect paths exist. This is called “partial control” by the mediating variable.
- The correlation of SES and Productivity increases compared to the original, unmediated model. This is called “suppression” and would occur in this example if the effect of SES directly on productivity and the effect of SES directly on Motivation were opposite in sign, creating a “push-pull” effect.



Moderating variables

The term “moderating variable” has been used in different and sometimes conflicting ways by various authors. Some writers use “mediating” and “moderating” interchangeably or flip the definition compared to other scholars. For instance, a mediating variable as described above does affect or “moderate” the relationship of variables it separates in a causal chain and thus might be called a moderating variable. It is also possible to model interactions between latent variables and latent variables representing interactions may be considered to involve moderating variables. Multigroup analysis of heterogeneity across groups, discussed further [below](#), is also a type of analysis of a moderating effect.

However, as used here, a moderating variable is an antecedent joint direct or indirect cause of two variables further down in the causal model. In the illustration below, SES is modeled as an antecedent cause of both Incentives and Motivation.



In the model above, adding SES to the model may cause the path from Incentives to Motivation to remain the same (no effect), drop to 0 (complete control effect of SES), drop part way to 0 (partial control effect), or to increase (suppression effect).

Spurious effects

If two variables share an antecedent cause, they usually are correlated but this effect may be spurious. That is, it may be an artifact of mutual causation. A classic example is ice cream sales and fires. These are correlated, but when the antecedent mutual cause of “heat of the day” is added, the original correlation goes away. In the model above, similarly, if the original correlation of Incentives and Motivation disappeared when the mutual antecedent cause SES was added to the model, it could be inferred that the originally observed effect of Incentives on Motivation was spurious.

Suppression

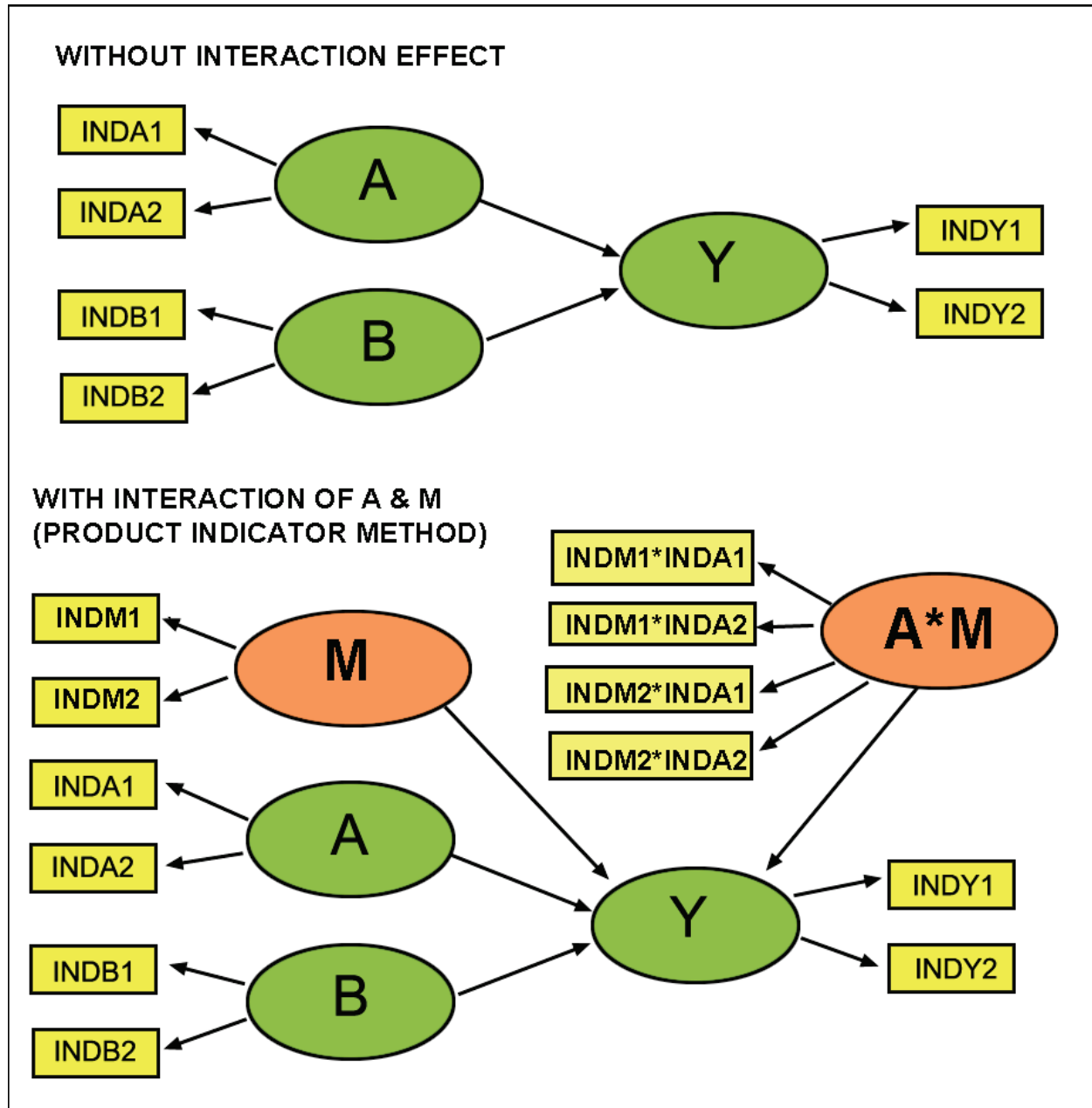
A suppression effect occurs when the antecedent variable is positively related to the predictor variable (ex., Incentives) and negatively related to the effect variable (ex., Motivation). In such a situation the antecedent variable has a suppressing effect in that the original Incentives/Motivation correlation without SES in the model will be lower than when SES is added to the model, revealing its push-pull effect as an antecedent variable. Put another way, the effect of

Incentives on Motivation initially appears weaker than it really is because, as seen when SES is added to the model, the correlation is suppressed by SES as a moderating variable.

Interaction terms

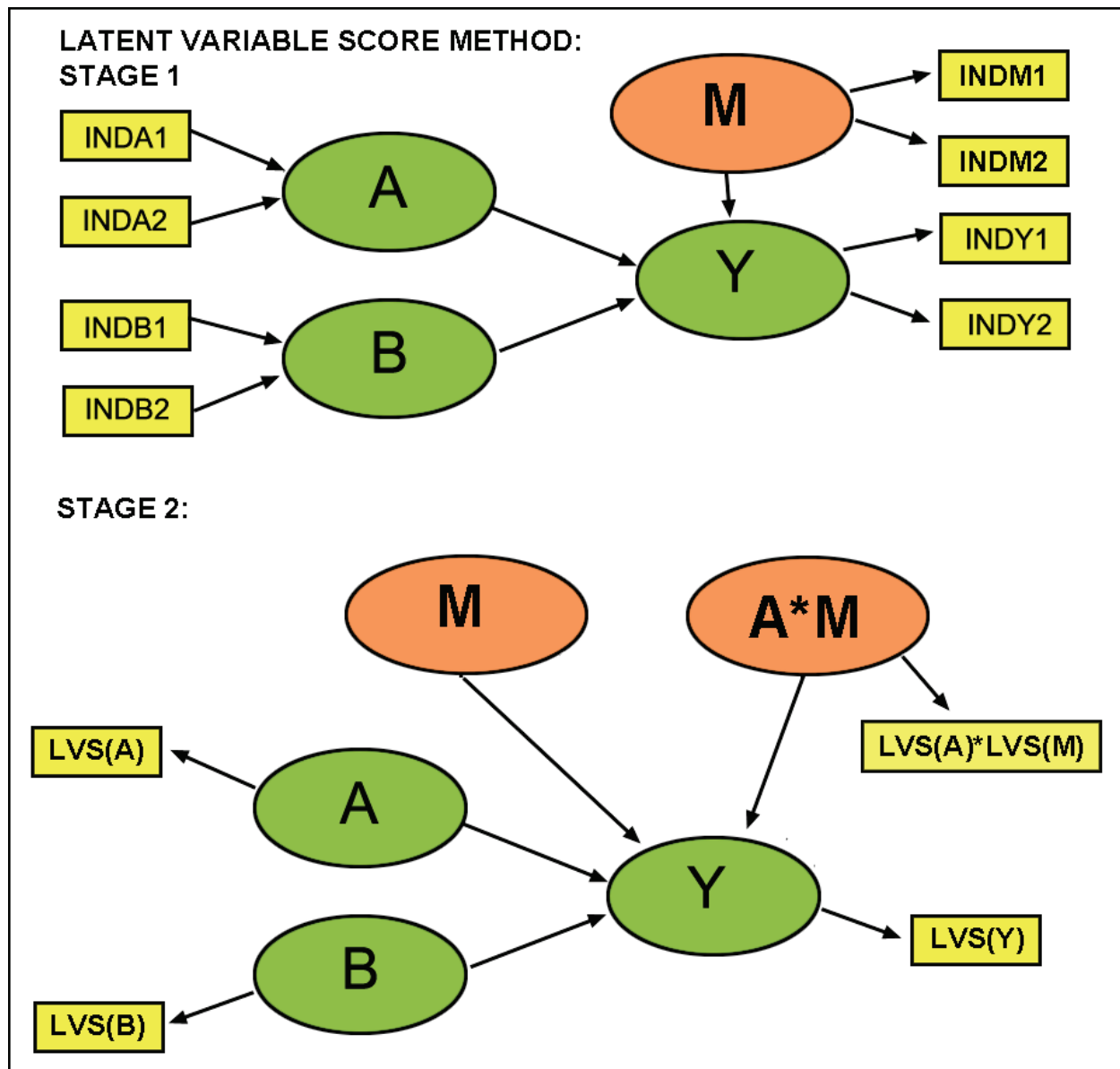
An interaction term is an exogenous moderator variable which affects an endogenous variable by way of a non-additive joint relation with another exogenous variable. While it may also have a direct effect on the endogenous target variable, the interaction is its non-additive joint relationship. In the diagram below, top, without interaction effect, latent variables A and B are modeled as causes of Y. Let moderator variable M be added as a third cause of Y. The researcher may suspect, however, that M and A have a joint effect on Y which goes beyond the separate A and M linear effects – that is, an interaction effect is suspected.

There are two popular methods for modeling such a hypothesized interaction. The first, the product indicator method, is illustrated below. This method may only be used for reflective models. In this approach, a new latent variable (the A*M factor) is added to the model whose indicators are the products of every possible pair of indicators for A and for M. For instance, its first indicator is INDM1*INDA1, being the product of the first indicator for M times the first indicator for A. If there is an interaction effect beyond the separate linear effects of A and M, then the path from A*M to Y will be significant.



A popular second approach to modeling interactions is depicted in the figure below. This is the latent variable score (LVS) approach, based on the product of latent variable scores. Unlike the product indicator approach, the latent variable score approach can be used when exogenous variables are modeled formatively, as in stage 1 of the figure below, or they may be modeled reflectively. The LVS approach requires two stages. In stage 1 (below top), A, B, and M are modeled as exogenous causes of Y, the endogenous variable. As part of stage 1, latent variable scores are created for all factors in the model.

In stage 2, all factors are modeled with a single indicator, which is their latent variable score from stage 1. Since latent variables with single indicators are set equal to their indicators, it does not matter whether they are modeled reflectively or formatively. Also, a new latent variable is created whose single indicator is the product of the stage 1 latent variable scores for A and for M. The A*M interaction is significant if its path to Y is significant in the stage 2 run of the model.



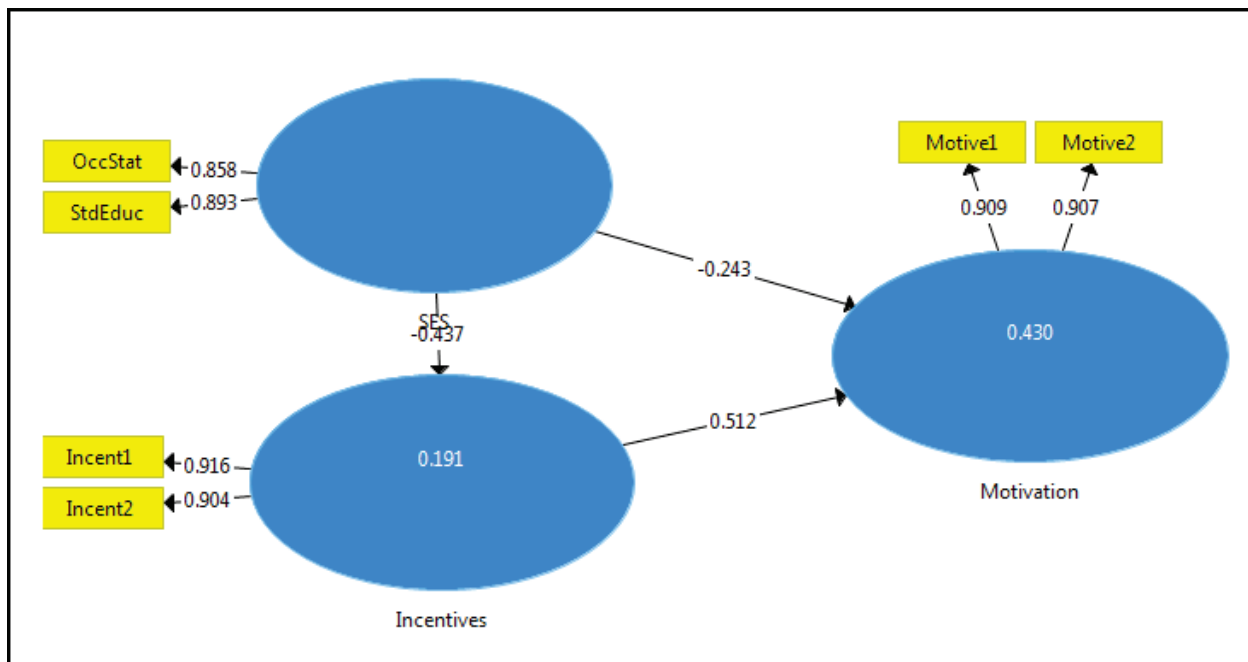
Simulation studies by Chin (2010) suggest that the product indicator approach produces more accurate parameter estimates than does the latent variable score method. Hair et al. (2014: 265) recommend the product indicator method when

the research purpose is hypothesis testing but recommend the latent variable score approach when the purpose is prediction.

Partitioning direct, indirect, and total effects

The path multiplication rule may be used to estimate direct and indirect effects when, as in the model depicted above, one variable (SES) has a direct effect on another (Motivation) as well as an indirect effect (from SES to Incentives to Motivation). The direct effect is the standardized structural coefficient, also known as the inner model loading of SES on Motivation. The indirect effect is the product of the path coefficient for SES-> Incentives times the path coefficient for Incentives -> Motivation. In more complex models there may be more than two paths multiplied together to get the indirect effect. The total effect of SES on Motivation is the sum of its direct and indirect effects.

Consider the model below, which has standardized path coefficients placed on its arrows.



The effects are these:

SES -> INCENTIVES: Direct = -0.437; Indirect = n/a; Total = -0.437

SES-> MOTIVATION: Direct = -0.243; Indirect = $-0.437 \times 0.512 = -0.224$; Total = $-0.243 + (-0.224) = -0.466$

INCENTIVES->MOTIVATION: Direct = 0.512; Indirect = n/a; Total = 0.512

Partitioning the effects shows that SES has a smaller total absolute effect on MOTIVATION than does INCENTIVES (-.467 vs. .512), with the total effect of SES being negative and that of INCENTIVES being positive.

The table below shows corresponding SmartPLS output. “Path Coefficients” are the direct effects which, when added to the “Indirect Effects” yield the “Total Effects”.

Path Coefficients			
	Incentives	Motivation	SES
Incentives		0.5124	
Motivation			
SES	-0.4369	-0.2425	

Indirect Effects			
	Incentives	Motivation	SES
Incentives	1.0000		
Motivation		1.0000	
SES		-0.2239	1.0000

Total Effects			
	Incentives	Motivation	SES
Incentives	1.0000	0.5124	
Motivation		1.0000	
SES	-0.4369	-0.4664	1.0000

Variables

PLS regression and modeling may involve any of the types of variables discussed below.

Case identifier variable

This is the case ID variable used for casewise output and saved datasets.

Measured factors and covariates

Measured covariates are the measured (manifest) continuous variables entered as measures for the dependent and independent variables. Measured factors are the measured categorical variables entered as dummy variables in the model. (Note this use of “factors” is not to be confused with the more common use of that term to refer to latent variables.) Multiple measured independent and dependent variables are used to construct PLS factors and PLS responses respectively.

Modeled factors and response variables

In other contexts, factors are categorical variables used as predictors. In the context of PLS-SEM, factors are the latent variables which are extracted as linear (usually equally weighted) combinations of the measured (indicator) variables. For PLS-regression, which uses a factor rather than path weighting scheme, the researcher may specify how many factors to extract from the measured indicator variables. For PLS-regression, ordinarily the first 3 - 7 factors will account for 99% of the variance (five factors is the default in PLS-regression in SPSS, for example).

Latent variables in PLS vs. SEM. Note that PLS factors are not the same as the latent variables in common factor analysis in the usual covariance-based structural equation modeling (SEM). Where SEM is based on common (principal) factor analysis, PLS-regression is based on principal component analysis (PCA). (PCA is discussed more fully in the separate Statistical Associates "Blue Book" on "Factor Analysis"). Many reserve the term "latent variable" for those created based on covariances, as in covariance based SEM, referring to PLS factors as “components” or “weighted composites.”

The term "composite" refers to the fact that PLS factors are estimated as exact linear combinations of their indicators. True latent variables in SEM, in contrast, are computed in a manner which reflects the covariation of their indicators (McDonald, 1996). While a PLS-SEM model of causal relations among composites may approximate a SEM path model of causal relations among latent variables

(McDonald, 1996) the two are not equivalent and under certain circumstances may diverge considerably. Only when the PLS weight vector is proportional to the SEM common factor loading vector will SEM and PLS factors be similar (see Schneeweiss, 1993).

Number of latent variables in PLS regression. In PLS-SEM modeling, the number of latent variables is determined a priori by theory. In PLS regression, however, both PLS responses and PLS factors are not specified a priori by the researcher, though researcher must specify how many latent variables to extract. Both predictor and response variables will have the same number of factors. There is no one criterion for deciding how many latent variables to employ. Common alternatives are:

Cross-validating the model with increasing numbers of factors, then choosing the number with minimum prediction error on the validation set. This is the most common method, where cross-validation is "leave-one-out cross-validation" discussed below, prediction error may be measured by the PRESS statistic discussed below, and models are computed for 1, 2, 3, c factors and the model with the lowest PRESS statistic is the most explanatory.

Alternatively one may use the method above to identify the model with the lowest prediction error, then choose the model with the least number of factors whose residuals are not significantly greater than that lowest prediction error model. See van der Voet (1994).

In a third alternative, models may be computed for 1, 2, 3, factors, and the process stopped when residual variation reaches a given level.

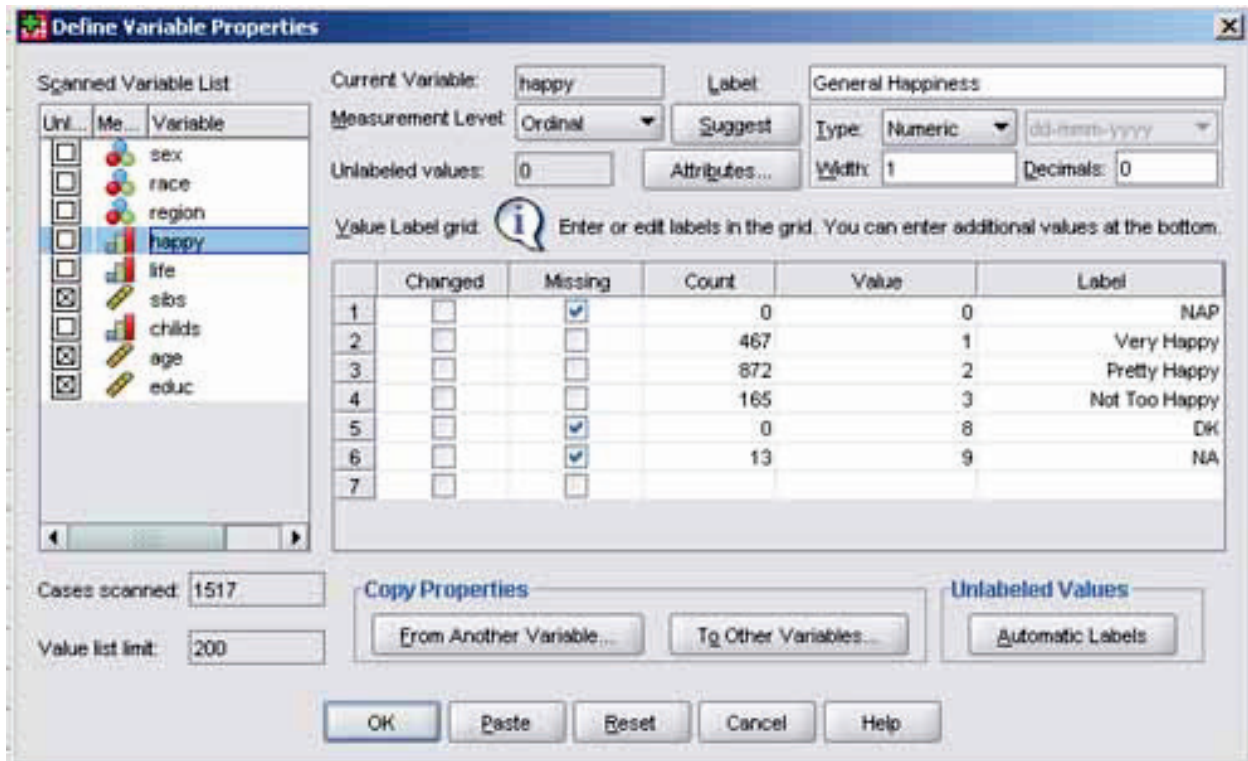
Single-item measures

Measures used in modeling, including PLS modeling, are often validated scales composed of multiple items, as in a scale of "authoritarian leadership." Multiple items generally increase reliability and improve model performance compared to single-item measures. In some cases, however, item reliability is not at issue because it may be assumed that measurement is without error or very close to it. Candidates for single-item measurement include such variables as gender, age, or salary. Also, single-item variables may cause identification and convergence problems in covariance-based SEM, but this is not a problem in PLS-SEM.

Measurement level of variables

The permitted measurement level of the indicator variables varies by package, as discussed [below](#) in the "Assumptions" section. In SPSS PLS regression, when first running PLS, the user must specify measurement levels. This is essential in SPSS, which uses a multiple regression algorithm for scalar dependent variables and a classification algorithm for categorical dependent variables, or a mixed model if both types of predictors are used. Note that in SPSS the user can temporarily change the measurement level setting for a variable to investigate what difference it makes, say, to treat an ordinal survey item as if it were interval (however, covariates must be coded as numeric).

Categorical variable coding. Both nominal and ordinal variables are treated the same, as categorical variables, by SPSS algorithms. Dummy variable coding is used. For a categorical variable with c categories, the first is coded (1, 0, 0,...0), where the last 0 is for the c th category. The last category is coded (0, 0, 0, 1). In the PLS dialog, the researcher specifies which dummy variable representing desired reference category is to be omitted in the model. When prompted at the start of the PLS run, click the "Define Variable Properties" button to obtain first a dialog letting the user enter the variables to be used, then proceed to the "Define Variable Properties" dialog, shown above. SPSS scans the first 200 (default) cases and makes estimates of the measurement level, classifying variables into nominal, ordinal, or scalar (interval or ratio). Symbols in front of variable names in the "Scanned variable list" on the left show the assigned measurement levels, though these initial assignments can be changed in the main dialog, using the drop-down menu for "Measurement Level". It is a good idea to check proper assignment of missing value codes and other settings in this dialog also. Clicking the "Help" button explains the many options available in the "Define Variable Properties" dialog.



Parameter estimates

Simulation studies comparing PLS-SEM and covariance-based SEM tend to confirm that PLS serves prediction purposes better when sample size is small (Hsu, Chen, & Hsieh, 2006: 364-365; see also discussion of sample size [below](#)). However, such studies also suggest that PLS exhibits a downward bias, underestimating path coefficients (Hsu, Chen, & Hsieh, 2006: 364; see also Chin, 1998; Dijkstra, 1983) and SEM serves prediction purposes better for large sample size.

Cross-validation and goodness-of-fit

Compared to covariance-based SEM, PL-SEM lacks the variety of goodness of fit measures to assess overall model fit. However, cross-validation indices (cv-redundancy and cv-communality) are supported by some existing PLS software programs. In cross-validation, the PLS model is developed for all the cases save one, then tested on that hold-out case. This is repeated n times, with each case used as the validation case in turn. In addition to this leave-one-out form of cross-validation (also called "full cross-validation"), software (ex., SAS) may support cross-validation by splitting the data into blocks or by reserved test set validation.

Leave-one-out cross-validation is recommended for small and medium datasets; split sample and reserved test set methods require large samples. The *cross-validation coefficient*, r^2_{cv} , is the percent of variance explained in the dependent variate by the predictions from the leave-one-out process (see Wakeling & Morris, 2005: 294). That is,

$$r^2_{cv} = (RSS - PRESS) / RSS$$

where RSS is the initial sum of squares for the dependent variable and PRESS is the PRESS statistic discussed below. Wakeling & Morris (2005: 298-300), using Monte Carlo simulation methods, have developed tables of critical values of r^2_{cv} for one-, two-, and three-dimensional models, for datasets with given numbers of rows and columns. Thus r^2_{cv} greater than the critical value may be taken as significant, and the researcher may select the model with the least number of dimensions with a significant cross-validation statistic as being the most parsimonious and therefore optimal model.

PRESS and optimal number of dimensions

In PLS regression in SPSS and some other packages, the predicted residual sum of squares (PRESS) for cross-validation is computed for the 0-factor model, the 1-factor model, the 2-factor model, etc. PRESS can be used to determine the optimal number of factors. Extracting the maximum number of factors (dimensions) gives a fully explanatory model which is overfitted and trivial. Correspondingly, as one adds dimensions, PRESS becomes lower and lower but then at some point may rise. Plotting PRESS by number of dimensions gives a scree plot, and the researcher may opt for the model (number of dimensions) where the scree plot curve forms an elbow and levels off. However, as in factor scree plots, there may be more than one "elbow" and researcher discretion is involved in selection of the exact number of dimensions for the best model. Alternatively, the researcher may select the first or the global minimum PRESS points as the basis for identifying the corresponding number of dimensions for the optimal model. In yet another alternative, the researcher may use the critical values of r^2_{cv} method discussed above. It may be noted that yet other, albeit less popular, criteria have also been proposed.

PLS-SEM in SPSS, SAS, and Stata

Overview

At this writing, PLS-SEM is not supported by SPSS, SAS, or Stata, which only support PLS regression, as discussed later in this volume.

PLS-SEM in SmartPLS

Overview

SmartPLS, a free, user-friendly modeling package for partial least squares analysis, is supported by a community of scholars centered at the University of Hamburg (Germany), School of Business, under the leadership of Prof. Christian M. Ringle. SmartPLS 3 is illustrated in this volume. The website is <http://www.smartpls.de>. Example projects are located at <http://www.smartpls.de/documentation/index>. As a side note, SmartPLS is a successor to the *PLSPath* software used in the 1990s.

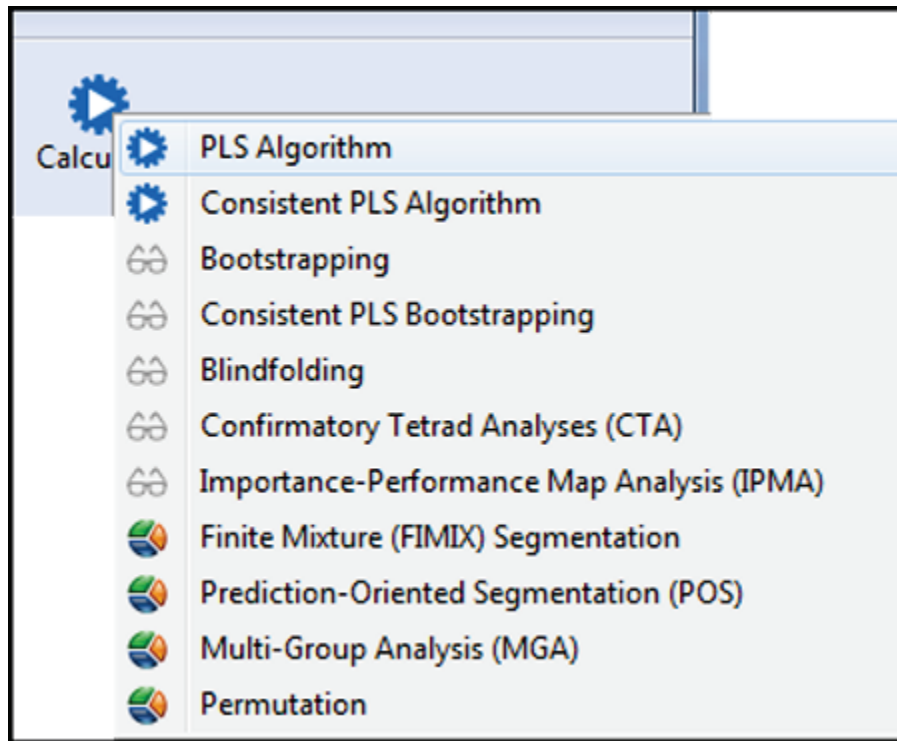
SmartPLS comes in four variants:

1. SmartPLS 3 Student: All algorithms are supported, but data are restricted to 100 observations although the number of projects is unlimited. Free.
2. SmartPLS 3 Professional: All algorithms; unlimited observations and projects; export results to Excel, R, and html; copy results to clipboard; export the graphical model; prioritized technical support; customizable display. Fee.
3. SmartPLS 3 Professional 30-day trial version: Free.
4. SmartPLS 3 Enterprise: Same as SmartPLS 3 Professional but for up to three installations and with method support service, results review service, and personal support via Skype. Fee.

After registering, a video-based manual is available by entering this url in a web browser: `file:///C:/SmartPLS/Handbook/index.html` (assuming SmartPLS is installed in this default folder). For further reference, see Ringle, Wende, and Will (2005) and Ringle (2006); Hair, Hult, Ringle, & Sarstedt (2014).

Estimation options in SmartPLS

From the SmartPLS menu, selecting the “Calculate” icon causes the menu shown below to appear, from which the researcher may select one of the estimation methods shown. The “PLS Algorithm” option computes in the standard (default) PLS solution.



Each of these estimation options is considered in a separate section below.

1. [PLS Algorithm](#)
2. [Consistent PLS Algorithm](#)
3. [Bootstrapping](#)
4. [Consistent PLS Bootstrapping](#)
5. [Blindfolding](#)
6. [Confirmatory Tetrad Analysis \(CTA\)](#)
7. [Importance-Performance Matrix Analysis \(IPMA\)](#)
8. [Finite Mixture Segmentation \(FIMIX\)](#)
9. [Prediction-Oriented Segmentation \(POS\)](#)
10. [Multi-Group Analysis \(MGA\)](#)
11. [Permutation](#)

Note that the section below on “Running the PLS algorithm” contains information on model construction and options which apply to other algorithms as well. For other estimation options, only unique output not discussed in the “PLS Algorithm” section is presented. The reader is therefore encouraged to read the “PLS Algorithm” section first before proceeding to other estimation option sections.

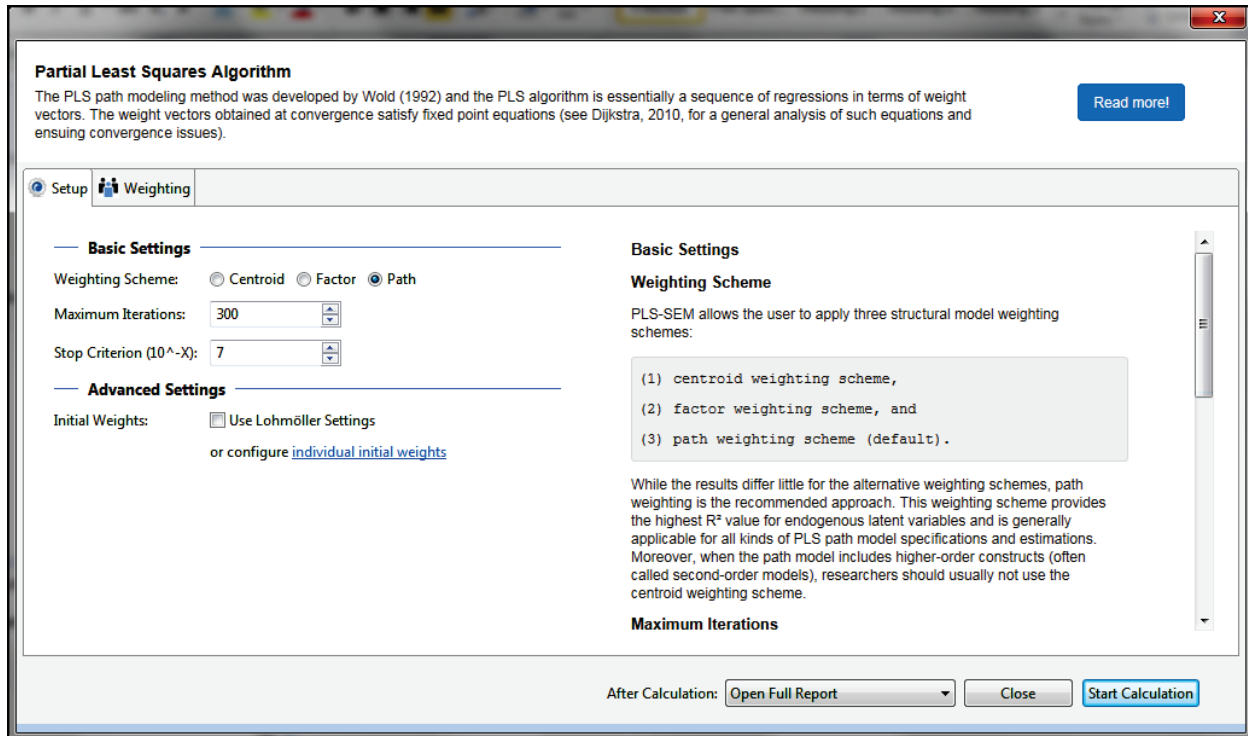
Running the PLS algorithm

Options

This section describes running the original PLS algorithm for the simple path model described [below](#). The “consistent PLS algorithm”, usually called just the “PLS algorithm”, is the default standard partial least squares modeling procedure.

The PLS algorithm may be run only after a model is created following steps described below. After the path model is created, the researcher double-clicks on the path model in the Project Explorer pane on the left. This will reveal the path diagram and above it an icon, the “PLS Algorithm” icon, which may be clicked to run the consistent PLS algorithm. Alternatively, selecting Calculate > PLS Algorithm from the main menus also instructs SmartPLS to run the model using default standard estimation methods.

Running the PLS algorithm brings up the options screen shown below. Typically, the researcher accepts all defaults and clicks the “Start Calculation” button in the lower right.



Elements of this dialog are described below. Description is also found in the dialog itself under “Basic Settings” in the right-side pane of the dialog.

- *“Read more!” button:* (Upper right). This opens a page of general description and bibliography about the PLS algorithm. This option is gives the same page as clicking the “PLS Algorithm” tab in the same dialog.
- *Weighting Scheme:* Weighting refers to assigning weights to the structural (inner model) path coefficients. In addition to the default “Path” choice, “Centroid” or “Factor” may be selected. Noonan & Wold (1982) found that the choice of weighting schemes made little difference in path estimates: $< .005$ for structural (inner) paths and $< .05$ for measurement (outer) paths.
 - The path method maximizes the R^2 value of endogenous latent variables in the current model, with the latent variable estimated based on regression. This method was introduced by Lohmöller (1989) and is the method recommended by Henseler, Ringle, & Sarstedt (2012), Hair et al. (2014), and many others. It is the default in SmartPLS.

- The factor method maximizes the variance of the principal component and estimates the latent variable based on the correlation of the exogenous and endogenous latent variables. It is not appropriate when the researcher is positing the directionality of the relationships connecting latent variables as, unlike the path method, directionality information is not taken into account. This method was also introduced by Lohmöller (1989).
- The centroid method, used if path or factor methods do not converge on a solution, is an older approach used when the correlation matrix of the latent variables is singular. The original approach used by Wold (1975), the “father of PLS”, the centroid method estimates the latent variable based on other latent variables in the model. The centroid method is not appropriate when there are second-order or higher latent variables in the model. Weights are based on the sign of the correlation of the exogenous and endogenous latent variables. When the correlation is close to 0, small data fluctuations may have strong effects on the model. See Henseler, Ringle, & Sinkovics (2009).
- *Maximum Iterations:* The default is 300 iterations while seeking convergence on a solution. The default is almost always selected by researchers. A larger number, such as 1,000, may be entered in one strategy for dealing with a convergence problem. Unlike covariance-based structural equation modeling (SEM), however, convergence problems in PLS-SEM are unusual. A model which stops due to the maximum iterations limit rather than the stop criterion has not yielded reliable results and the model should be respecified. Setting maximum iterations to 0 causes SmartPLS to run the “sum scores” approach (see discussion [above](#) on sum scores).
- *Stop Criterion:* SmartPLS will stop when the change in outer weights (path weights connecting the indicator variables to the latent variables) do not change more than a very small amount. The default amount is 10^{-7} . When dealing with a convergence problem, a slightly larger amount might be selected, such as 10^{-5} . Changing the stopping criterion in such a rare instance would have negligible impact on the resulting coefficients. This default is very rarely overridden by the researcher.

- *Initial Weights*: The outer weights (paths connecting the indicator variables to their latent variables) must be initialized to some value before the iterative PLS estimation process begins. The default, which is almost always taken by researchers, is to set these weights to +1. Alternatives are (1) to click “individual initial weights” and enter user-desired weights manually, or (2) to check “Use Lohmöller Settings”. The Lohmöller setting is an attempt to speed up convergence by setting all weights to +1 but setting the last weight to -1. Online help documentation states, however, “this initialization schema can lead to counterintuitive signs of estimated PLS path coefficients in the measurement models and/or in the structural model” and is thus disparaged.
- *Weighting tab*: Clicking the “Weighting” tab opens a new dialog pane which prompts the researcher for a “Weighting Vector”. A pull-down menu allows the researcher to select one of the variables in the current data as a weighting variable. For instance, the weighting variable might be one generated by weighted least squares (WLS), which attempt to compensate for heterogeneity by weighting each observation by the inverse of its point variance. Any such weights are computed outside of and prior to running SmartPLS. Weights could also be used to compensate for differences in sampling proportions for different subgroups of the sample. In a third use, weights might be the probabilities of group memberships as computed in a PLS-FIMIX run of the model (FIMIX is discussed [below](#)).
- *Open Full Report button*: Usually the researcher will want automatic generation of the full report. Other options are “Close Calculation Dialog” or “Leave Calculation Dialog Open”.

Data input and standardization

SmartPLS needs raw data input, not standardized data. Standardization is implemented automatically and all indicator weights and latent variable scores are always standardized. Correlation matrix input (correlations are standardized coefficients) is not supported by PLS 3 for this reason. This differs from SmartPLS 2, where there was a dialog choice for data standardization.

Single indicator latent variable: If there is only a single indicator for a latent variable, the latent variable score will be the standardized score of the indicator.

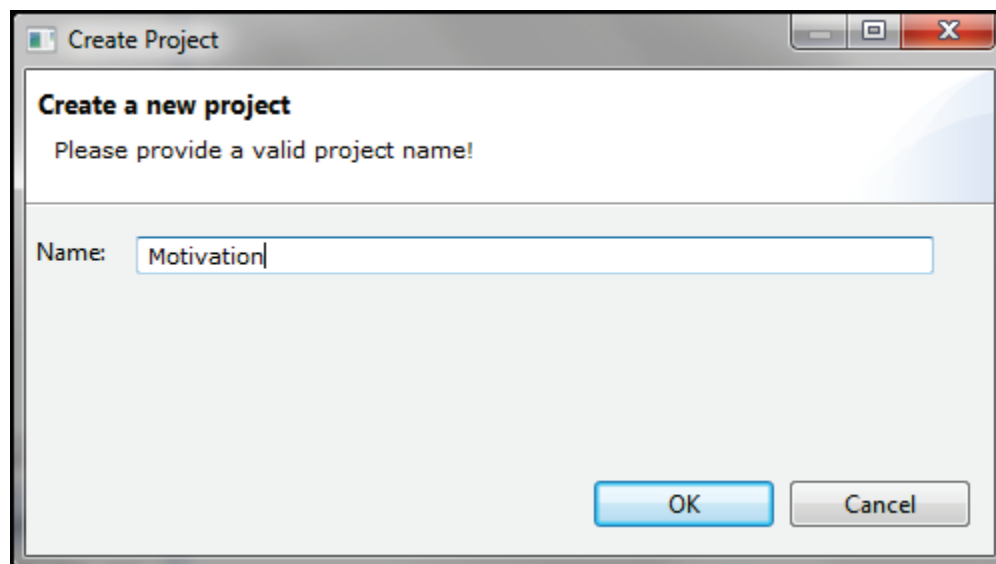
Interaction effects: If an indicator is a product variable (ex., income*education), using mean-centered variables is recommended (Jan-Michael Becker, 2014, post to the SmartPLS Forum). Note, however, this affects the interpretation of results as discussed in the literature on moderated multiple regression. At present SmartPLS supports only two-variable interaction effects.

Setting the default workspace

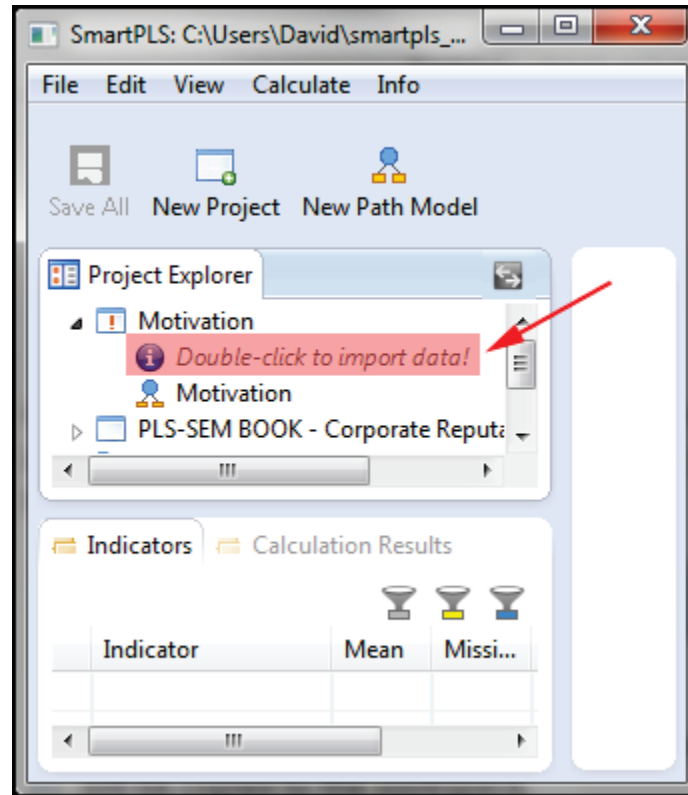
By default, SmartPLS will save projects and data to a workspace located in a directory similar to C:\Users\YourName\smartpls_workspace\. This can be changed by selecting File > Switch Workplace.

Creating a PLS project and importing data

Select File > Create new project (or click the “New Project” icon) to view the window illustrated below. When prompted, assign a project name (in the example, the project name is "Motivation"). Click the "OK" button.



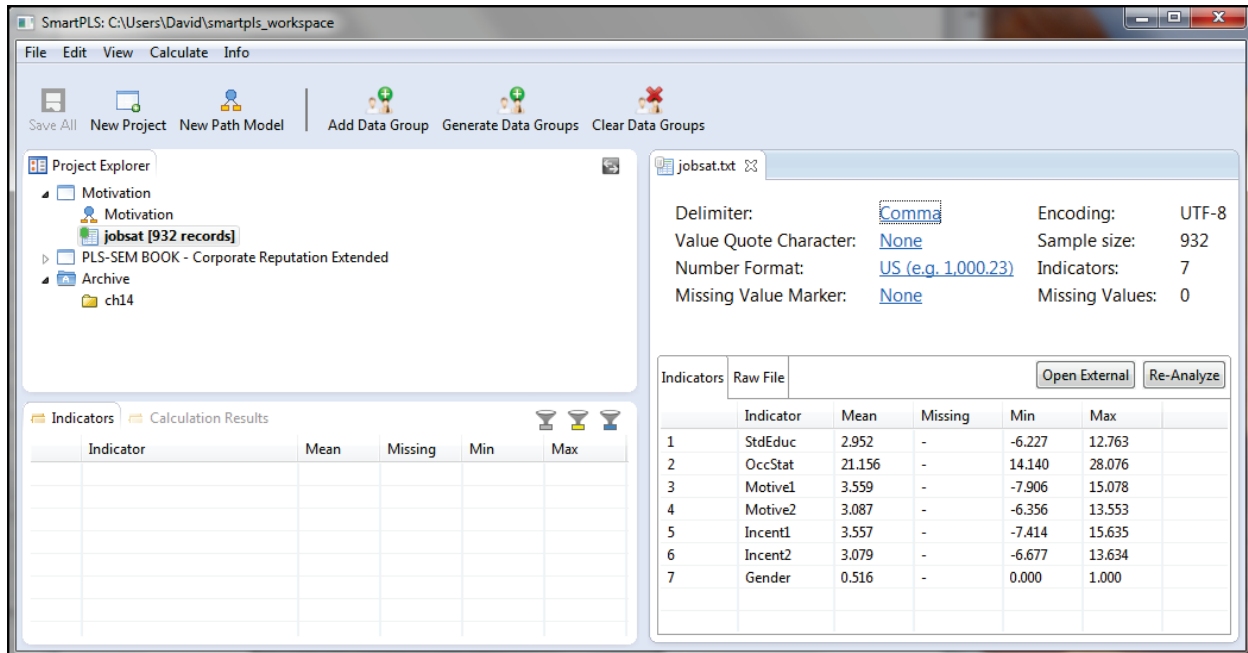
After clicking “OK”, the screen below appears. Double-click where indicated by the red arrow in the figure below.



After double clicking, the usual Windows-type catalog browsing screen will appear (not shown). Browse to the folder where the data file is located, which here is jobsat.csv – a comma-delimited file described [above](#). SmartPLS supports importation only of .csv and .txt text-type data files. Note, however, that SPSS, SAS, and Stata can save .csv files for use by SmartPLS.

On loading this file, the main SmartPLS program screen will appear as shown below. Note that “jobsat” appears as a dataset under the just-created “Motivation” project in the upper left of the screen. The variable list and summary statistics about each variable appear in the lower right (later the variable list will appear in the “Indicators” area in the lower left). Sample size, missing value information, and certain other information appears in the upper right.

If there is a missing-values code, it may be entered by clicking the “None” link shown below after “Missing Value Marker , such as “-99”. The example dataset does not include missing values. Only one missing value code is supported. If there are more, the researcher may need to impute missing values in SPSS or another package prior to running SmartPLS.



At this point, the default workspace will contain the following files:

- Motivation.splsm: This is the SmartPLS project file.
- jobsat.txt: This is the jobsat.csv file re-saved as a .txt file. If the “Raw File” tab in the figure above is clicked (in the lower right), the raw jobsat data are displayed.
- jobsat.txt.aggregated: This is an internal file containing means and other descriptive statistics on the variables. Much of this information is displayed when, as shown above, the “Indicators” tab is selected in the lower right.
- jobsat.txt.meta: This is another internal file containing information on the missing value token, the value separator, and other metadata.

Note the user interface allows switching among multiple projects and datasets, according to the tab pressed in the Project Explorer area at the top left.

Validating the data settings

With the “Indicators” tab selected (see previous figure above), notice it the variable names, ranges, and means appear correctly. Normally they will be correctly displayed automatically as they are for the current example, which uses a comma delimiter, no quotes around values, U.S. rather than European number format, and no missing value markers.

If not displaying correctly, the researcher may need to change the settings for Delimiter, Value Quote Character, Number Format, or Missing Value Marker by clicking the corresponding links in the upper right quadrant of the display. It is also possible to inspect the raw data file by clicking on the “Raw File” tab for insight into the proper setting. When a setting is changed, the display for the “Indicator” tab will change but not for the “Raw File” tab. Change settings until the “Indicator” tab display appears to be correct.

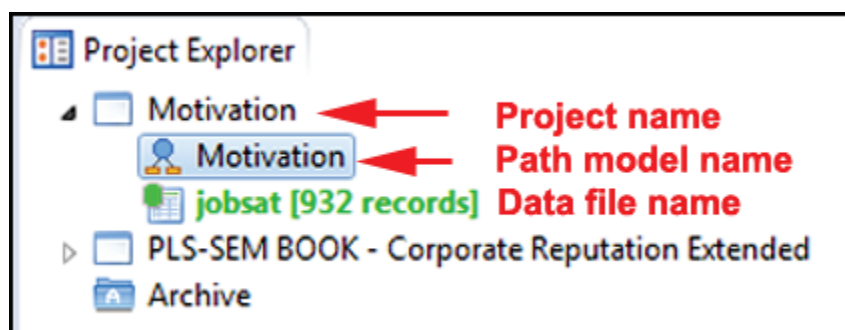
These and additional settings may also be changed under the menu selection File > Preferences.

If there are illegal cell entries, such as blanks, the researcher must quit, make the corrections, then restart.

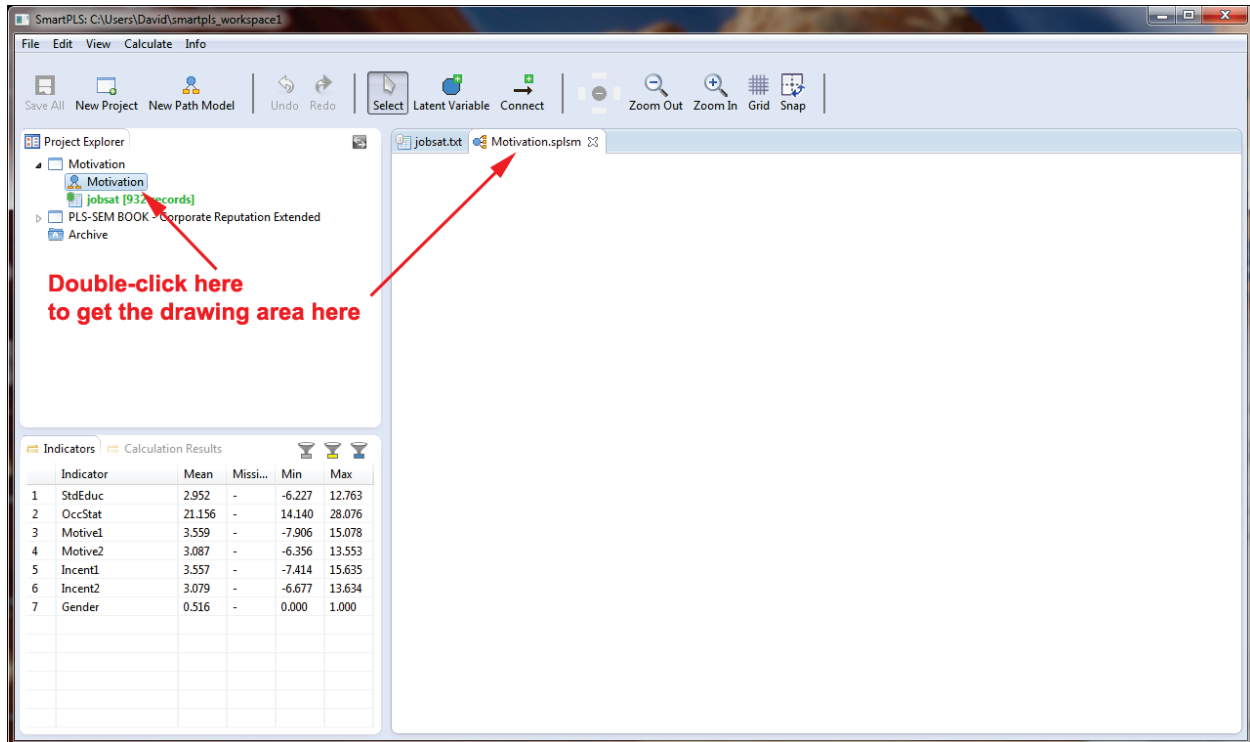
Drawing the path model

Below, a model is created in which Motivation is caused by Incentives and Socioeconomic Status (SES), with each variable being measured by two indicators.

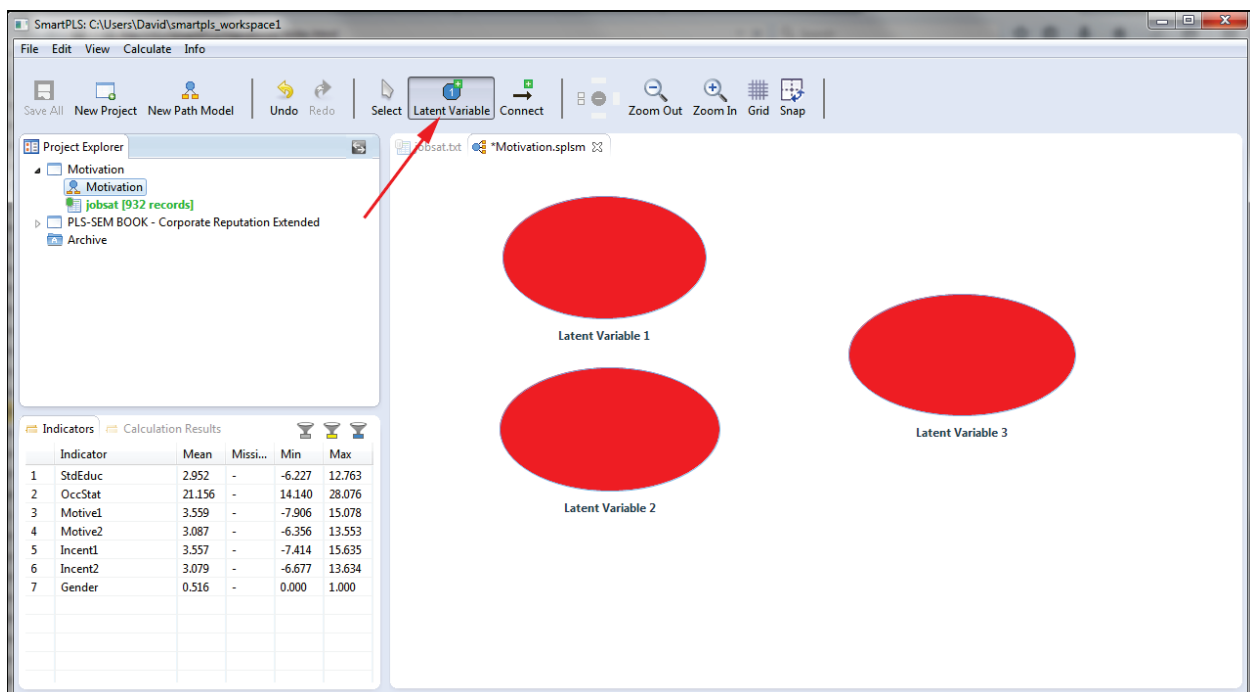
Double-click on the Motivation path diagram (the motivation.splsm file) in the upper left of the screen above, in the Project Explorer area, to display the model viewing area, which initially is blank, as shown below. Note this is the lower “Motivation” label. The upper “Motivation” label is the project name. A project might have multiple path diagrams, though in this example there is only one.



Measured variables in the dataset appear in the Indicators window in the lower left.

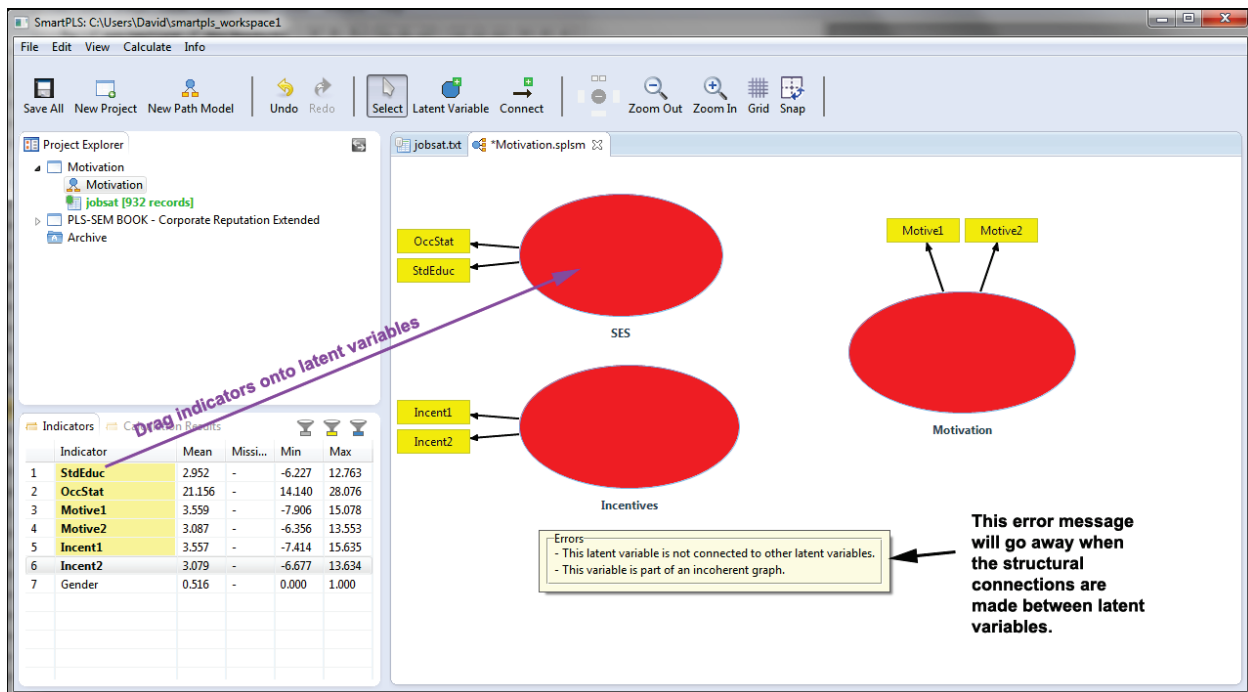


To create the path model, select the Latent Variable tool, shown by the arrow pointer in the figure below, to drag and draw the three ellipses. The researcher may also select Edit > Add latent variable(s) to be able to create multiple latent variables while holding down the Shift key.

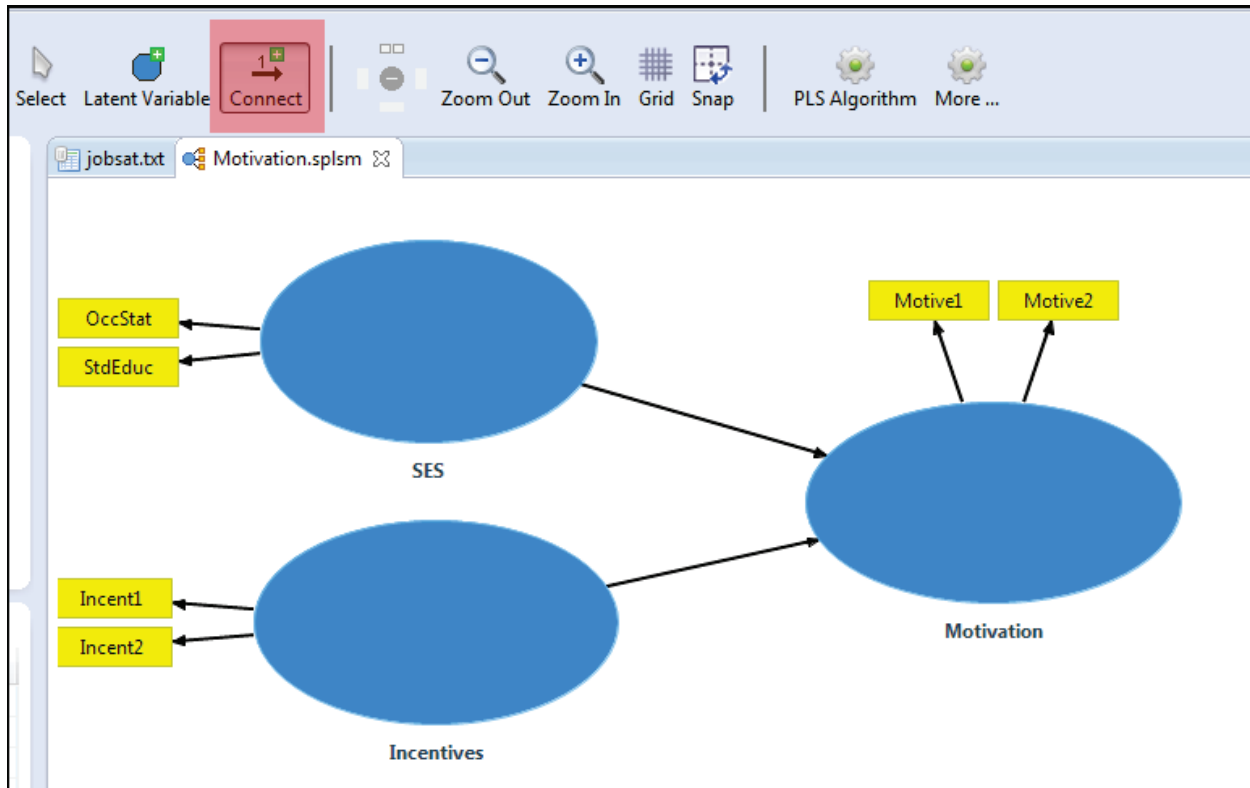


Right-click on the ellipses to reveal a context menu, from which choose “Rename”. Rename the latent variables as Incentives, SES, and Motivation, using the context menu shown below.

Then drag the corresponding indicators from the Indicators pane in the lower left and drop on their respective ellipses. In the display area, indicators will appear as yellow rectangles. By default, reflective arrows (ones from the latent variables to the indicator variables) will connect the latent variables to their indications, which may be dragged using the Select tool to desired positions. For greater placement control, select View > Show Grid and View > Snap Elements to the Grid. At this point, the model appears as shown below.



Then use the Connection tool, highlighted in the figure below, to draw the arrows connecting the ellipses representing latent variables. When connected, the ellipses turn blue.



By default, indicators will appear to the left of the latent variable ellipses. Their location can be rotated by selecting a given latent variable with the Select tool (white arrow), then right-clicking and from the context menu that appears, choose Align > Indicators Top (or whatever position is wanted).

Note also that right-clicking in the Projects pane in the upper left also allows the researcher to copy models or data from one project to another.

Reflective vs. formative models

As discussed [above](#), models may be reflective or formative (or rarely, mixed). The diagram above is reflective because the indicators are shown as effects of the factors. Reflective models are the most common type. To create a formative model, common in PLS-SEM literature but not in covariance-based SEM literature, right-click each factor (ellipse) and from the context menu which appears, select "Change mode of measurement model".

Switching between reflective and formative modes

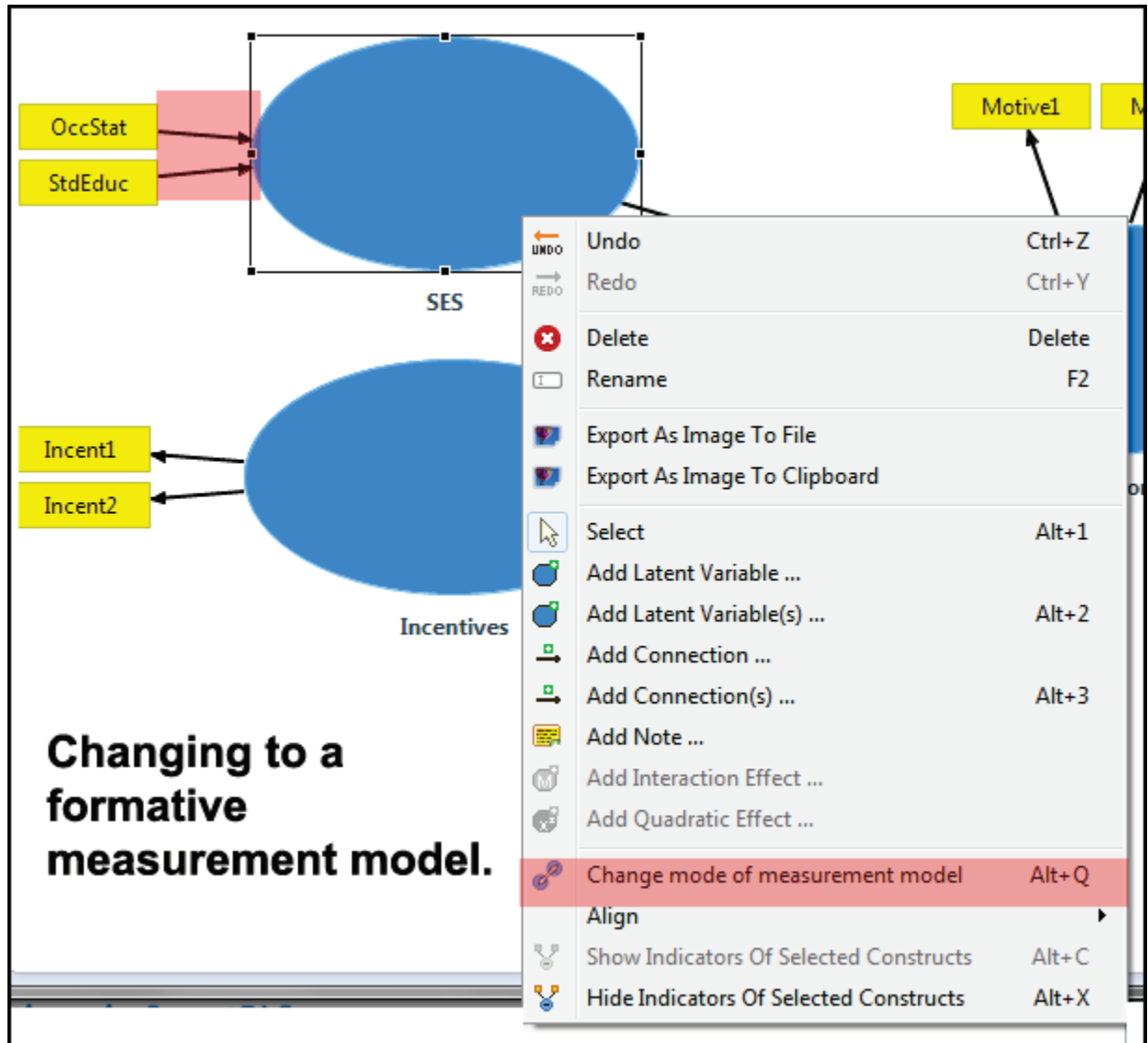
To switch modes from reflective to formative or vice versa, follow these steps:

1. Right-click on the existing reflective model (here, Motivation) in the Project Explorer pane and from the context menu which appears, select “Copy”.
2. Right-click again and select “Paste”, giving a new model name such as MotivationF for the formative model.
3. Optionally, right-click again on Motivation and select “Rename”, renaming the original model as MotivationR for the reflective model.
4. Double-click on the MotivationF model to bring up its graphic display, which is still reflectively modeled.
5. Right-click on any indicator and from the context menu select “Change Mode of Measurement Model”. All constructs will now be formatively modeled.

The same process is used to switch from formative to reflective modeling. It is also possible to have mixed models, with some factors modeled reflectively and some modeled formatively. In a mixed model, selecting “Change Mode of Measurement Model” will switch reflective arrows to formative and vice versa.

Displaying/hiding the measurement model

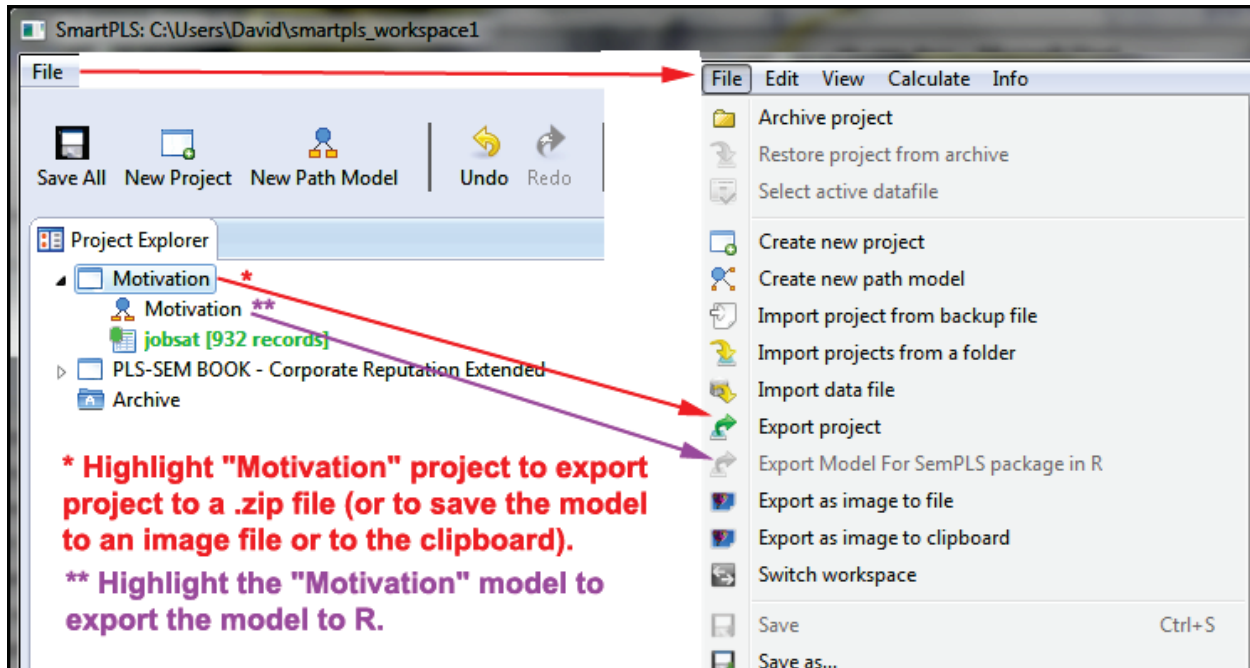
When the model is complex and/or the indicators are many, the right-clicking on any latent variable brings up a context menu with an option to "Hide Indicators of Selected Constructs" (see figure below). Toggling this menu choice between “Show” and "Hide" causes the indicator variables shown as yellow rectangles, and their connecting arrows, to be displayed or hidden in the diagram, though they are still active for estimation purposes. Similarly, right-clicking on an indicator brings up a context menu with the choices “Hide Indicators of All Constructs” or “Show Indicators of All Constructs”.



Saving the model

With the desired project highlighted in the Project Explorer window, select File > Export project, to save the project file as a compressed .zip archive file, which archives in the zip file the graphical model file (Motivation.splsm) and the data file (jobsat.csv). Other choices include exporting the path model to an image file (in .png, .bmp, .jpg, or .svg formats) or to the clipboard.

The researcher may also highlight the desired model in the Project Explorer to export the model for use with R (ex., to save a file which in this example is called Motivation.splsm), as illustrated in the figure below.



Other formatting of the model, including icons for saving the model to .png or .svg graphic file formats, are available in the formatting sidebar shown below.



Model report output

An output report is available after running the PLS algorithm as discussed [above](#). The researcher should have accepted the “Open Full Report” default at the bottom of the opening screen for the PLS algorithm.



Selecting Report > HTML (Print) Report causes output to be displayed, or use one of the other report options illustrated below. In addition, as illustrated above, the Calculate command causes the path coefficients to be entered on the graphical model.

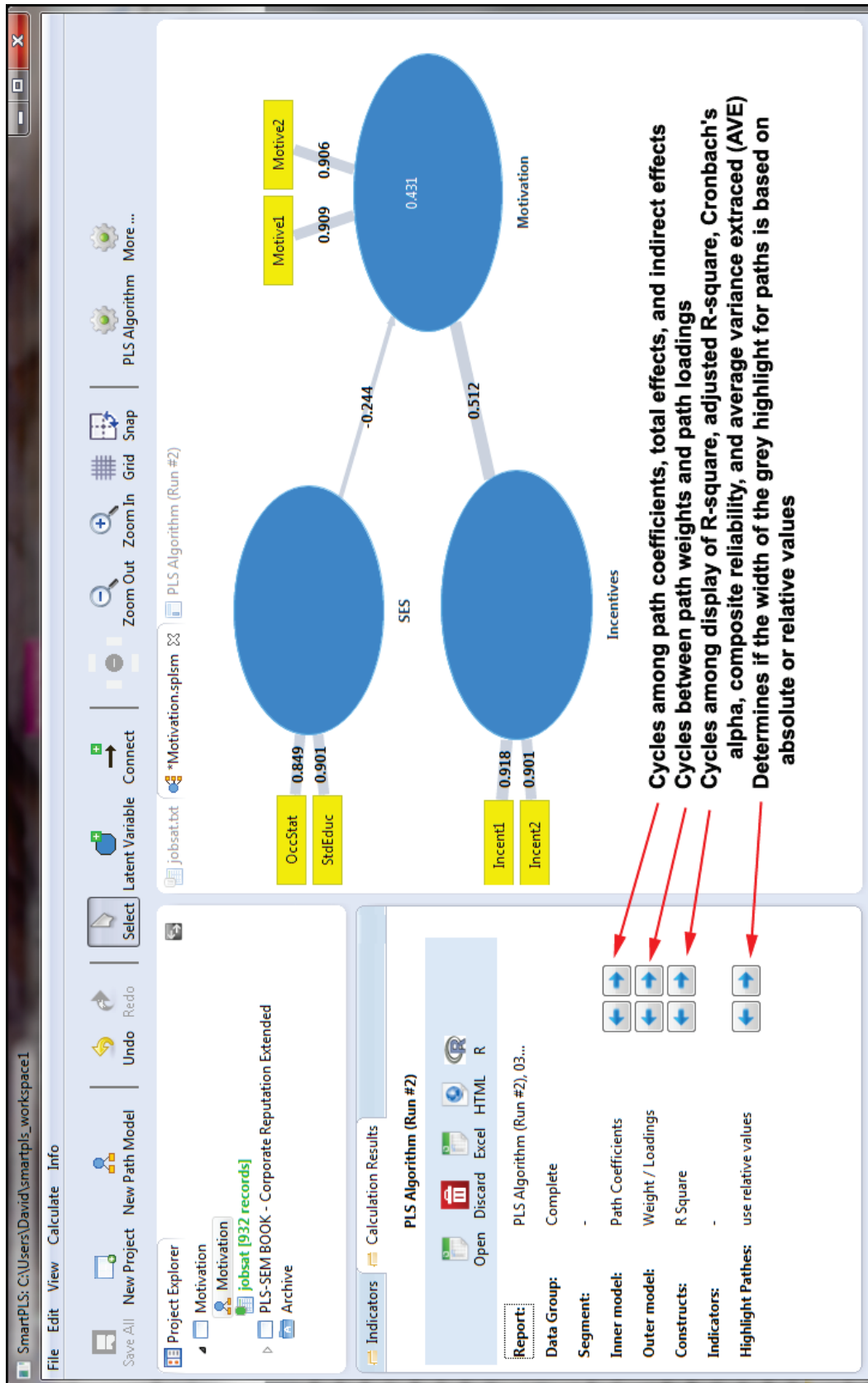
Graphical view of the report

The figure below illustrates the graphical view of the report. For this view, note that the “Motivation” model is highlighted in the Project Explorer window and the “Motivation.splsm” tab is selected in the display area.

What is displayed in the graphical view depends on selections in the lower left of the figure below. The figure display I for path coefficients connecting the latent variables (the inner model), weights assigned to the paths from the latent variables to the indicators (the outer model), and the R-square value displayed for endogenous latent variables. Highlighting in grey is wider for path with large relative values.

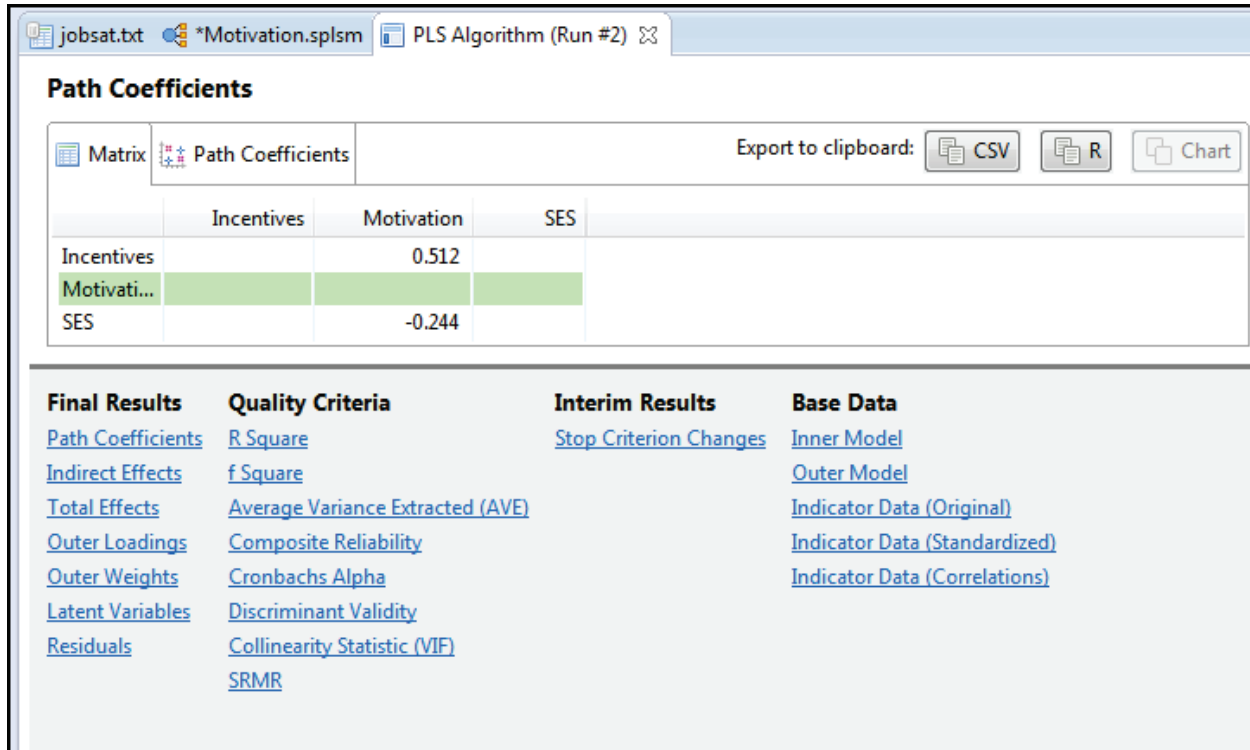
As explained in the figure, the right-left arrow buttons in the lower left will change which coefficients are displayed.

- *Inner model:* Cycle among path coefficients, total effect coefficients, and indirect effect coefficients
- *Outer Model:* Cycle between path coefficients and path loadings
- *Constructs:* Cycle among R-square, adjusted R-square, Cronbach’s alpha, composite reliability, and average variance extracted (AVE)
- *Highlighted paths:* Cycle between absolute and relative values as the basis for the width of the gray highlight for paths.

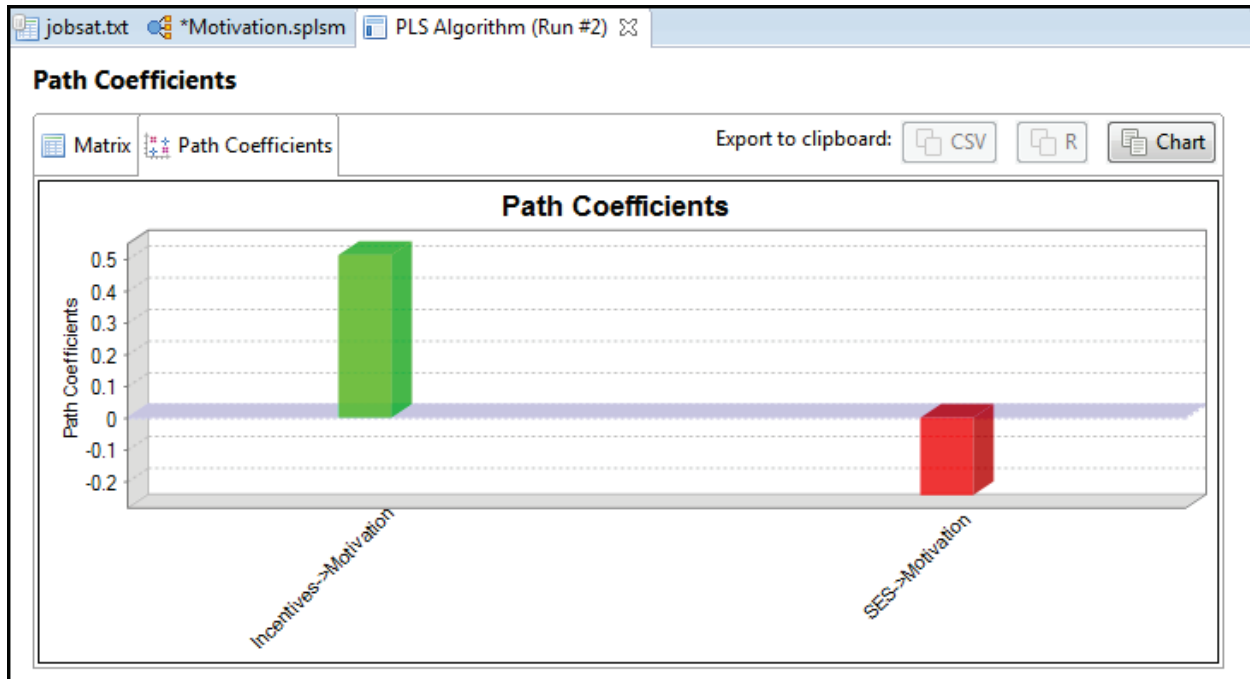


Path coefficients hyperlink view of the report

If the “PLS Algorithm” tab is selected instead of the “Motivation.splsm” tab, a display such as that below appears. In the figure below, the “Matrix” (table format) tab is selected and the default hyperlink to “Path Coefficients” output is also selected. The hyperlinks in the bottom half of the figure provide for display of many different coefficients, settings, and data specifications.



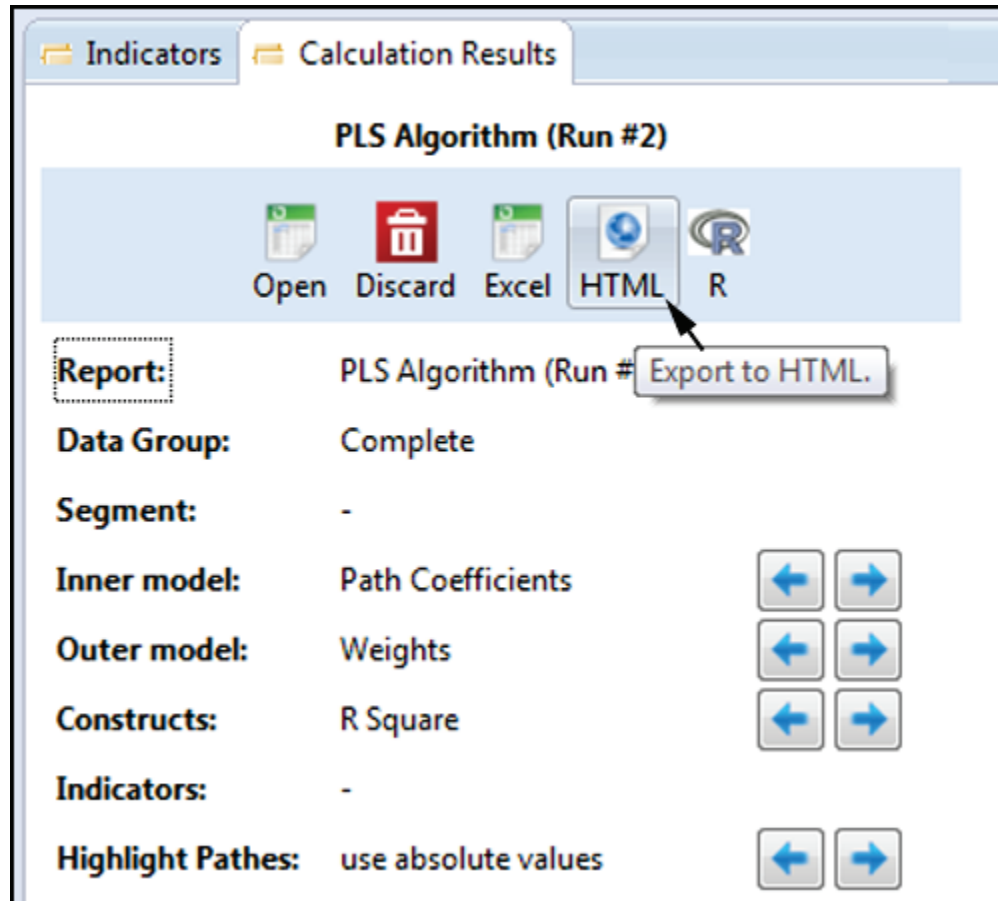
In some cases, graphical output is available. For instance, clicking the “Path Coefficients” tab shown in the figure below displays the path coefficient matrix entries in bar graph form, as shown below.



Printed or web output

Researchers may prefer all output be sent to an html web display from which it can easily be printed in entirety. The “Calculation Results” tab in the lower left of the screen contains options shown below for exporting the results to html (web display), Excel, or R. The “HTML” option will cause a prompt for all results to be saved in a single web page file (ex., file:///C:/Temp/Motivation.html-files/Motivation.html). Using Windows Explorer or some other program, the researcher can browse to the saved file, double-click it, and view the output. Html output may be very long but at the top will be a hyperlink table of contents linking to lower sections, which include both matrix (tabular) and graphical output. Most of the output discussed in output sections below was reproduced in this manner.

Likewise, for this example, the “Excel” option prompts the user to save the file “Motivation.xls”. The R option prompts the user to save the file “Motivation.rData”. The “Open” option flips the display to the “Path coefficients hyperlink view” display discussed above.



Student/demo/free version

In the student version, results still appear in the "Calculation Results" tab in the lower left but in the student version the user cannot export the report to HTML, Excel, or R views. Instead, click "Open" to go to the "Path coefficients hyperlink view" display discussed above. Use the right (Next) and left (Previous) arrows for the output you want. For example:

- *Inner model:* Path coefficients
- *Outer Model:* Loadings
- *Constructs:* R Square

After making these settings, choose the option to export to the clipboard. Go to Word and select Home > Paste to place an image of the selected output as a Word document.

Checking for convergence

While convergence is not often a problem in PLS-SEM, if the solution fails to converge then coefficients in output are unreliable. Therefore it is a good first step to check for convergence after running the PLS algorithm. This is done in a three-step process outlined in the figure below.

1. Go to the “the “Path coefficients hyperlink view” discussed above.
2. Select the hyperlink “Stop Criterion Changes”
3. Note the matrix output in the upper portion of the display. If the number of listed iterations is below the maximum (default = 300), the solution converged. In the figure below, convergence was reached in six iterations.

The screenshot shows the 'Stop Criterion Changes' window in a software application. The window title is 'PLS Algorithm (Run #2)'. It features a 'Matrix' tab and 'Export to clipboard' buttons for 'CSV' and 'R'. The matrix displays the following data:

	Incent1	Incent2	Motive1	Motive2	OccStat	StdEduc
Iteration 0	1.000	1.000	1.000	1.000	1.000	1.000
Iteration 1	0.574	0.525	0.553	0.549	0.514	0.625
Iteration 2	0.574	0.525	0.554	0.548	0.514	0.625
Iteration 3	0.574	0.525	0.554	0.548	0.514	0.625
Iteration 4	0.574	0.525	0.554	0.548	0.514	0.625
Iteration 5	0.574	0.525	0.554	0.548	0.514	0.625
Iteration 6	0.574	0.525	0.554	0.548	0.514	0.625

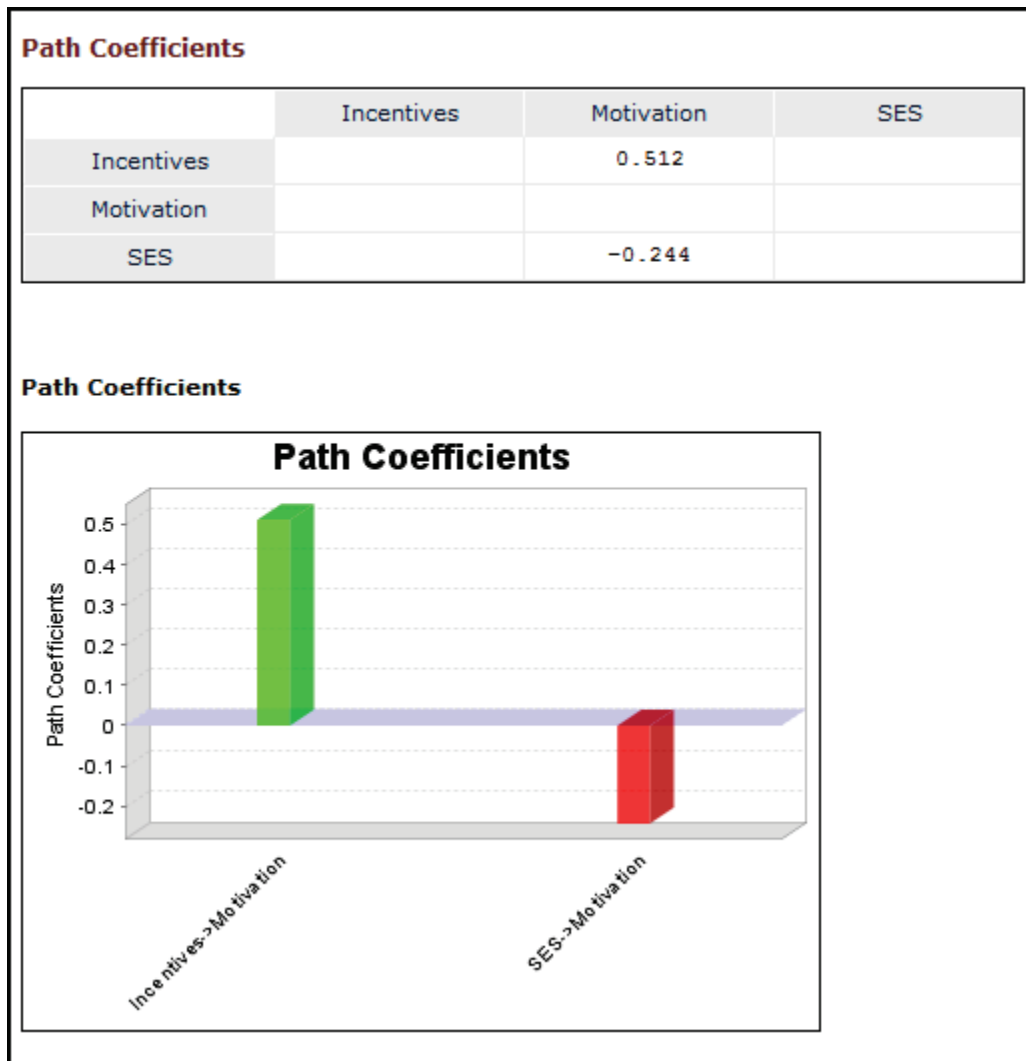
Below the matrix is a navigation menu with four columns: 'Final Results', 'Quality Criteria', 'Interim Results', and 'Base Data'. A red arrow points to the 'Stop Criterion Changes' link in the 'Interim Results' column.

Final Results	Quality Criteria	Interim Results	Base Data
Path Coefficients	R Square	Stop Criterion Changes	Inner Model
Indirect Effects	f Square		Outer Model
Total Effects	Average Variance Extracted (AVE)		Indicator Data (Original)
Outer Loadings	Composite Reliability		Indicator Data (Standardized)
Outer Weights	Cronbachs Alpha		Indicator Data (Correlations)
Latent Variables	Discriminant Validity		
Residuals	Collinearity Statistic (VIF)		
	SRMR		

OUTPUT

Path coefficients for the inner model

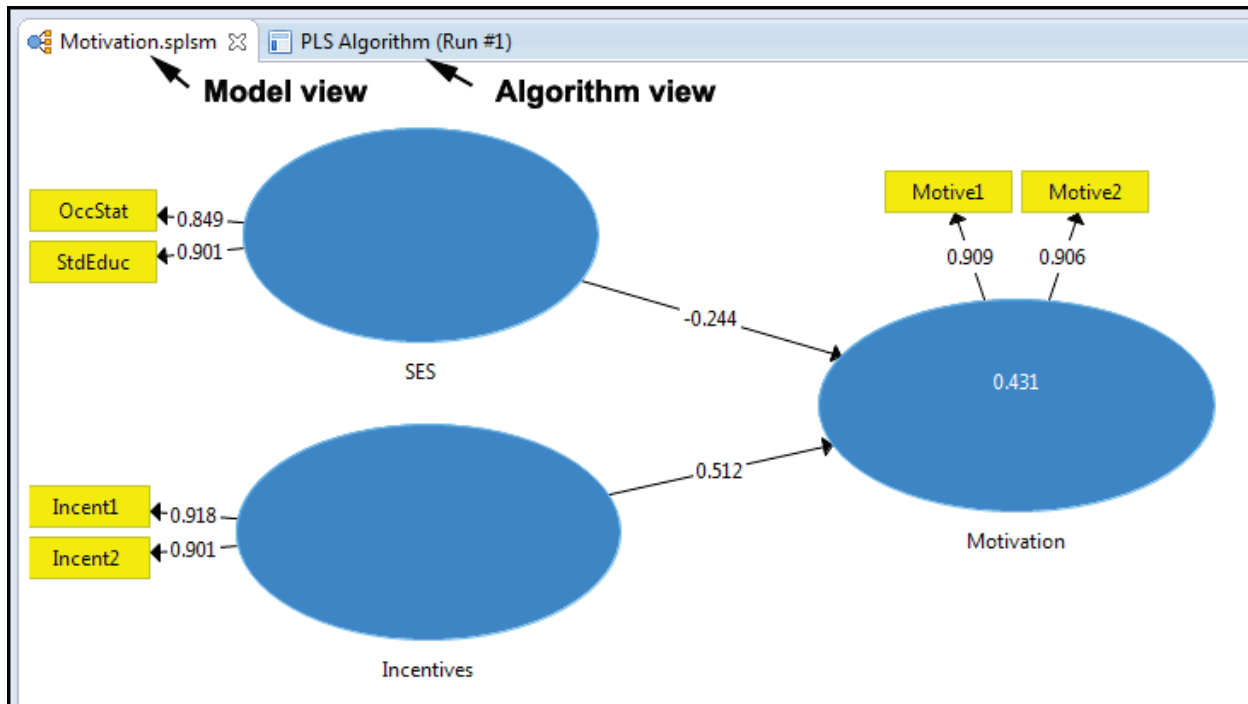
At the top of the HTML output are the path coefficients for the inner model (the arrows connecting latent variables). For the present simple example, the path from Incentives to Motivation has a coefficient of positive .512. The path from SES to Motivation has a coefficient of negative .244.



Path coefficients are always standardized path coefficients. Given standardization, path weights therefore vary from -1 to +1. Weights closest to absolute 1 reflect the strongest paths. Weights closest to 0 reflect the weakest paths. Above, the path weight of 0.512 shows Incentives have a positive effect on Motivation. SES,

at -0.244, has a negative effect. Since standardized data are involved, it can also be said based on these path coefficients that the absolute magnitude of the Incentives effect on Motivation is approximately twice that of SES.

If the researcher switches to model view, it will be seen that these standardized path coefficients are the ones placed on the corresponding paths in the graphical model, shown below.



If requested (see [above](#)), the R-square values are shown inside the blue ellipses for endogenous latent variables (factors). This is the most common effect size measure in path models, carrying an interpretation similar to that in multiple regression. In this example, only Motivation is an endogenous variable (one with incoming arrows). For the endogenous variable Motivation, the R-square value is 0.431, meaning that about 43% of the variance in Motivation is explained by the model (that is, jointly by SES and Incentives). See further discussion of R-square, see [below](#).

Direct, indirect, and total path coefficients

Following the inner model path coefficients, HTML output lists the coefficients for direct effects (the same as the corresponding standardized path coefficients just

discussed above), indirect effects (effects of one latent variable on an endogenous latent variable mediated through one or more additional latent variables), and total effects (the sum of direct and indirect effects). In the present simple model, there are no indirect effects and thus output is not displayed here. However, similar output for a model to which an arrow from SES to Incentives was added, thereby introducing the indirect path SES-> Incentives -> Motivation, is discussed and illustrated [above](#).

Outer model measurement loadings and weights

The "outer model" is the measurement model consisting of the indicators and the paths connecting them to their respective factors. Both weights and loadings are output for both reflective and formative models

- Outer model loadings are the focus in reflective models, representing the paths from a factor to its representative indicator variables. Outer loadings represent the absolute contribution of the indicator to the definition of its latent variable.
- Outer model weights are the focus in formative models, representing the paths from the constituent indicator variables to the composite factor. Outer weights represent the relative contribution of the indicator to the definition of its corresponding latent variable (component or composite).

Loadings

Measurement loadings are the standardized path weights connecting the factors to the indicator variables. As data are standardized automatically in SmartPLS, the loadings vary from 0 to 1. The loadings should be significant. In general, the larger the loadings, the stronger and more reliable the measurement model. Indicator reliability may be interpreted as the square of the measurement loading: thus, $.708^2 = .50$ reliability (Hair et al., 2014: 103).

Outer model loadings appear in the graphical model ([above](#)). They may be considered a form of item reliability coefficients for reflective models: the closer the loadings are to 1.0, the more reliable that latent variable. By convention, for a well-fitting reflective model, path loadings should be above .70 (Henseler, Ringle, & Sarstedt, 2012: 269). Note that a loading of .70 is the level at which about half

the variance in the indicator is explained by its factor and is also the level at which explained variance must be greater than error variance. On the value 0.70 as a criterion for minimum measurement loadings, see Ringle, 2006: 11).

Another rule of thumb is that an indicator with a measurement loading in the .40 to .70 range should be dropped if dropping it improves composite reliability (Hair et al., 2014: 103).

Outer Loadings				Outer Weights			
	Incentives	Motivation	SES		Incentives	Motivation	SES
Incent1	0.918			Incent1	0.574		
Incent2	0.901			Incent2	0.525		
Motive1		0.909		Motive1		0.554	
Motive2		0.906		Motive2		0.548	
QccStat			0.849	QccStat			0.514
?StdEduc			0.901	?StdEduc			0.625

Weights

Outer model “weights,” in contrast to loadings, do not vary from 0 to plus or minus 1. Weights vary from 0 to an absolute maximum lower than 1. The more the indicators for a latent variable, the lower the maximum and the lower the average outer model weight.

It is possible for an indicator’s outer loading to be high and significant while its outer weight is not significant. If an indicator has a nonsignificant outer weight and its outer loading is not high (Hair et al., 2014: 129 suggest that “not high” means not > .50) and it is not the only indicator for a theoretically important

dimension in a formative model, then the indicator is a candidate for being dropped from the model even if its loading is significant. As a corollary, even a path with a non-significant weight should be retained in the model if it is the only indicator for a theoretically significant dimension or has a high loading.

Bootstrapped significance output

The reader may have noticed that path coefficient output discussed thus far are not presented with the usual p-value significance levels. As path coefficients in PLS do not assume a normal, chi-square, or other known distribution, the usual asymptotic significance levels cannot be computed. Rather, bootstrapped significance coefficients must be employed. In SmartPLS this requires running the model after requesting “Bootstrapping” rather than “PLS Algorithm” from the “Compute” button menu. Bootstrapped significance is discussed in the subsequent section [below](#).

Assessing model fit: Overview

There is no global goodness of fit measure available in PLS-SEM, unlike covariance-based SEM. Such global measures are based on how closely the model-implied covariance matrix approximates the observed covariance matrix. As such the focus is on reproducing the relationships among the variables. In contrast, goodness of fit measures in PLS-SEM, similar to OLS regression, emphasize how close the predicted values of the dependent variables are to the observed values. As such, the focus of PLS-SEM is on prediction. This is a central reason why it is often said that covariance-based SEM is appropriate for testing hypotheses and causal models, while PLS-SEM may be preferred when the research purpose is prediction. However, as discussed [above](#), covariance-based SEM may return better predictions than PLS for large samples when its assumptions are met.

While no global fit coefficient is available in PLS-SEM, immediately after the listing of the input data, the SmartPLS report displays various coefficients related to model fit ("model quality"), as shown below.

Not all measures are appropriate for assessing all types of fit. There are three types of fit with which the researcher may be concerned.:

- *Measurement fit for reflective models:* This deals with fit of the measurement (outer) model when factors are modeled reflectively, which is the usual approach.
- *Measurement fit for formative models:* This deals with fit of the measurement (outer) model when factors are modeled formatively.
- *Structural fit:* This deals with fit of the structural (inner) model.

Measurement fit for reflective models

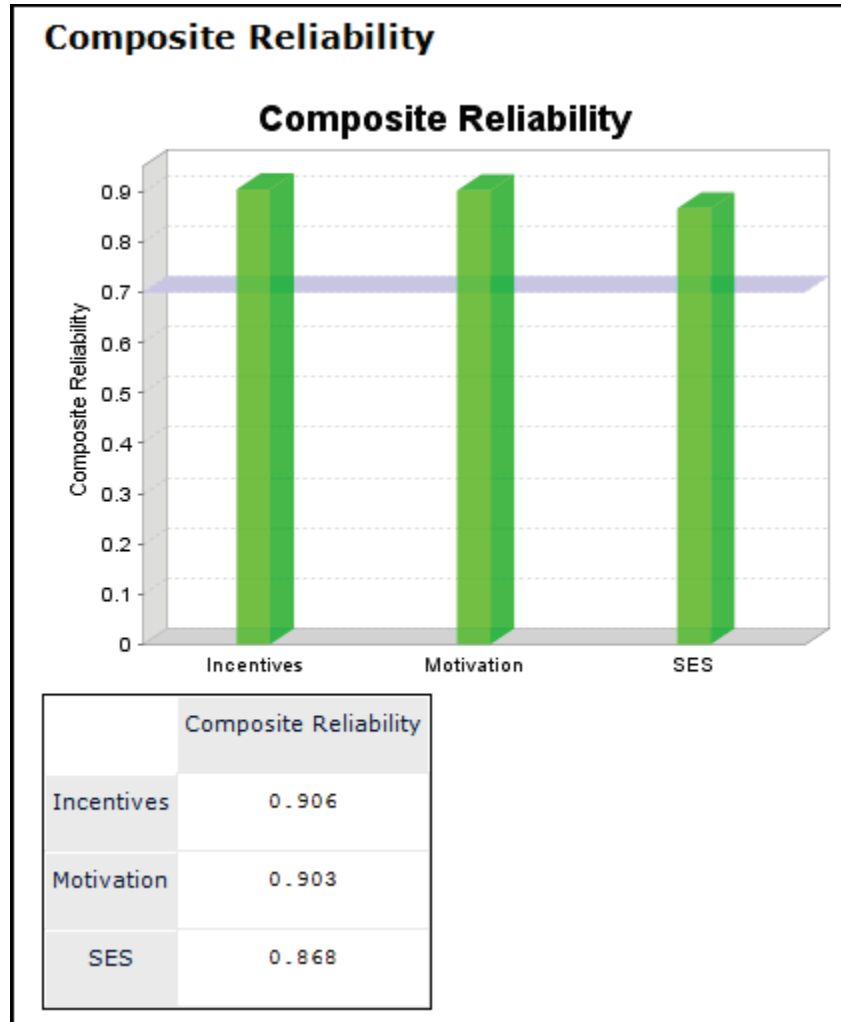
In a reflective model, arrows go from the factor to the indicator variables, signifying that a unidimensional underlying construct determines the values of the measured and representative indicator variables. Testing for convergent validity through such measures as composite reliability or Cronbach's alpha is appropriate in reflective models but not in formative models. Goodness of fit measures appropriate for reflective measurement models, are those below.

Composite reliability

Composite reliability is a preferred alternative to Cronbach's alpha (see below) as a test of convergent validity in a reflective model. It may be preferred as a measure of reliability because Cronbach's alpha may over- or underestimate scale reliability, usually the latter. For this reason, composite reliability is preferred among researchers in PLS-based research. Compared to Cronbach's alpha, composite reliability may lead to higher estimates of true reliability. The acceptable cutoff for composite reliability is the same as for any measure of reliability, including Cronbach's alpha. Composite reliability varies from 0 to 1, with 1 being perfect estimated reliability. In a model adequate for exploratory purposes, composite reliabilities should be equal to or greater than .6 (Chin, 1998; Höck & Ringle, 2006: 15); equal to or greater than .70 for an adequate model for confirmatory purposes (Henseler, Ringle, & Sarstedt, 2012: 269); and equal to or greater than .80 is considered good for confirmatory research (for ex., Daskalakis & Mantas, 2008: 288).

Very high composite reliability ($> .90$) may indicate that the multiple indicators are minor wording variants of each other rather than being truly representative measures of the construct the factor represents. The researcher should consider if

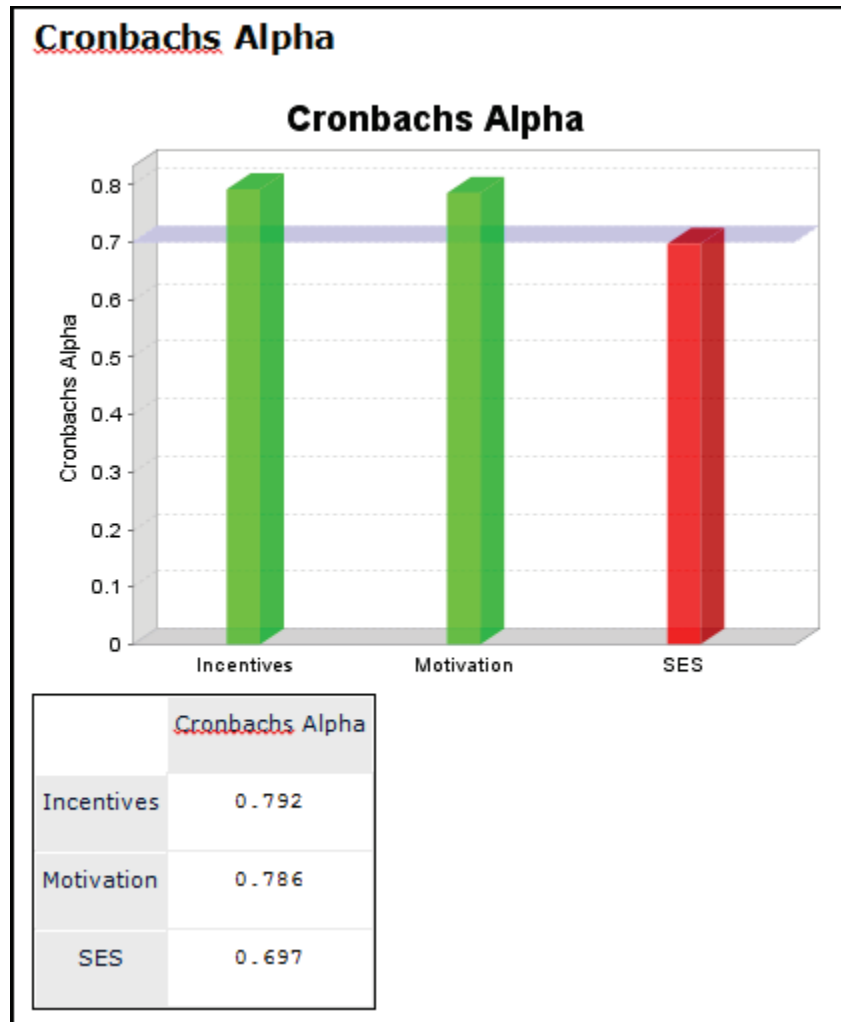
very high composite reliability reflects this design problem, or if the indicators are representative of the desired dimension and simply correlate highly. For further discussion and the formula, see Hair et al. (2014: 101).



Cronbach's alpha

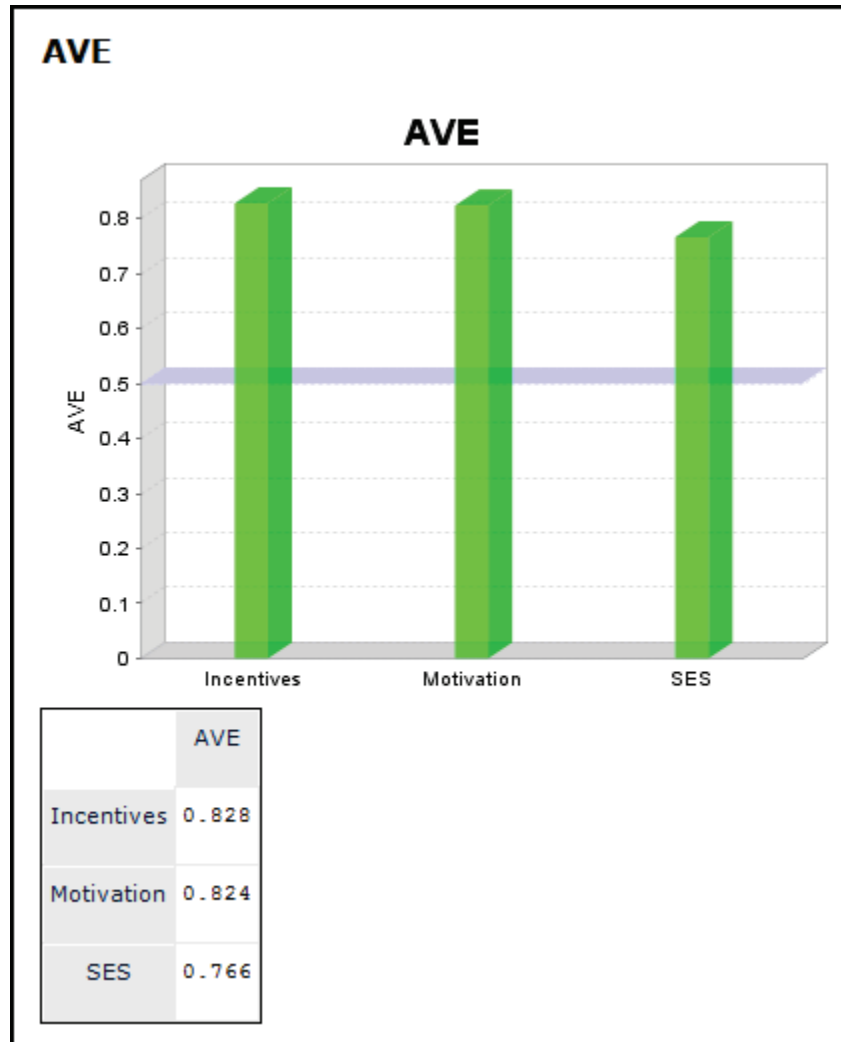
Cronbach's alpha also addresses the question of whether the indicators for latent variables display convergent validity and hence display reliability. By convention, the same cutoffs apply: greater or equal to .80 for a good scale, .70 for an acceptable scale, and .60 for a scale for exploratory purposes. Note, however, Cronbach's alpha is a conservative measure which tends to underestimate reliability. For these data, the Incentives and Motivation latent factors are measured at an acceptable level for confirmatory research. The SES latent factor

falls short of this cut-off. As Cronbach's alpha is biased against short scales of two or three items as in the current example, this small discrepancy falling short of the cutoff for an adequate confirmatory scale would usually be ignored. .



Average variance extracted (AVE)

AVE may be used as a test of both convergent and divergent validity. *AVE* reflects the average communality for each latent factor in a reflective model. In an adequate model, *AVE* should be greater than .5 (Chin, 1998; Höck & Ringle, 2006: 15) as well as greater than the [cross-loadings](#), which means factors should explain at least half the variance of their respective indicators. *AVE* below .50 means error variance exceeds explained variance. For the seminal paper on *AVE*, see Fornell & Larcker (1981).



Communality

SmartPLS 2 reported “communalities”. These coefficients were identical to the AVE coefficients and therefore are no longer reported in SmartPLS 3. In SmartPLS 2 output where the rows are the factors and communality is a column, the communality coefficient measures the average percent of variance in the indicators for a row factor (e.g., Incent1 and Incent2) explained by that row factor (e.g., Incentives) and is a fourth test of convergent validity. Communality may be interpreted as a measure of the reliability of row factor. Like any measure of reliability, the same cutoff criteria as described above apply.

The Fornell–Larcker discriminant validity criterion

AVE may also be used to establish discriminant validity by the Fornell–Larcker criterion: for any latent variable, the square root of AVE should be higher than its correlation with any other latent variable. This means that for any latent variable, the variance shared with its block of indicators is greater than the variance it shares with any other latent variable. In SmartPLS output, in the Fornell-Larcker criterion table, the square root of AVE appears in the diagonal cells and correlations appear below it. Therefore, in absolute value terms, if the top number (which is the square root of AVE) in any factor column is higher than the numbers (correlations) below it, there is discriminant validity. Cross-loadings, discussed [below](#), also are useful in establishing discriminant validity.

Discriminant Validity

Fornell-Larcker Criterium

	Incentives	Motivation	SES
Incentives	0.910		
Motivation	0.619	0.908	
SES	-0.437	-0.467	0.875

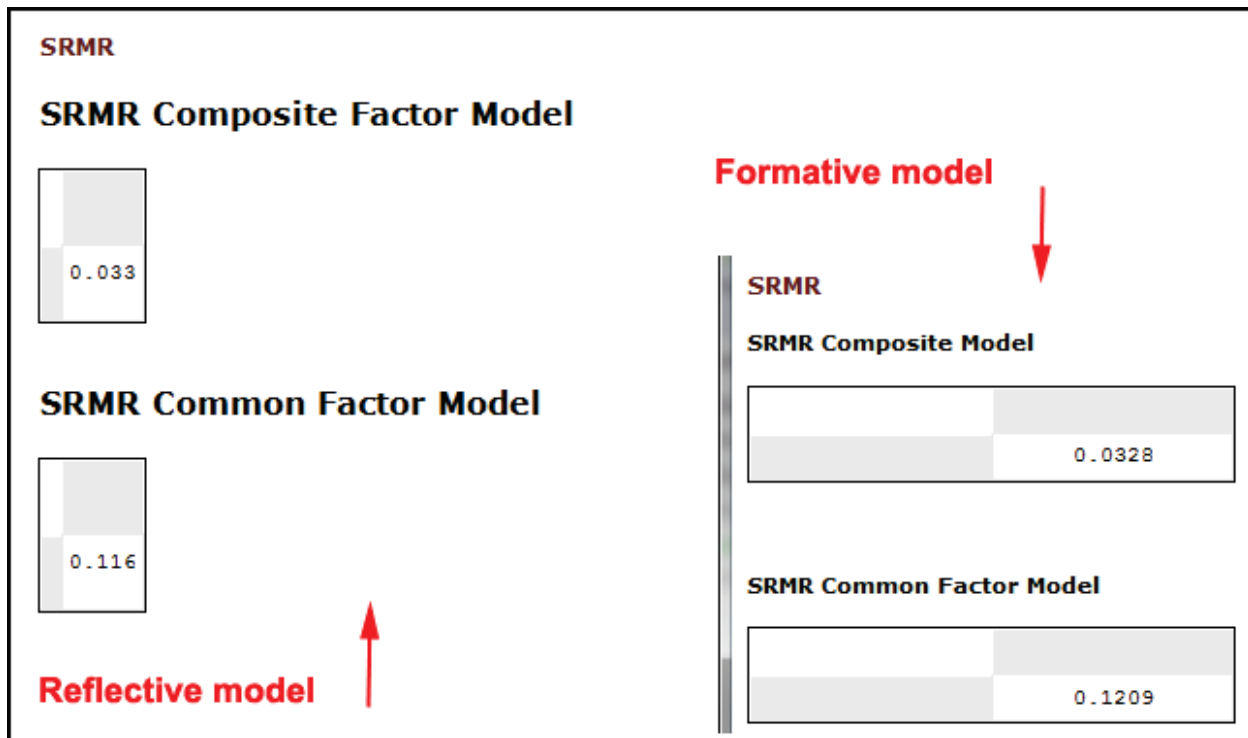
Indicator reliability

Outer (measurement) model path loadings and weights provide another set of criteria for evaluating the reliability of indicators in the model, whether reflective or formative. See previous discussion [above](#).

The standardized root mean square residual (SRMR)

SRMR is a measure of approximate fit of the researcher's model. It measures the difference between the observed correlation matrix and the model-implied correlation matrix. Put another way, the SRMR reflects the average magnitude of such differences, with lower SRMR being better fit. By convention, a model has good fit when SRMR is less than .08 (Hu & Bentler, 1998). Some use the more lenient cutoff of less than .10. For discussion in the context of partial least squares modeling, see Henseler, Dijkstra, et al. (2014).

SRMR output illustrated below provides two versions: SRMR for composite factor models and SRMR for common factor models. SmartPLS documentation states, "Usually, when using PLS, the composite model SRMR is relevant. When all your measurement models are reflective and PLSc has been used, then, the common factor model SRMR is the relevant model fit assessment criterion" (<http://www.smartpls.de/documentation/srmr>).



Cross-loadings

In a good model, indicators load well on their intended factors and cross-loadings with other factors they are not meant to measure should be markedly. Ideally,

there is simple factor structure, by rule of thumb taken to mean that intended loadings should be greater than .7 (some use .6) and cross-loadings should be under .3 (some use .4). The table below does not achieve simple factor structure due to cross-loadings at the .4 and .5 levels. Lack of simple factor structure diminishes the meaningfulness of factor labels (ex., the Incentives factor here still has substantial cross-loadings with the indicators for Motivation).

	Incentives	Motivation	SES
Incent1	0.918	0.587	-0.398
Incent2	0.901	0.537	-0.398
Motive1	0.568	0.909	-0.419
Motive2	0.555	0.906	-0.429
OccStat	-0.370	-0.367	0.849
?StdEduc	-0.394	-0.446	0.901

Cross-loadings are an alternative to AVE as a method of assessing discriminant validity for reflective models. At a minimum, no indicator variable should have a higher correlation with another latent variable than with its own latent variable. If it does, the model is inappropriately specified.

Heterotrait-Monotrait Ratio (HTMT)

As noted in SmartPLS documentation, although examination of cross-loadings and use of the Fornell-Larcker criterion are accepted methods for assessing the discriminant validity of a PLS model, these methods have shortcomings. Henseler, Ringle & Sarstedt (2015) used simulation studies to demonstrate that lack of discriminant validity is better detected by the heterotrait-monotrait (HTMT) ratio they developed. Guidelines for the use of HTMT coefficients are found in the above-cited article.

The HTMT ratio is the geometric mean of the heterotrait-heteromethod correlations (i.e., the correlations of indicators across constructs measuring different phenomena) divided by the average of the monotrait-heteromethod correlations (i.e., the correlations of indicators within the same construct). Averaging using the geometric mean is necessary because there are two monotrait-heteromethod submatrices (sets of within-construct correlations), for example, when there are two constructs. See Henseler, Ringle, & Sarstedt (2015: 121).

In a well-fitting model, heterotrait correlations should be smaller than monotrait correlations, meaning that the HTMT ratio should be below 1.0, as they are in the example output below. Henseler, Ringle, & Sarstedt (2015: 121) suggest that if the HTMT value is below 0.90, discriminant validity has been established between a given pair of reflective constructs. Gold et al. (2001) and Teo et al. (2008) also use the .90 cutoff, though Clark & Watson (1995) and Kline (2011) use the more stringent cutoff of .85.

	Incentives	Motivation	SES
Incentives			
Motivation	0.783		
SES	-0.587	-0.626	

Factor scores

The factor scores table lists each observation's scores on each factor. For the standardized factor scores table, observations with scores higher than 1.96 may be considered outliers. The greater the proportion of outlier cases, the worse the measurement fit.

Factor scores in standardized form are displayed by default in the "Latent Variable Scores" table, shown in partial format below. The correlation of these observation scores produces the "Latent Variable Correlations" table discussed further below.

The factor scores can also be analyzed to identify outlier cases (those with a greater absolute value than 1.96 are outliers at the .05 level, those greater than 2.58 are outliers at the .01 level, etc.).

Latent Variable Scores

	Incentives	Motivation	SES
	0.243	0.237	1.276
	-0.055	-0.652	1.145
	0.902	1.694	-0.782
	1.524	1.403	-1.230
	2.589	2.671	-1.681
	0.742	0.191	-0.503

Partial table of the first six observations

Multicollinearity in reflective models

In OLS regression, multicollinearity exists when two or more independent variables are highly intercorrelated. Multicollinearity in OLS regression inflates standard errors, makes significance tests of independent variables unreliable, and prevents the researcher from assessing the relative importance of one independent variable compared to another. A common rule of thumb is that problematic multicollinearity may exist when the variance inflation factor (VIF) coefficient is higher than 4.0 (some use the more lenient cutoff of 5.0). VIF is the inverse of the tolerance coefficient, for which multicollinearity is flagged when tolerance is less than .25 (some use the more lenient cutoff of .20).

Formative models are a type of regression model, in which multiple indicators predict the value of the dependent variable, which is the latent variable value. The multicollinearity issue for formative models is discussed [below](#).

For reflective models, the latent variable is modeled as a single predictor of the values of each of the indicator variables, which are dependent variables. Therefore in a reflective measurement model, multicollinearity is not an issue, even though SmartPLS will output the VIF statistic for the outer (measurement) model, whether the model is reflective or formative.

In either a reflective or a formative model, there is potentially multicollinearity at the structural level. That is, the latent variables which are modeled as causes of an endogenous latent variable may be multicollinear. Structural multicollinearity is a problem in either reflective or formative models for the same reason it is in OLS regression models. VIF coefficients for the structural model are printed by SmartPLS in the “Inner VIF Values” table shown further [below](#). In a well-fitting model, the structural VIF coefficients should not be higher than 4.0 (some use the more lenient criterion of 5.0).

Criterion validity

Criterion validity is not part of SmartPLS output but may supplement it. If there is a measure of a construct used in the PLS model which is also used and widely accepted in the discipline, then the factor scores of that factor should correlate highly with the criterion construct used in the discipline. In the data collection phase, this requires that the researcher have administered the survey items for the criterion construct as well as for his/her own indicators of the constructs in the model.

Goodness of fit (GoF)

GoF is a measure combining effect size with convergent validity, suggested by Tenenhaus et al. (2005). However, use of GoF is now disparaged due to various statistical shortcomings (e.g., Hair et al., 2014: 185). Shortcomings include not being suitable for model validation (Henseler & Sarstedt, 2012: 565) and not handling misspecified models well (Hair et al., 2014: 78). GoF is not output by SmartPLS but must be computed manually. GoF is the geometric mean of average communality for the outer model and average R-square for the inner model. That is, goodness-of-fit equals the square root of communality times R-square. GoF will vary from 0 to 1. Henseler & Sarstedt (2012: 565) note that GoF may still be useful in assessing which datasets PLS-SEM explains better than others, with higher reflecting better explanation.

Redundancy

The redundancy coefficient reported in SmartPLS 2 is no longer reported in SmartPLS 3 for the standard PLS algorithm. Redundancy reflects how well the response factor (and endogenous factors generally) is capable of predicting the variance in its indicator variables. The redundancy coefficient measures the percent of variance in the indicators for the dependent factor (Motivation) explained by the exogenous factors (SES and Incentives). This may modify the evaluation of R^2 as a model fit measure. .

In SmartPLS 3, the blindfolding algorithm discussed [below](#) outputs cross-validated redundancy coefficients and cross-validated communality coefficients for constructs as well as indicators.

Measurement fit for formative models

In a formative measurement model (that portion dealing with the latent variables and their indicators), arrows in the model diagram go from the indicator variables to the factors. This signifies that a formatively modeled factor is a composite variable reflecting the indicators, which represent different dimensions of the factor. Because the indicators represent different dimensions, the researcher would not expect that the indicators would correlate highly, implying that composite reliability and Cronbach's alpha might not be high. Likewise, the researcher would not expect that the composite factor would necessarily predict the values of the indicator variables well, implying that communality and redundancy might not be particularly high because any type of average of different dimensions will not predict any one dimension well. Rather, measurement fit for formative models is assessed by other means discussed below.

Face validity

The face meaning of the indicator variables should present a relevant and convincing set of all the dimensions of the construct for which the factor is labeled.

Path loading significance

Measurement path loadings should be significant in a formative model with acceptable fit. In principle every formative indicator should have been intended to represent one of the dimensions of the meaning of a factor in a comprehensive set of indicators for that factor and as such should not be dropped. That is, for formative models, measurement model path coefficients, which are the path loadings discussed [above](#), should be significant (Henseler, Ringle, & Sarstedt, 2012: 270).

However, in empirical practice, if the indicator's path loading is not high (<.5) and is non-significant, the data do not support the contention that the indicator is relevant to the measurement of its factor and it may be dropped from the model (Cenfetelli & Bassellier, 2009). Some suggest any indicator with a low path loading, significant or not, might be considered for removal unless it seems relevant from a content validity viewpoint, meaning it is the only indicator of a theoretically important dimension of the construct represented by the factor (Hair et al., 2014: 130-131).

Measurement weights

Measurement weights, also illustrated and discussed [above](#), are the path weights connecting the factors to the indicator variables. These should also be significant. The larger, the stronger the model.

Cross-loadings

Cross-loadings of the indicators on the latent variables, discussed [above](#), apply in the same manner for formative as well as for reflective models. In a good formative model, indicators load on their intended composite factors and cross-loadings with the composite scores of other factors they are not meant to measure should not be high (Klein & Rai, 2009). Ideally, there is simple factor structure, also discussed above. However, Henseler, Ringle, & Sarstedt (2015:131) note, based on simulation studies, "considering the poor performance of cross-loadings in our study, its use in formative measurement models appears questionable. Against this background, future research should seek alternative means to consider formatively measured constructs when assessing discriminant validity."

Factor scores

The factor scores table, shown [above](#), lists each observation's scores on each factor. For the standardized factor scores table, cases with scores higher than 1.96 may be considered outliers. The greater the proportion of outlier cases, the worse the measurement fit.

Criterion validity

Criterion validity, discussed [above](#), also applies to formative measurement models.

Convergent validity

This model fit procedure, which is a special type of criterion validity, creates a reflective factor parallel to the formative factor. In a well-fitting model, it is assumed that the formative factor should be correlated with and be able to predict values of the reflective factor, which is the criterion latent variable.

For a given formative construct (ex., IncentivesF), create a corresponding reflective construct (ex., IncentivesR). The indicators for the reflectively-modeled construct IncentivesR should be representative of the overall underlying construct (Incentives) and should be different from the indicators for its formative counterpart IncentivesF, whose indicators should each represent a dimension of Incentives. For reasons given earlier [above](#), the indicators of IncentivesR should be above the cutoff for composite reliability (see [above](#)) or Cronbach's alpha (see [above](#)), but this will not necessarily be true of the indicators for IncentivesF.

Convergent validity is said to exist if the standardized path loading coefficient for the structural arrow from the formative factor IncentivesF to the reflective factor IncentivesR is high. Chin (1998) suggests a cutoff of .90 or at least .80. This implies that the R-squared value for the reflective factor should be 0.81 or at least 0.64. Note that this method of assessment requires that the indicators for the reflective construct be identified beforehand and included in the data gathering phase of the research project...

The standardized root mean square residual (SRMR)

SRMR is an approximate measure of model goodness of fit which may be used for formative models. See discussion in a previous section [above](#).

Multicollinearity of the indicators in formative models

A well-fitting formative measurement model should not display excessive multicollinearity of indicator variables in the set for any given formatively modeled factor according to Hair et al. (2014: 97). Since formative models embody a form of OLS regression, in which factors are linear combinations of the indicator variables as predictors, the usual regression test for multicollinearity problems may be applied.

Multicollinearity may be a problem according to these authors if tolerance is less than 0.20 or if the variance inflation factor (VIF) exceeds 5. Some researchers used the more stringent cutoff values of .25 and 4, respectively. VIF is the inverse of tolerance and contains the same information (tolerance < 0.20 corresponds to VIF > 5), so only one of these tests is applied. Tolerance is 1.0 minus R-squared for the factor. This means that when R-squared for a formative factor is less than .80, multicollinearity is not a problem by the criteria or tolerance < .20 or VIF > 5. Standard error is doubled when VIF is 4.0 and tolerance is .25, corresponding to $R_j = .87$. Therefore VIF ≥ 4 is a more stringent but common alternative cutoff criterion.

Hair et al. (2014: 125) suggest formative factors flagged for high multicollinearity by the tolerance or VIF tests must be dropped from the model or operationalized in some different manner. This author disagrees. While it is true that multicollinearity among the indicators for a formative factor inflates standard errors and makes assessment of the relative importance of the independent variables unreliable, nonetheless such high multicollinearity does not affect the efficiency of the regression estimates.

For purposes of sheer prediction (as opposed to causal analysis), such high multicollinearity is not necessarily a problem in formative models in this author's view. Rather, the concern of the researcher should be that the indicator items for a formative factor should include coverage of all the constituent dimensions of that factor. To take an example, for the factor "Philanthropy", formative items

might be dollars given to church, dollars given to environmental causes, dollars given to civil rights causes, etc. If it were the case that respondents who contributed a certain amount for church tended to contribute the same amount for environmental or other forms of giving, the fact that very high correlations might result would not change the fact that the set of types of giving were the dimensions of “Philanthropy” and appropriate measurement would be by way of a linear combination of the constituent types of giving. Hair et al. are correct, however, that high multicollinearity undermines the researcher’s ability to make judgments about the relative importance of the indicators in giving meaning to the formative factor and if high multicollinearity is present, the researcher must avoid comparative analysis of indicator importance based on path weights.

The “Outer VIF Values” table shown below contains VIF coefficients for the formative measurement model (for latent variables as predicted by their indicators). Note that the VIF value is the same for indicators in the same set (e.g., 1.756 for Incent1 and Incent2 as predictors of Incentives in a formative model).

The foregoing discussion applied to multicollinearity in the formative measurement model. The story is different for the inner (structural) portion of the model, where arrows connect latent variables. The VIF values in the “Inner VIF Values” table are the ones for endogenous latent variables (here, only Motivation is endogenous) as predicted from other latent variables for which the endogenous variable has incoming causal arrows in the model diagram.

In either a reflective or a formative model, there is potentially multicollinearity at the structural level. Structural multicollinearity is a problem in either reflective or formative models for the same reason it is in OLS regression models (see [above](#)). VIF coefficients for the structural model are printed by SmartPLS in the “Inner VIF Values” table shown below. In a well-fitting model, the structural VIF coefficients should not be higher than 4.0 (some use the more lenient criterion of 5.0).

SmartPLS outputs the VIF statistic as shown in the table below. Though here based on the reflectively modeled example, the output format is the same for formative models.

Collinearity Statistic (VIF)

Inner VIF Values

	Incentives	Motivation	SES
Incentives		1.236	
Motivation			
SES		1.236	

Outer VIF Values

	VIF
Incent1	1.756
Incent2	1.756
Motive1	1.721
Motive2	1.721
QccStat	1.402
?StdEduc	1.402

As noted earlier, the table above is for the reflectively modeled example. The format is the same for a formatively modeled example. In the output shown below for the equivalent formative model, the VIF values for the outer (measurement) model remain the same, rounding apart, but the VIF values for the inner (structural) model differ somewhat because formative modeling alters the values computed for the latent variables.

Collinearity Statistic (VIF)		For equivalent formative model	
Inner VIF Values			
	Incentives	Motivation	SES
Incentives		1.2284	
Motivation			
SES		1.2284	
Outer VIF Values			
	VIF		
Incent1	1.7564		
Incent2	1.7564		
Motive1	1.7214		
Motive2	1.7214		
OccStat	1.4021		
?StdEduc	1.4021		

Goodness of fit for structural models

Structural fit is examined only after measurement fit is shown to be acceptable. The structural or inner model consists of the factors and the arrows that connect one factor to another. The loadings of the direct paths connecting factors are standardized regression coefficients. Appropriate model fit criteria are discussed in sections below.

Structural path coefficients

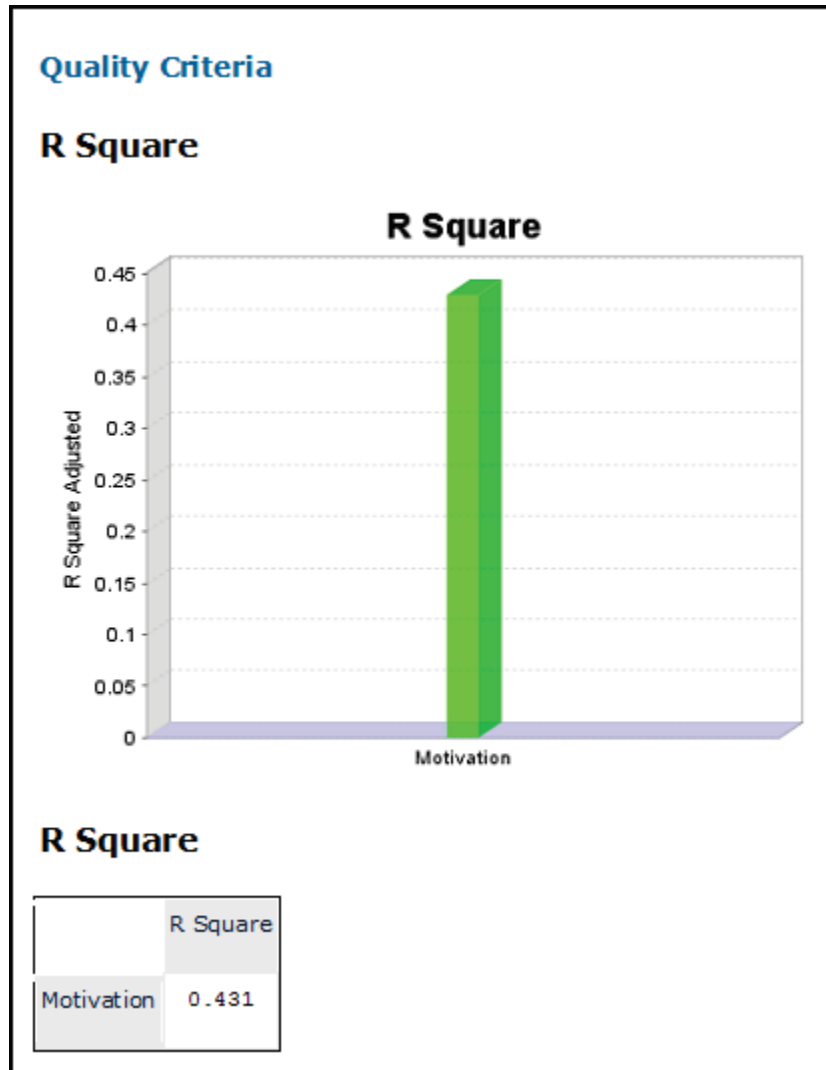
Structural path coefficients (loadings), illustrated in the path diagram after computation, are the path weights connecting the factors to each other. As data are standardized, path loadings vary from 0 to 1. These loadings should be significant (using bootstrapping). The larger, the stronger that path in the structural (inner) model. A non-significant path may call for respecifying the model without that path, or for reasons of theoretical importance and discussion, the researcher may nonetheless wish to retain the path in the model. Note,

however, that in unusual instances, dropping a non-significant path may affect the significance of other paths in the model.

R-square

R-square, also called the coefficient of determination and previously discussed and illustrated [above](#), is the overall effect size measure for the structural model, as in regression, indicating below that 43.1% of the variance in the Motivation variable is explained by the model. No R-square is shown for SES or Incentives as these are exogenous latent factors. Chin (1998: 323; see also Höck & Ringle, 2006: 15) describes results above the cutoffs 0.67, 0.33 and 0.19 to be “substantial”, “moderate” and “weak” respectively. The R-square here would be considered to be of moderate strength or effect. However, what is “high” is relative to the field: a value of .25 might be considered “high” if the state of the art in the given subject and field had previously led to values even lower.

Adjusted R-square (here, 0.430) is also output, not shown here but illustrated and discussed [below](#).



Multicollinearity.

As for any form of linear regression, multicollinearity may be present. If present, the researcher cannot use structural path coefficients to reliably assess the relative importance of predictor variables, including of predictor latent variables in the structural (inner) model. For a structural model, the predictor variables for an endogenous factor are other factors associated with incoming structural arrows (paths).

To assess multicollinearity in the inner (structural) model, tolerance or VIF criteria may be applied, discussed and illustrated previously [above](#). Recall that tolerance equals $1.0 - R^2$, and tolerance $< .20$ flags possible multicollinearity. This is equivalent to saying that $R^2 > .80$ suggests a possible multicollinearity problem.

This corresponds to VIF greater than 5, though some use the more stringent cutoffs of .25 for tolerance and 4 for VIF.

In any PLS-SEM model, there will be as many R^2 values as there are endogenous variables. For the present example, there is only one endogenous variable (Motivation) and hence only one R^2 , which is well below the level where one would think multicollinearity might be a problem (see figure [above](#)).

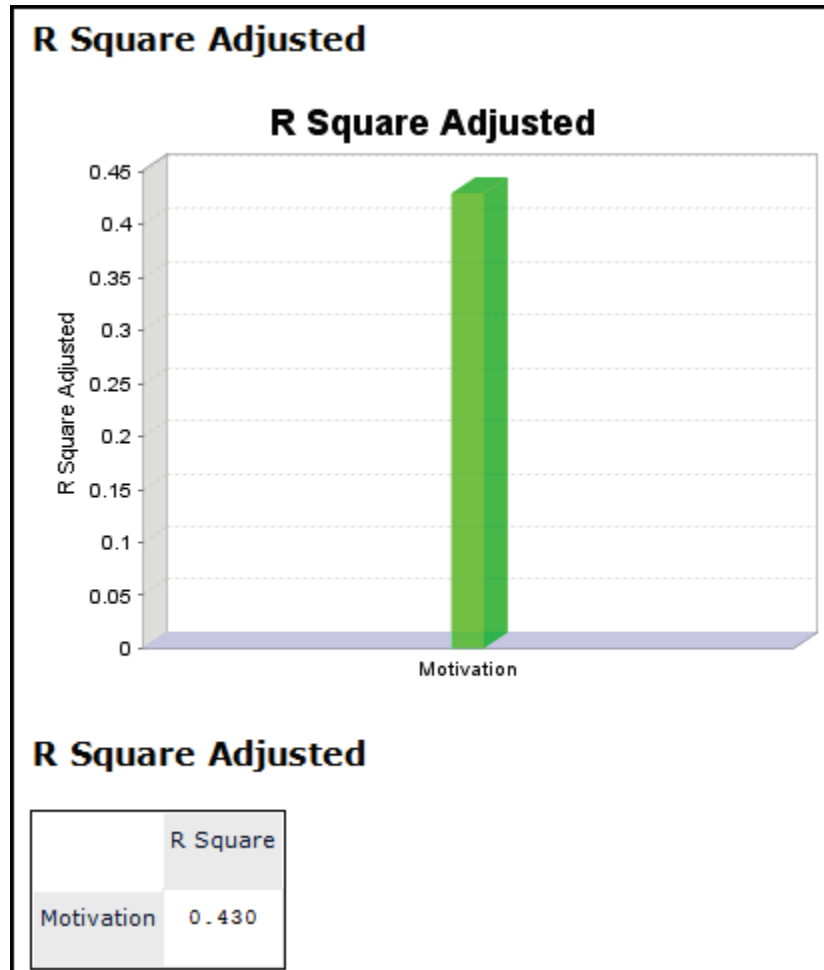
If multicollinearity is flagged as a possible problem, the researcher should consider if the highly correlated factors should be merged into a more general factor or if one is redundant and might be dropped. Factors should be retained in the model if it is clear they measure different things (thus should not be merged) and are theoretically relevant (thus should not be dropped). However, though such a factor might be retained, it would still be true that multicollinearity would mean that the standard errors of the path coefficients would be inflated and judgments about the relative importance of the predictor factors, based on the size of standardized structural (path) coefficients, would not be reliable.

Adjusted R^2

Note that adding predictors to a regression model tends to increase R^2 , even if the added predictors have only trivial correlation with the endogenous variable. To penalize for such a bias, adjusted R^2 may be used. Adjusted R^2 , which is output by SmartPLS as illustrated below, is easily computed by the formula below:

$$\text{Adjusted } R^2 = 1 - \left\{ \frac{[(1 - R^2) * (n-1)]}{[n-k-1]} \right\}$$

Where R^2 is the unadjusted R^2 , n is sample size, and k is the number of predictor variables. In the PLS-SEM structural model, k is the number of exogenous factors used to predict a given endogenous factor. Note that the term “ $(n-1)$ ” is used for samples, whereas n is used for populations (enumerations). Because of the small number of variables in the example model, adjusted R^2 is very close to unadjusted R^2 .



R-square change and f-square effect size of exogenous factors

R-square change is the change in R^2 when a causal (exogenous) factor is removed from the model. To illustrate, the “Motivation” model (see [above](#)) was run three times:

- (1) with the SES and Incentives factors as causes of Motivation (the original model, described previously);
- (2) a model in which SES was dropped; and
- (3) a model in which Incentives was dropped.

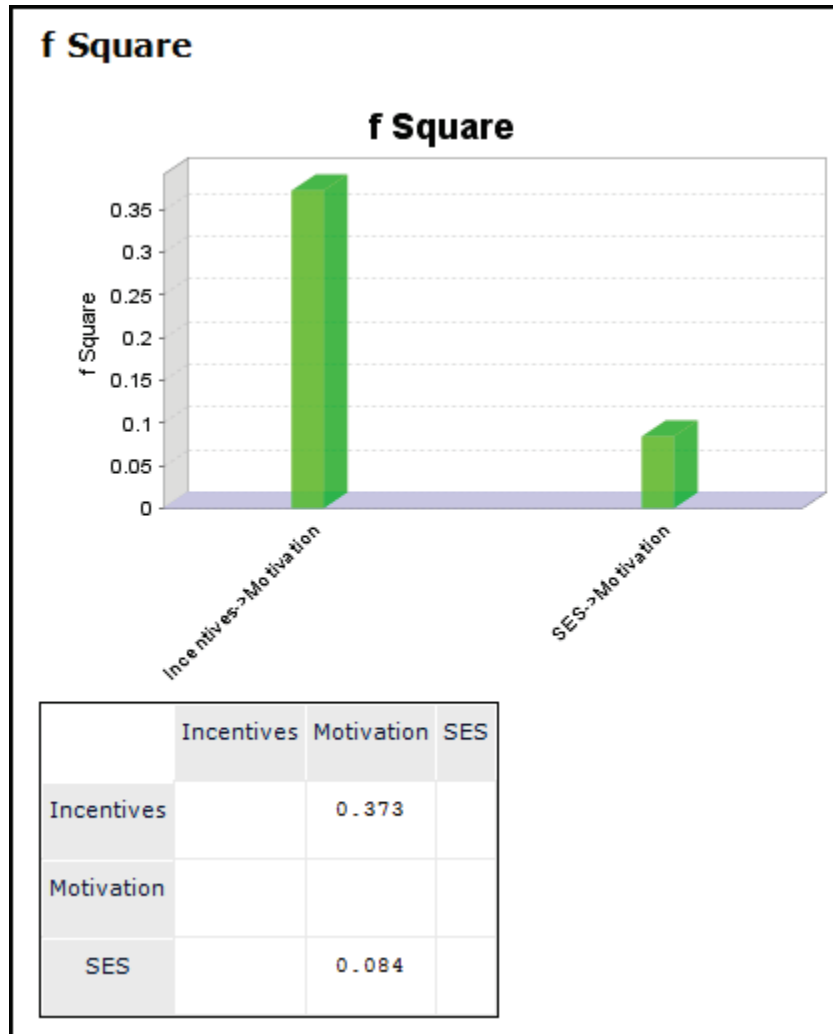
The R^2 for model 1 was .4308, for Model 2 R^2 was .3828, and for Model 3 R^2 was .219. For Model 2 compared to the original model, R^2 change was 0.043 and for Model 3 it was 0.2186. The larger the R^2 change, the more omitting that factor reduced the explained variance in Motivation. Specifically, dropping Incentives led to a greater drop in explained variance than did dropping SES. Incentives is thus

the more important explanatory variable of the two. As was also evident from the standardized structural paths (inner model loadings) shown [above](#).

EXPLAINING MOTIVATION	
WITH & WITHOUT SES	
WITH SES AND INCENTIVES	0.4308
UNEXPLAINED	0.5692
WITHOUT SES	0.3828
R2 CHANGE	0.0480
f2 EFFECT	0.0843
WITH & WITHOUT INCENTIVES	
WITH INCENTIVES AND SES	0.4308
UNEXPLAINED	0.5692
WITHOUT INCENTIVES	0.2186
R2 CHANGE	0.2122
F2 effect	0.3728

The f-square effect size measure is another name for the R-square change effect. The f-square coefficient can be constructed equal to $(R^2_{\text{original}} - R^2_{\text{omitted}})/(1 - R^2_{\text{original}})$. The denominator in this equation is “Unexplained” in the table above. The f-square equation expresses how large a proportion of unexplained variance is accounted for by R² change (Hair et al., 2014: 177). Again, Incentives has a larger effect on Motivation than does SES.

The figure above is a manual calculation using Excel. However, SmartPLS outputs the f-square values for the researcher, as illustrated below.



Following Cohen (1988), .02 represents a “small” f^2 effect size, .15 represents a “medium” effect, and .35 represents a “high” effect size. We can say that the effect of dropping Incentives from the model is high.

Latent variable correlations output

This table shows the correlation coefficients for the factor scores for the three factors in this example. Factor scores were discussed [above](#). The coefficients in the “Latent Variable Correlations” table show that Incentives is tied to Motivation at a higher absolute level than is SES, and that the SES effect is negative. In addition, this table shows the extent of correlation between the exogenous latent variables. The covariances table is redundant since data are standardized, making covariances equal to correlations.

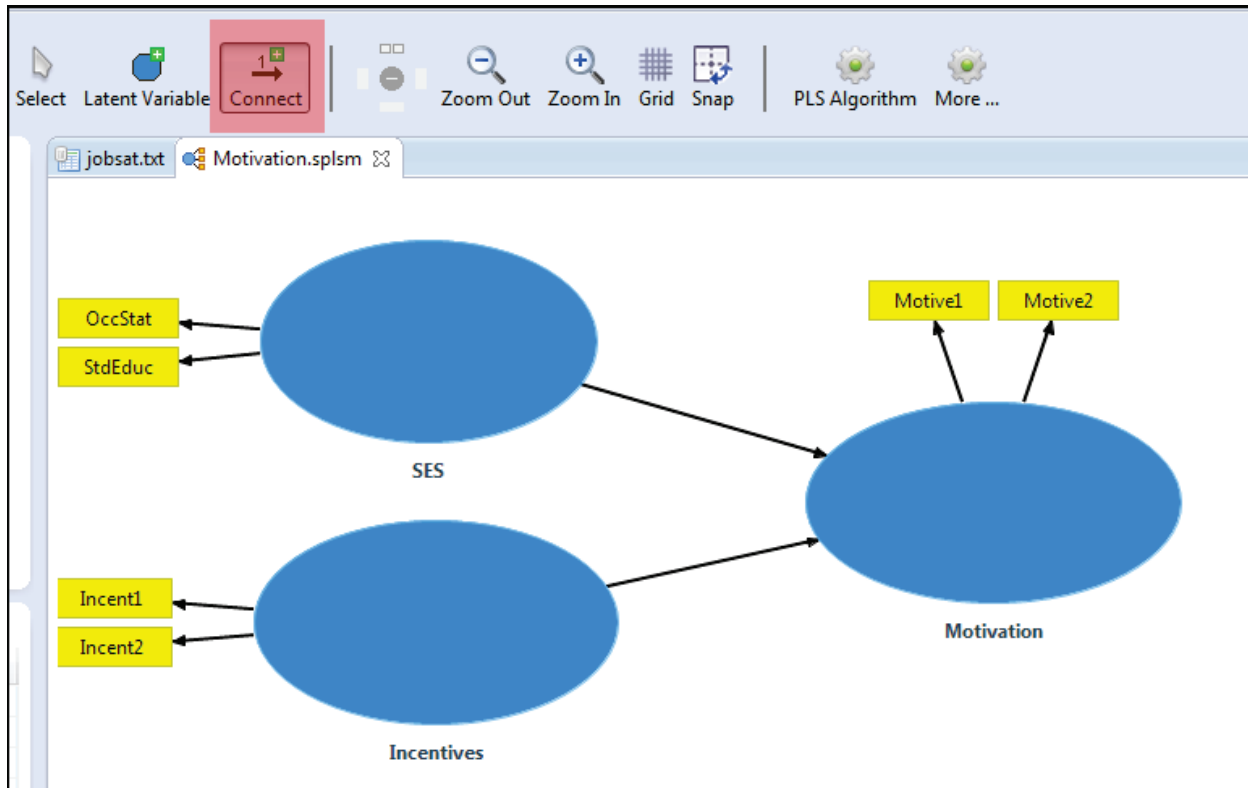
Latent Variable Correlations			
	Incentives	Motivation	SES
Incentives	1.0000		
Motivation	0.6214	1.0000	
SES	-0.4312	-0.4699	1.0000

Latent Variable Covariances			
	Incentives	Motivation	SES
Incentives	1.0000		
Motivation	0.6214	1.0000	
SES	-0.4312	-0.4699	1.0000

Analyzing residuals

Residuals may be analyzed to identify outliers in the data. Since residuals reflect the difference between observed and expected values, there is good model fit when residuals are low. Since data are standardized and assuming normal distribution of scores, residuals greater than absolute 1.96 may be considered outliers at the .05 level. The presence of a significant number of outliers may flag the omission of one or more explanatory variables from the model, which may therefore require respecification.

For convenience, the example model and residual score output is reproduced below. An observation may be an outlier on an of the indicator variables in the outer (measurement) model or on any of the latent variables in the inner(structural) model.



Residuals

Outer Model Residual Scores

Incent1	Incent2	Motive1	Motive2	OccStat	?StdEduc
0.269	-0.294	-0.181	0.184	0.694	-0.571
-0.549	0.600	0.476	-0.481	0.241	-0.198
0.183	-0.200	0.470	-0.475	0.028	-0.023
0.245	-0.268	0.213	-0.215	-0.313	0.258
-0.003	0.004	0.238	-0.241	-0.573	0.472
-0.429	0.469	-0.312	0.315	0.323	-0.265

Inner Model Residual Scores

Incentives	Motivation	SES
0.122	0.237	1.333
0.278	-0.652	0.987
0.035	1.694	-0.370
0.805	1.403	-0.888
1.220	2.671	-1.030
0.644	0.191	-0.456

Partial tables for first six observations.

Default SmartPLS output also includes tables of the covariances of residuals, shown below. In a well-fitting model, residuals are random normal and covariances should be low and non-significant. Significance testing requires

bootstrapped estimation in SmartPLS. Note also, a correlation may be trivial but nonetheless may be flagged as significant when sample size is large. Large residual covariances may flag the omission of important predictor variables from the model and hence the need for its respecification.

Outer Model Residual Covariance						
	Incent1	Incent2	Motive1	Motive2	OccStat	?StdEduc
Incent1	0.157	-0.171	0.043	-0.044	-0.006	0.005
Incent2	-0.171	0.187	-0.047	0.048	0.007	-0.006
Motive1	0.043	-0.047	0.174	-0.176	-0.014	0.012
Motive2	-0.044	0.048	-0.176	0.178	0.015	-0.012
OccStat	-0.006	0.007	-0.014	0.015	0.279	-0.229
?StdEduc	0.005	-0.006	0.012	-0.012	-0.229	0.189

Inner Model Residual Covariance			
	Incentives	Motivation	SES
Incentives	1.000	0.134	-0.237
Motivation	0.134	1.000	-0.245
SES	-0.237	-0.245	1.000

Estimation with the consistent PLS (PLSc) algorithm

Overview

Dijkstra & Schermelleh-Engel (2014) proposed “consistent PLS” (PLSc) as an algorithm intended to produce consistent and asymptotically normal estimates of path loadings and of correlations among latent variables for reflectively-modeled

constructs. As such, PLSc is meant to overcome statistical inconsistency associated with the traditional PLS estimation algorithm. Built on Nunally's (1978) correction for attenuation, PLSc is a correction to the traditional PLS algorithm (Dijkstra, 2010; Dijkstra and Henseler, 2015a, 2015b).

Lack of "consistency" means that in traditional PLS, estimates do not approach true values as sample size increases. With PLSc, estimates do approach true values asymptotically. PLSc consistently estimates path coefficients, inter-construct correlations, and indicator loadings in reflective models. Also, Dijkstra & Henseler (2015a: 299) found in simulation studies that PLSc was only slightly lower in power than full information maximum likelihood (FIML) SEM but had advantages in handling non-normally distributed data.

Note that traditional PLS displays what Wold called "consistency at large": the traditional PLS algorithm approaches true values as the number of reflective indicator variables for a given construct increases (Dijkstra & Henseler, 2015a: 298, n.2). Also note that simulation studies of the statistical power of traditional PLS have tended to show it to be comparable to the power of traditional covariance-based structural equation modeling (Goodhue, Lewis, & Thompson, 2006; Lu et al., 2011; Reinartz, Haenlein, & Henseler, 2009). Nonetheless, PLS and PLSc estimates may differ substantially.

The traditional PLS algorithm "tends to overestimate the loadings in absolute value, and to underestimate multiple and bivariate (absolute) correlations between the latent variables....The advantage of PLSc is that it is 'well calibrated', i.e. it will produce the true parameter values for the models we discuss when applied to the 'population'" (Dijkstra & Schermelleh-Engel, 2015: 586). Traditional PLS also underestimates the R-squared value of endogenous latent variables (Dijkstra, 2010).

Without correction, the more inconsistent the estimates, the more the error and the more the error, the more the probable attenuation of inter-construct correlations (Goodhue, Lewis, & Thompson, 2012; Dijkstra & Henseler, 2015a: 298). PLSc is designed to increase power and to reduce Type II error in reflective models: the researcher is less likely to reject a true model. Inconsistency of estimate in traditional PLS also means that in the case where PLS would overestimate these parameters, Type I error is higher for PLS than for PLSc.

In their conclusion, these authors note that the PLSc approach is least problematic for non-recursive reflectively-modeled linear models. Put another way, PLSc is designed for fully connected common factor models in which all constructs are reflectively measured. Because indicator correlations are not informative for gauging reliability in composite and formative models, PLSc is not appropriate, nor is it recommended for mixed formative and reflective models (Dijkstra & Henseler, 2015a: 311). Traditional PLS remains the estimation algorithm of choice for formative models and mixed models, and in some cases may be preferred even for reflective models where the research goal is sheer prediction rather than causal analysis.

PLSc output

Consistent PLS produces the same output tables as discussed [above](#) for the traditional PLS output. The coefficients are different and may even be substantially different, however, because the PLSc algorithm adjusts for consistency of estimate. Though the coefficients differ, interpretation of output is the same as discussed above for traditional PLS except that for a reflective common factor model, PLS estimates an approximation whereas PLSc yields more consistent estimates (e.g., as consistent as SEM in LISREL).

As illustration, below are tables for path coefficients from traditional PLS and from PLSc for the same simple model as discussed previously in the traditional PLS section.

Path Coefficients				Path Coefficients			
	Incentives	Motivation	SES		Incentives	Motivation	SES
Incentives		0.512		Incentives		0.6330	
Motivation				Motivation			
SES		-0.244		SES		-0.2570	

Traditional PLS **Consistent PLS**

Estimation with PLS bootstrapping

Overview

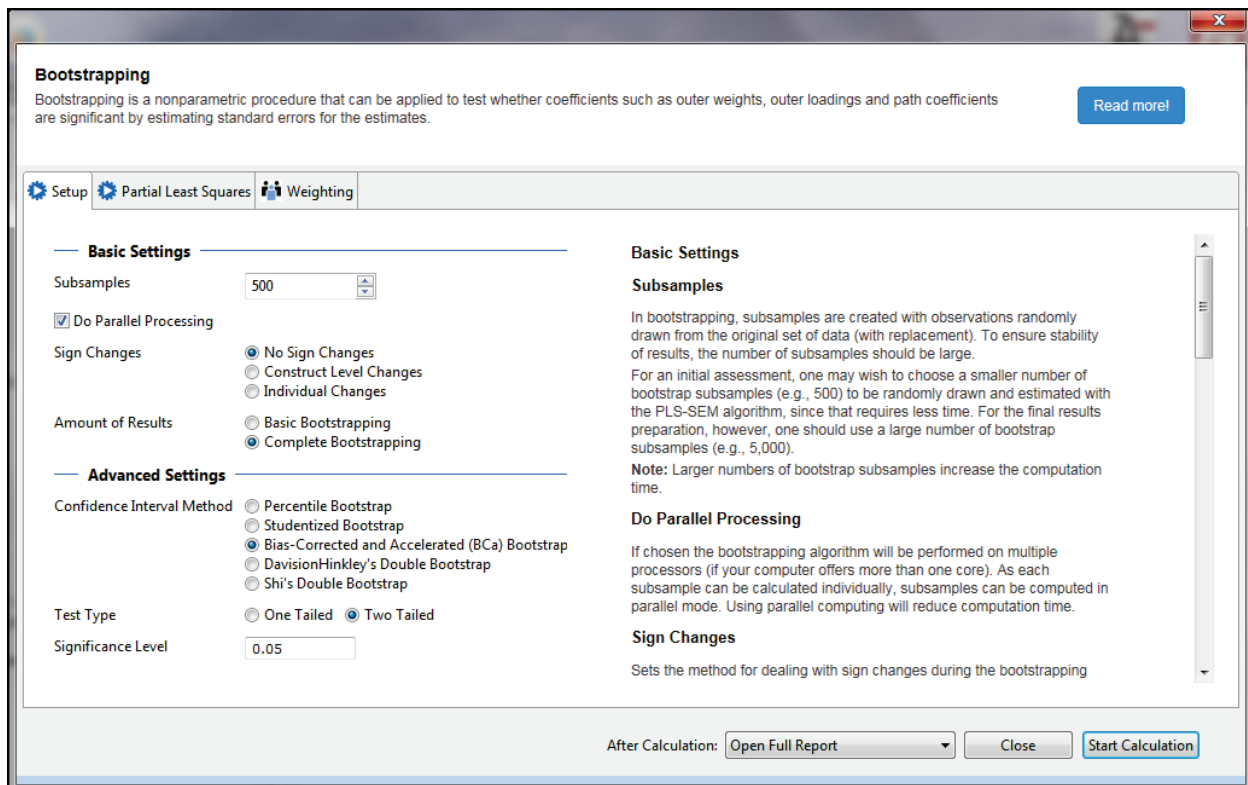
Bootstrapping uses resampling methods to compute the significance of PLS coefficients. It may be used with the traditional PLS estimation algorithm or with the consistent PLS (PLSc) algorithm, though this section focuses on the former. If the researcher wants output of significance levels, a bootstrapping option must be selected. Bootstrapped significance, though common in many statistical settings of which PLS is only one context, is not the same as the usual asymptotic tests of significance familiar to users of regression and other random-normal data applications.

In traditional asymptotic significance tests, a probability level of .05 means there is one chance in 20 that a result as strong or stronger in absolute terms will occur due to the chance of sampling (taking another sample from the population), assuming random sampling from a normal distribution. If the data are an enumeration rather than a sample, significance is moot as all effects, however small, are real and there is no possibility of “another sample”. If the sample is non-random, the computed significance level is in error to an unknown degree. A significant can be generalized to the population when random normal assumptions are met.

Bootstrapped significance is often used when data cannot be assumed to be normal. The distributional properties of PLS estimates are not known for the population and thus bootstrapping is appropriate. As typically computed, bootstrapping takes a large number of “leave one out” samples from the researcher’s data. This enables computation of a given coefficient of interest (ex., a correlation) for a large number of such samples, allowing a standard deviation to be computed. Counting standard deviations from the observed coefficient to 0 yields a significance level. For bootstrapped significance, a probability level of .05 means there is one chance in 20 that a result as strong or stronger in absolute terms will occur due to chance of sampling (taking another sample from the data). Though bootstrapping will handle any distribution, the researcher cannot generalize to the population unless the sample is randomly drawn from the population. Otherwise the researcher can generalize only to the data at hand. That is, bootstrapped estimates address the problem of non-normal distribution of data but do not address the problem of non-random sampling.

Running the PLS bootstrapping algorithm

To obtain traditional PLS estimates with bootstrapped significance, select “Bootstrapping” after selecting the desired model (here, the same ‘Motivation’ model is selected as in the PLS example above) and clicking on the “Calculate” button. This brings up the dialog shown below.



While the researcher may wish to accept all bootstrapping defaults by clicking on the “Start Calculation” button in the lower right, various options may be adjusted. These options fall under the three tabs of the dialog above: Setup, Partial Least Squares, and Weighting. (To skip discussion of bootstrapping option and proceed directly to discussion of bootstrapping output, click [here](#).)

The seven options for the “Setup” tab are shown in the enlarged figure below, with explanations under the figure (and explained on the right-hand side of the dialog itself).

The screenshot displays the 'Partial Least Squares' settings window. It is divided into two main sections: 'Basic Settings' and 'Advanced Settings'. In the 'Basic Settings' section, 'Subsamples' is set to 500, 'Do Parallel Processing' is checked, 'Sign Changes' is set to 'No Sign Changes', and 'Amount of Results' is set to 'Complete Bootstrapping'. In the 'Advanced Settings' section, 'Confidence Interval Method' is set to 'Bias-Corrected and Accelerated (BCa) Bootstrap', and 'Test Type' is set to 'Two Tailed'. The 'Significance Level' is set to 0.05.

1. *Subsamples*: The default is 500 leave-one-out samples, with replacement. This default is suitable for exploratory purposes. For confirmatory purposes, a larger number (e.g., 5000) is recommended, though this will take more computational time.
2. *Do Parallel Processing*: By default, subsamples are computed using multiple processing cores if available on the researcher's computer, thereby reducing computation time.
3. *Sign Changes*: Sign changes have to do with change in the sign of a coefficient (e.g., a path in the outer model) in a given subsample (iteration) compared to the sign when the entire sample is used.
 - a) The default is "No Sign Changes", meaning that sign changes in the resamples are accepted as is, resulting in larger standard errors.
 - b) "Construct Level Changes" makes signs consistent with those in the entire sample if in any group of coefficients (e.g., the outer model group of coefficients for a given construct) but only if a majority of signs in the group are reversed in the given subsample.

- c) “Individual Changes” makes all signs consistent with those in the entire sample.
4. *Amount of Results*: “Basic Bootstrapping” computes bootstrapped significance for path coefficients, indirect effects, total effects, outer loadings, and outer weights. “Complete Bootstrapping”, which is the default, also computes bootstrapped significance for R-square, average variance extracted (AVE), Cronbach’s alpha, and the heterotrait-monotrait ratio (HTMT). Complete bootstrapping takes more computational time.
5. *Confidence Interval Method*: Bootstrapping has several variants, of which SmartPLS offers five:
- a) Bias-Corrected and Accelerated (BCa) Bootstrap: This is the default and is a stable method producing relatively narrow confidence intervals and which is not intensive in computation time. BCa adjusts for bias and skewness in the distribution of bootstrap estimates.
 - b) Percentile Bootstrap: Confidence intervals are constructed using percentiles of the bootstrap distribution of estimates of a given coefficient. Not recommended when the distribution is asymmetrical, the median and mean diverge, or when sample size is small (e.g., < 50).
 - c) Studentized Bootstrap: Confidence intervals are constructed using quantiles from the bootstrap distribution of Student’s t-test, which is considered superior to the percentile bootstrap method.
 - d) Davison Hinkley's Double Bootstrap: Each resample is resampled again, requiring extra computational time. See Davison & Hinkley (1997).
 - e) Shi's Double Bootstrap: See Letson & McCullough (1998) for a Monte Carlo simulation study finding Shi’s method to converge quickly and to produce confidence intervals with better coverage (likelihood true values are within the limits) than single bootstrap methods. Differences In confidence limits from single bootstrap methods are modest.
6. *Test Type*: The researcher may determine if one-sided or two-sided significance tests are desired. The usual two-tailed test is the default. One-

sided would be selected only if the researcher could be certain that one side of the distribution (e.g., negative coefficients) were impossible.

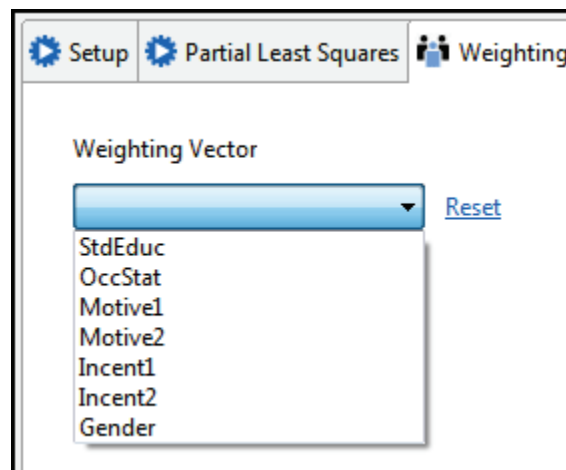
7. *Significance Level*: The usual .05 cutoff for a coefficient being significantly different from 0 is the default, but the researcher may reset this (e.g., to .10 for exploratory research).

The “Partial Least Squares” tab provides four additional optional settings for bootstrapping, shown in the figure below.

1. *Weighting Scheme*: The path weighting method., which is the default, maximizes the R-square value of endogenous latent variables in the model. Using the centroid and factor methods will generally make little difference. The centroid method should not be used when there are second-order latent variables (latent variables whose indicators are themselves latent variables) in the model.
2. *Maximum Iterations*: By default, the bootstrap algorithm will take up to 300 iterations in an attempt to achieve convergence as defined by the stop criterion. The researcher may override this default, typically to increase iterations when convergence is not achieved..

3. *Stop Criterion (10^{-X}):* Convergence I considered achieved when the change in coefficients is less than the stop criterion, which by default is 10^{-7} , which is .0000001. The researcher may adjust the stop criterion.
4. *Initial Weights:* By default, initial outer model weights (path weights connecting a latent variable and its indicator variables) are set to +1. This default can be overridden by checking the “Lohmöller Settings” checkbox, which sets the initial value to +1 for all indicators except the last, which is set to -1. While the Lohmöller method leads to faster convergence, the signs may be counterintuitive. There is also an option for user-defined initial weights set by the researcher (click “Individual Settings”).

The “Weighting” tab allows the researcher to enter the name of a weighting variable in the current dataset. This causes the program to compute a weighted PLS solution. For the example, there is no weighting variable, which is the default.



Typical uses of a weighting variable are:

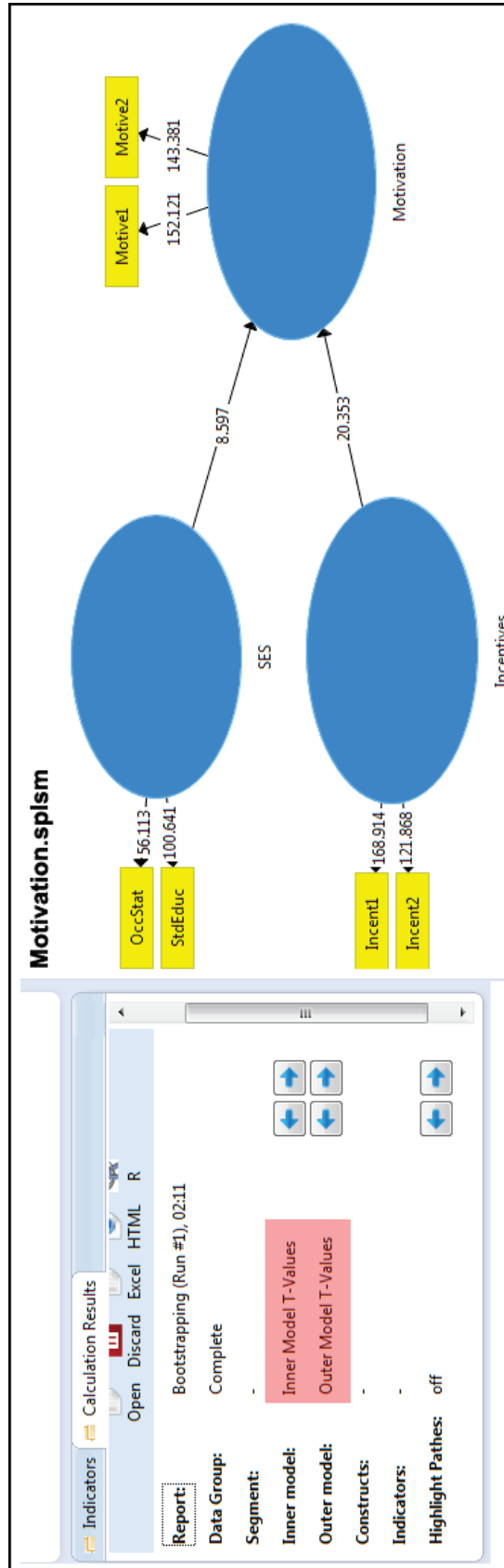
1. To adjust for oversampling of some observations compared to others (e.g., the sample may have oversampled Hispanic-Americans by a factor of two).
2. Using weighted least squares (WLS) weights to adjust for differences in point variance of the observations on a dependent variable, or for differences in some other criterion of relative observation importance.
3. Following finite mixture PLS (discussed [below](#)), probabilities of group membership in a given group may be used to obtain estimates for a given group, based on all observations.

PLS bootstrap output

After running the bootstrapping option as described above (using the default settings for the example model, “Motivation”, values in the path diagram are values for t-tests of significance. View this diagram by being in the “Motivation.splsm” tab after calculation. Be sure “Calculation Results” on the left is set to “Inner Model T-Values” and “Outer Model T Values”, as shown in the figure below.

All t values above 1.96 are significant at the .05 level, which is the case for all t values for the example model. “Calculation Results” may also be set to “P Values” to get probability levels, which are all 0.000 for this example, also meaning all paths are significant at better than the .001 probability level.

Note that because of random processes built into the bootstrapping algorithm, the exact t values reported will vary a little with each run of bootstrapping. Changing the requested number of samples will change the t values only modestly.



These values can be seen in output, either interactively under the “Bootstrapping (Run #1)” tab or as part of the full report. Here we use the latter, as sent to HTML format as described earlier [above](#). At the top of the HTML report is output for the “Path Coefficients”, by which is meant the paths in the inner model (arrows connecting the latent variables). This is shown in the figure immediately below (red highlight added):

Path Coefficients					
Mean, STDEV, T-Values, P-Values					
	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O/STERR)	P Values
Incentives -> Motivation	0.5122	0.5125	0.0252	20.3535	0.0000
SES -> Motivation	-0.2436	-0.2436	0.0283	8.5970	0.0000

Confidence Intervals				
	Original Sample (O)	Sample Mean (M)	2.5%	97.5%
Incentives -> Motivation	0.5122	0.5125	0.4618	0.5584
SES -> Motivation	-0.2436	-0.2436	-0.2995	-0.1918

Confidence Intervals Bias Corrected					
	Original Sample (O)	Sample Mean (M)	Bias	2.5%	97.5%
Incentives -> Motivation	0.5122	0.5125	0.0003	0.4618	0.5584
SES -> Motivation	-0.2436	-0.2436	-0.0000	-0.3006	-0.1919

In the output above, the “T Statistics” column contains the same value of t as appeared in the diagram above. The “P Values” column shows the corresponding significance (probability) levels for the row path. Confidence intervals appear in a separate table immediately below. Some 2.5% of cases lie below the lower confidence limit and another 2.5% (100-97.5) lie above the upper confidence limit, making these the 95% confidence limits.

“Bias corrected” confidence limits are shown in a third table in the set. The formula for this bias correction is found in Sarstedt, Henseler, & Ringle (2011):

205). For further discussion of bootstrapped confidence limits, see Efron & Tibshirani (1998), who state that bias-corrected confidence intervals yield more accurate values. Interpretation of bias-corrected confidence intervals is the same as for any other confidence interval: If 0 is not within the confidence limits, the coefficient is significant. Bias correction has been used particularly in PLS tetrad analysis (see [below](#)) to assess path significance (Gudergan, Ringle, Wende, & Will, 2008).

T-values, P-values, confidence limits, and bias-corrected confidence limits are also output for indirect and total effects, but are not shown here as the simple example model has no indirect effects and thus total effects are the same as direct effects above.

Likewise, T-values, P-values, and confidence limits are output for the outer (measurement) model, under the heading “Outer Loadings”, as shown below. A bias-corrected confidence limit table is also output, not shown here. For the example model, all outer model loadings are highly significant also.

The same three confidence/significance tables are also produced for “Outer Weights”, not shown here.

Outer Loadings**Mean, STDEV, T-Values, P-Values**

	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O/STERR)	P Values
Incent1 <- Incentives	0.9182	0.9180	0.0054	168.9144	0.0000
Incent2 <- Incentives	0.9014	0.9009	0.0074	121.8676	0.0000
Motive1 <- Motivation	0.9087	0.9080	0.0060	152.1207	0.0000
Motive2 <- Motivation	0.9064	0.9055	0.0063	143.3811	0.0000
OccStat <- SES	0.8493	0.8480	0.0151	56.1125	0.0000
?StdEduc <- SES	0.9007	0.9003	0.0089	100.6409	0.0000

Confidence Intervals

	Original Sample (O)	Sample Mean (M)	2.5%	97.5%
Incent1 <- Incentives	0.9182	0.9180	0.9062	0.9280
Incent2 <- Incentives	0.9014	0.9009	0.8854	0.9142
Motive1 <- Motivation	0.9087	0.9080	0.8961	0.9187
Motive2 <- Motivation	0.9064	0.9055	0.8922	0.9163
OccStat <- SES	0.8493	0.8480	0.8187	0.8751
?StdEduc <- SES	0.9007	0.9003	0.8835	0.9180

T-values, P-values, confidence limits, and bias-corrected confidence limits are also output for model “quality criteria”, such as R-square, as shown below, demonstrating the R-square value to be significant for the example model. Similar sets of tables are output for adjusted R-square, f-square, average variance extracted (AVE), composite reliability, Cronbach’s alpha, the heterotrait-monotrait ratio (HTMT), the SRMR for the common factor model, and the SRMR for the composite model, all not shown here. These measures were all discussed previously in the traditional PLS estimation algorithm sections on assessing model fit.

Quality Criteria**R Square****Mean, STDEV, T-Values, P-Values**

	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O/STERR)	P Values
Motivation	0.4308	0.4320	0.0237	18.1387	0.0000

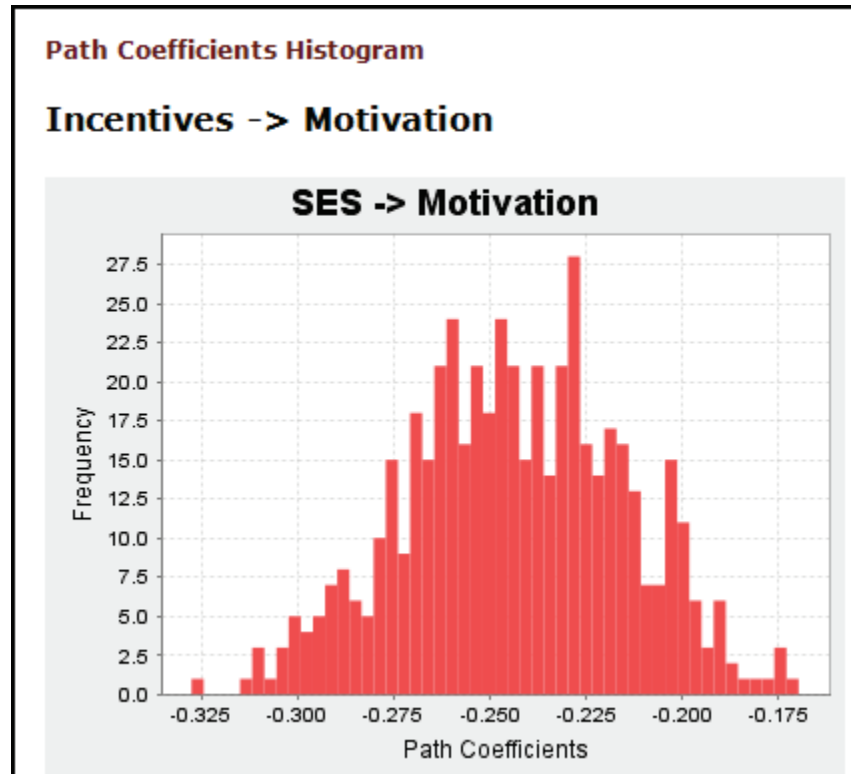
Confidence Intervals

	Original Sample (O)	Sample Mean (M)	2.5%	97.5%
Motivation	0.4308	0.4320	0.3870	0.4755

Confidence Intervals Bias Corrected

	Original Sample (O)	Sample Mean (M)	Bias	2.5%	97.5%
Motivation	0.4308	0.4320	0.0013	0.3888	0.4797

Bootstrap output also includes histograms showing the dispersion of estimated values across iterations. For instance, the histogram below shows the distribution of path loading coefficients for the model's path from SES to Motivation. Other histograms are output for indirect effects and total effects. This is a graphical way of displaying the same information as is contained in confidence intervals. There are no histograms for the outer (measurement) model.



Dropping indicators

It may be asked whether indicators with non-significant paths should be dropped from the model.

For reflective models, indicators are representative of the factor and in principle, dropping one does not change the meaning of the factor. Assuming enough other representative indicator variables exist for the given factor, dropping one whose path is non-significant is appropriate. When an indicator is dropped, all coefficients in the model will change, sometimes crossing the border between significance and non-significance. For this reason, as for coefficients in other statistical procedures, it is recommended to drop one at a time, re-running the model each time.

For formative models, however, each indicator measures one of the set of dimensions of which the factor is composed. Dropping such an indicator changes the meaning of the factor because that dimension of meaning is omitted. Therefore, unless there are redundant indicator items for the dimension in question, indicators usually are not dropped from formative models even if non-significant

Estimation with consistent PLS bootstrapping

Overview

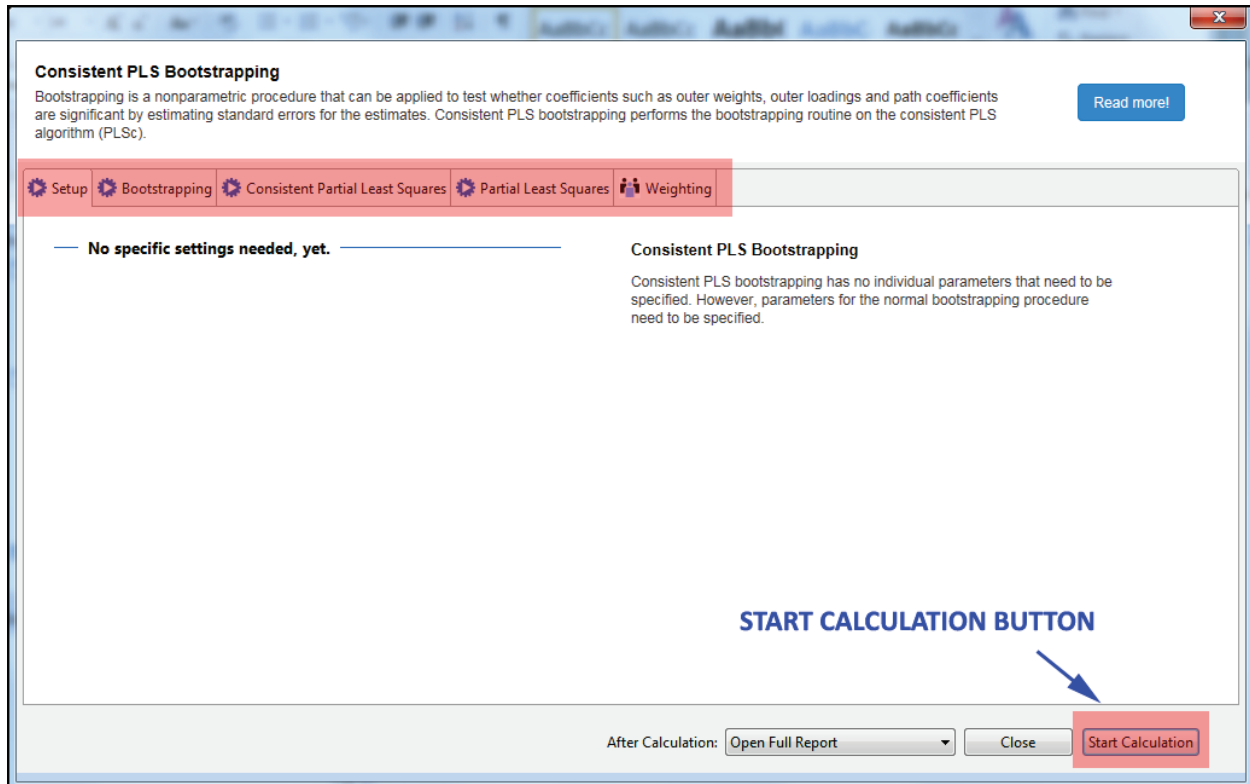
Consistent PLS (PLSc) was discussed [above](#) and, also [above](#), bootstrapping using the default PLS algorithm was discussed and pros and cons presented. The “consistent PLS bootstrapping” method combines the two, using bootstrapping methods but in conjunction with the PLSc algorithm. As a form of bootstrapping, PLSc bootstrapping is a nonparametric method which may be used to derive standard errors and significance tests for coefficients in the partial least squares model.

For the example in this section we use MotivationR.splsm, which is the reflexively modeled version of the Motivation model. This was created in a previous section [above](#).

Running the PLSc bootstrapping algorithm

After selecting Calculate > Consistent PLS Bootstrapping from the SmartPLS menu, a dialog appears with five tabs:

1. Setup
2. Bootstrapping
3. Consistent Partial Least Squares
4. Partial Least Squares
5. Weighting



Under each tab, the user may accept or reset various default parameters. These are discussed below in turn.

SETUP

Unlike regular PLS bootstrapping (recall prior figure [above](#)), consistent PLS bootstrapping does not require setting any parameters under this tab.

BOOTSTRAPPING

The default settings for the “Bootstrapping” tab in SmartPLS are shown in the figure below.

The screenshot shows the 'Bootstrapping' tab in the SmartPLS software interface. The settings are as follows:

- Basic Settings:**
 - Subsamples: 500
 - Do Parallel Processing:
 - Sign Changes: No Sign Changes, Construct Level Changes, Individual Changes
 - Amount of Results: Basic Bootstrapping, Complete Bootstrapping
- Advanced Settings:**
 - Confidence Interval Method: Percentile Bootstrap, Studentized Bootstrap, Bias-Corrected and Accelerated (BCa) Bootstrap, DavisionHinkley's Double Bootstrap, Shi's Double Bootstrap
 - Test Type: One Tailed, Two Tailed
 - Significance Level: 0.05

In the example described below in this section, we accepted the defaults as shown. Comments on the options are presented next:

- *Subsamples:* Bootstrapping requires repeated sampling from the given data. The default 500 samples is for exploratory purposes, keeping computation time minimal. For final analysis, however, a much larger number (e.g., 5,000) is recommended for stability of estimates.
- *Parallel Processing:* If this is checked (the default) and the researcher’s computer has multiple processors, they will be used to speed computation time. If the computer lacks multiple processors, checking this box has no effect.

- *Sign Changes*: Options are the same as discussed [above](#) for ordinary PLS bootstrapping. Sign changes refer to the sign of a coefficient flipping from positive to negative, or vice versa, for a particular sample compared to the mode for all samples. The default is “No Sign Changes”, meaning that sign changes in the resamples are accepted as is, resulting in larger standard errors. It is possible to force signs to conform to other resample results.
- *Amount of Results*: Basic Bootstrapping” computes bootstrapped significance for path coefficients, indirect effects, total effects, outer loadings, and outer weights. “Complete Bootstrapping”, which is the default, also computes bootstrapped significance for R-square, average variance extracted (AVE), Cronbach’s alpha, and the heterotrait-monotrait ratio (HTMT). Complete bootstrapping takes more computational time.
- *Confidence Interval Method*: Bias-corrected and accelerated (BCa) bootstrapping is the default method of computing confidence intervals. It is considered to be a stable method producing relatively narrow confidence intervals and is not intensive in computation time. The BCa method and alternatives were discussed [above](#) in the section on ordinary PLS bootstrapping.
- *Test Type*: As in most social research, two-tailed significance tests are specified as the default. One-sided would be selected only if the researcher could be certain that one side of the distribution (e.g., negative coefficients) were impossible.
- *Significance level*: Also following common social science practice, the usual .05 cutoff for a coefficient being significantly different from 0 is the default. This may be reset by the researcher.

CONSISTENT PARTIAL LEAST SQUARES

This tab (not shown) has a single option. The researcher can check a box labeled “Connect all LVs for Initial Calculation”. The default is not to check this box, meaning that the connections involving the latent variables (LVs) in the model are accepted as drawn by the researcher. Dijkstra and Henseler (2012) have suggested that more stable results may follow if all latent variables are connected in the model. The default (no check) option, however, preserves the researcher’s

original model and test coefficients refer to this model, not a more saturated model.

PARTIAL LEAST SQUARES

The screenshot shows the 'Partial Least Squares' tab in a software interface. It is divided into two sections: 'Basic Settings' and 'Advanced Settings'. In the 'Basic Settings' section, the 'Weighting Scheme' is set to 'Path' (indicated by a selected radio button). The 'Maximum Iterations' is set to 300, and the 'Stop Criterion (10^-X)' is set to 7. In the 'Advanced Settings' section, the 'Use Lohmöller Settings' checkbox is unchecked, and there is a link to 'configure individual initial weights'.

In the example described below, we accepted the defaults as shown. Comments on the options are presented next:

Weighting Scheme: Initial weights were discussed earlier [above](#). The “Path” weighting method is recommended because it is thought to generate the highest R^2 values. Differences among methods are sufficiently small that the choice of weighting scheme typically does not affect substantive interpretations of results.

Maximum Iterations: In the initial, exploratory phase of research, computational time is minimized by the default 300 iterations. Later, in the confirmatory stage of research, a much higher number is recommended (e.g., 1,000 or even 5,000).

Stop Criterion: The number entered here (by default 10^{-7}) specifies how small the change in outer weights must be on a successive iteration to judge that iterations should stop. In the rare event that convergence is a problem, a slightly larger stop criterion might be used (e.g., 10^{-5}).

Initial Weights: Initial outer weights by default are set to +1. If the “Use Lohmöller Settings” box is checked, however, all initial weights are set to +1 except the last,

which is set to -1. While the Lohmöller method speeds convergence, it is not generally adopted as it may lead to counter-intuitive signs for path coefficients.

WEIGHTING TAB

This tab (not shown) allows the user to specify a variable in the current dataset (the “weighting vector”) whose values are used to weight observations. There are three common weighting purposes.

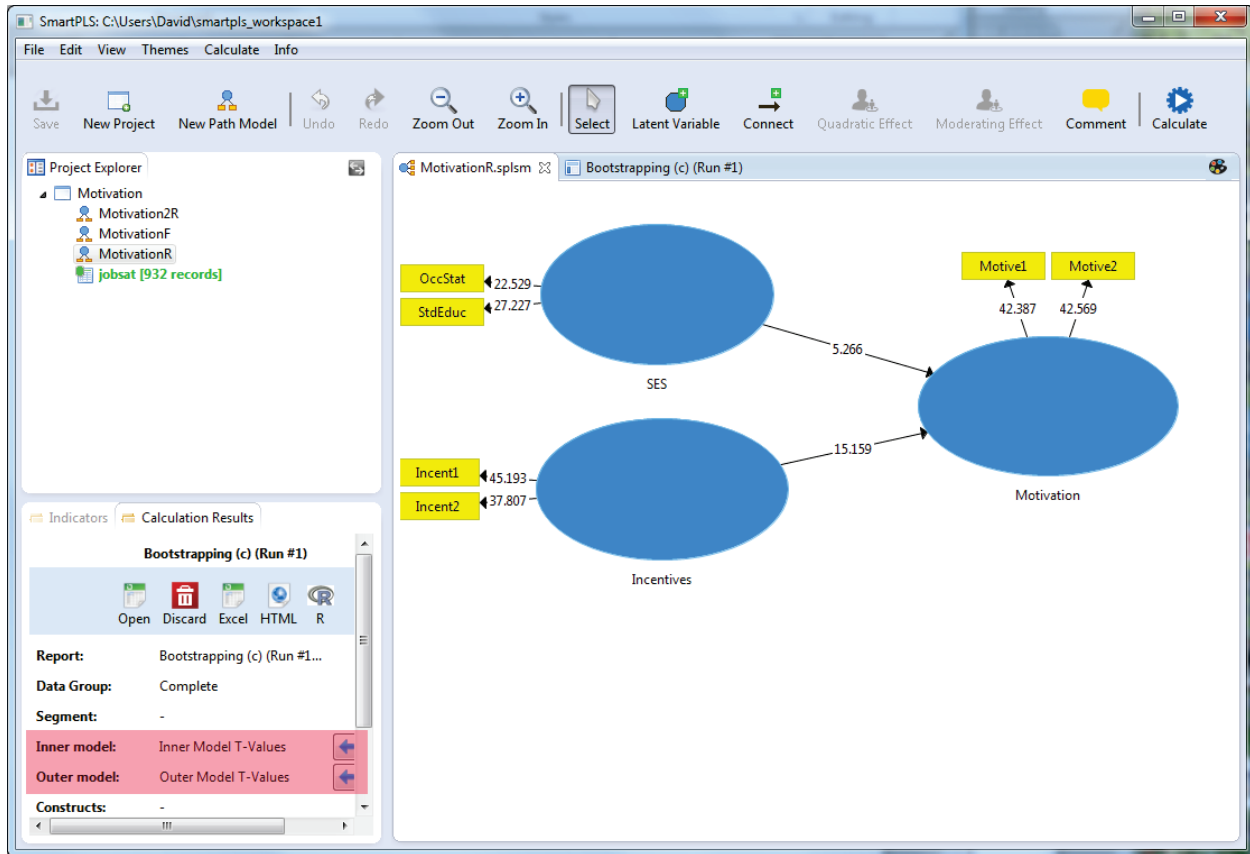
1. Weights may compensate for differential sampling of the population (e.g., oversampling of a subgroup of special interest).
2. Weights may reflect probabilities of membership in various groups identified by finite mixture analysis (FIMIX), discussed [below](#).
3. Weights may compensate for differential reliability of some observations (e.g., WLS weights may be used. See the separate Statistical Associates “Blue Book” on “Weighted Least Squares”).

Consistent PLS bootstrap output

For the output below, the defaults for all options described above were accepted.

Run the analysis by clicking the “Start Calculation” button in the lower-right corner of the Consistent PLS shown [above](#).

After calculation is completed, values in the path diagram are values for t-tests of significance. View this diagram by being in the “MotivationR.splsm” tab after calculation. Be sure “Calculation Results” on the left is set to “Inner Model T-Values” and “Outer Model T Values”, as shown highlighted in the lower left of the figure below.



All t values above 1.96 are significant at the .05 level, which again is the case for all t values in the example model. “Calculation Results” may also be set to “P Values” to get probability levels, which are all 0.000 for this example, as in ordinary PLS bootstrapping.

Note that because of random processes built into the bootstrapping algorithm, the exact t values reported will vary a little with each run of bootstrapping. Changing the requested number of samples will change the t values only modestly.

These values can be seen in output, either interactively under the “Bootstrapping (c) (Run #1)” tab shown in the figure above, or as part of the full report. Here we use the latter. Click the “Export to Web” button to send the full report in HTML format to a file location of choice. It will also appear in a web browser.

At the top of the HTML report is output for the “Path Coefficients”, which here are the paths in the inner model (arrows connecting the latent variables). This is shown in the figure immediately below (red highlight added). While the

coefficients differ from those produced by ordinary PLS bootstrapping (see [above](#)), substantive inferences about path significance or lack thereof are usually the same. Note also that if the reader is following along, random processes inherent in bootstrapping will yield coefficients which differ from those in the figure below.

Path Coefficients					
Mean, STDEV, T-Values, P-Values					
	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O/STERR)	P Values
Incentives -> Motivation	0.6330	0.6319	0.0418	15.1591	0.0000
SES -> Motivation	-0.2570	-0.2609	0.0488	5.2657	0.0000

Confidence Intervals				
	Original Sample (O)	Sample Mean (M)	2.5%	97.5%
Incentives -> Motivation	0.6330	0.6319	0.5487	0.7140
SES -> Motivation	-0.2570	-0.2609	-0.3549	-0.1724

Confidence Intervals Bias Corrected					
	Original Sample (O)	Sample Mean (M)	Bias	2.5%	97.5%
Incentives -> Motivation	0.6330	0.6319	-0.0011	0.5501	0.7155
SES -> Motivation	-0.2570	-0.2609	-0.0039	-0.3720	-0.1777

In the figure above, the “T Statistics” column contains the same value of t as appeared in corresponding diagram above. The “P Values” column shows the corresponding significance (probability) levels for the path for the given row (e.g., the first row is the path from Incentives to Motivation). Confidence intervals appear in a separate table immediately below. Coefficients of some 2.5% of cases lie below the lower confidence limit and another 2.5% lie above the upper limit, making these the 95% confidence limits.

The “Bias corrected” confidence limits shown in the third table in the set are discussed [above](#) in the previous section on ordinary PLS bootstrap estimates. T-values, P-values, confidence limits, and bias-corrected confidence limits are also output for indirect and total effects, but are not shown here as a the simple

example model has no indirect effects and thus total effects are the same as direct effects above.

In a similar manner, T-values, P-values, and confidence limits are output for the outer (measurement) model, under the heading “Outer Loadings”, as shown below. A bias-corrected confidence limit table is also output, not shown here. For the example model using consistent PLS bootstrapping, all outer model loadings are highly significant also. The same three confidence/significance tables are also produced for “Outer Weights”, not shown here.

Outer Loadings					
Mean, STDEV, T-Values, P-Values					
	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O/STERR)	P Values
Incent1 <- Incentives	0.8471	0.8472	0.0187	45.1932	0.0000
Incent2 <- Incentives	0.7747	0.7739	0.0205	37.8066	0.0000
Motive1 <- Motivation	0.8094	0.8083	0.0191	42.3870	0.0000
Motive2 <- Motivation	0.7998	0.7990	0.0188	42.5688	0.0000
OccStat <- SES	0.6638	0.6632	0.0295	22.5289	0.0000
?StdEduc <- SES	0.8067	0.8062	0.0296	27.2267	0.0000

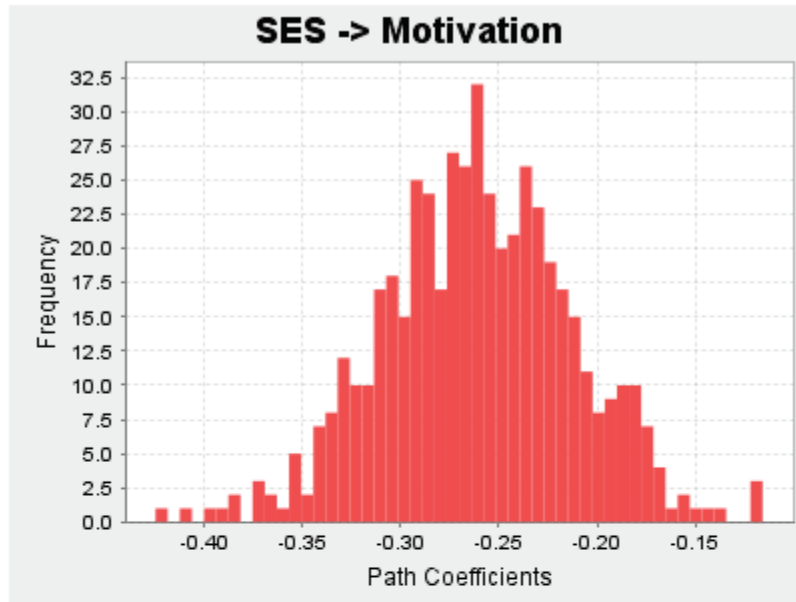
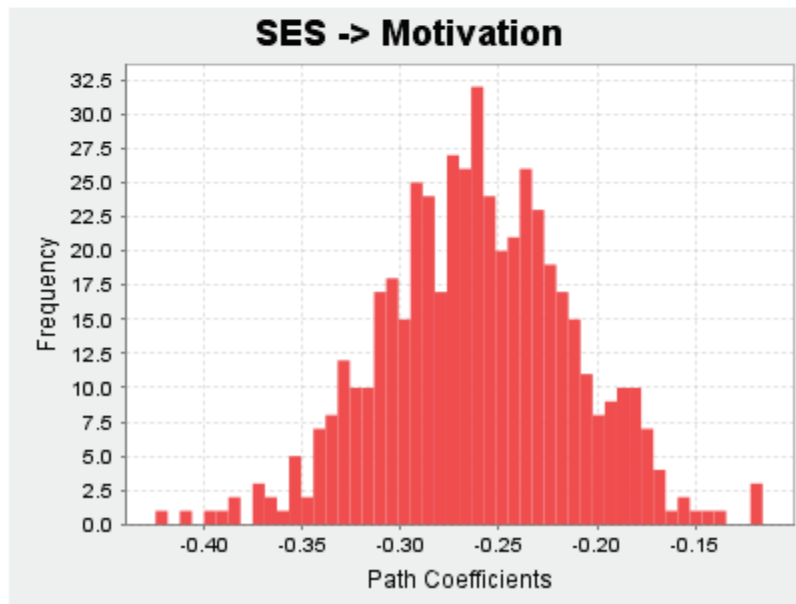
Confidence Intervals				
	Original Sample (O)	Sample Mean (M)	2.5%	97.5%
Incent1 <- Incentives	0.8471	0.8472	0.8099	0.8842
Incent2 <- Incentives	0.7747	0.7739	0.7329	0.8117
Motive1 <- Motivation	0.8094	0.8083	0.7691	0.8423
Motive2 <- Motivation	0.7998	0.7990	0.7615	0.8343
OccStat <- SES	0.6638	0.6632	0.6023	0.7214
?StdEduc <- SES	0.8067	0.8062	0.7461	0.8635

T-values, P-values, confidence limits, and bias-corrected confidence limits are also output for model “quality criteria”, such as R-square, as shown below, demonstrating the R-square value to be significant for the example model. Similar sets of tables are output for adjusted R-square, f-square, average variance extracted (AVE), composite reliability, Cronbach’s alpha, the heterotrait-

monotrait ratio (HTMT), the SRMR for the common factor model, and the SRMR for the composite model, all not shown here. These measures were all discussed previously in the traditional PLS estimation algorithm sections on assessing model fit.

Quality Criteria					
R Square					
Mean, STDEV, T-Values, P-Values					
	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O/STERR)	P Values
Motivation	0.6550	0.6602	0.0362	18.0992	0.0000
Confidence Intervals					
	Original Sample (O)	Sample Mean (M)	2.5%	97.5%	
Motivation	0.6550	0.6602	0.5860	0.7250	
Confidence Intervals Bias Corrected					
	Original Sample (O)	Sample Mean (M)	Bias	2.5%	97.5%
Motivation	0.6550	0.6602	0.0052	0.5938	0.7310

PLSc bootstrap output also includes histograms showing the dispersion of estimated values across iterations. For instance, the histogram below shows the distribution of path loading coefficients for the model's paths from Incentives to Motivation, and from SES to Motivation. Other histograms are output for indirect effects and total effects. This is a graphical way of displaying the same information as is contained in confidence intervals. There are no histograms for the outer (measurement) model.

Path Coefficients Histogram**Incentives -> Motivation****SES -> Motivation**

Dropping indicators

Whether indicators with non-significant paths by PLS bootstrapping should be dropped from the model is a question involving the same considerations as previously discussed [above](#) for ordinary PLS bootstrapping.

Estimation with blindfolding

Overview

Blindfolding utilizes a cross-validation strategy and reports cross validated communality and cross validated redundancy for constructs as well as indicators. SmartPLS documentation calls these “predictive accuracy” criteria. Unlike bootstrapping, no standard errors or significance coefficients are calculated. Rather, the purpose is to calculate cross-validated measures of model predictive accuracy (reliability), of which there are four:

- Construct cross-validated redundancy
- Construct cross-validated communality
- Indicator cross-validated redundancy
- Indicator cross-validated communality

The cross-validated redundancy for a reflectively modeled endogenous factor is the Stone-Gleisser Q^2 value, a model fit measure discussed further below ((Stone, 1974; Geisser, 1974). As shown in the user dialog for the blindfolding choice shown below, the researcher must set a distance value called the “omission distance” (d). The blindfolding algorithm omits every d th data point for the indicators for the selected endogenous factor (below, every 7th data point for the indicators for Motivation) and does d iterations. Estimates from the d iterations are combined to compute a total estimate of the cross-validated redundancy, which is Q^2 . There is a Q^2 value for each reflectively-modeled endogenous factor in the model. A Q^2 value above 0 indicates that the model is relevant to predicting that factor. For more regarding computation of Q^2 , see Hair et al. (2014: 178-197).

For the example in this section we use MotivationR.splsm, which is the reflexively modeled version of the Motivation model. This was created in a previous section [above](#).

Warning: The blindfolding procedure should only be applied to reflective models, as in the example below.

ONLINE HELP

Blindfolding is a sample re-use technique that starts with the first data point and omits every d th data point in the endogenous construct's indicators. Then, the procedure estimates the PLS path model parameters by using the remaining data points. The omitted data points are considered missing values and treated accordingly when running the PLS-SEM algorithm (e.g., by using mean value replacement). The resulting estimates are then used to predict the omitted data points. The difference between the true (i.e., omitted) data points and the predicted ones is then used as input for the Q^2 measure.

Blindfolding is an iterative process. In the next iteration, the algorithm starts with the second data point and omits every d th data point and continues as described before. After d iterations, every data point has been omitted and the model re-estimated.

When PLS-SEM exhibits predictive relevance, it accurately predicts the data points of indicators in reflective measurement models of endogenous constructs and endogenous single-item constructs (the procedure does not apply for formative constructs). In the structural model, a Q^2 value larger than zero for a certain reflective endogenous latent variable indicate the path model's predictive relevance for this particular construct.

END ONLINE HELP

Running the blindfolding algorithm

After selecting Calculate > Blindfolding from the SmartPLS menu, a dialog appears with four tabs. These are discussed in turn below.

1. Setup
2. Partial Least Squares
3. Weighting
4. Blindfolding

SETUP

The “Setup” tab (not shown) has a single parameter, “omission distance”. The user may reset the default value of 7 to some other value between 5 and 12. The omission distance parameter, d , specifies how far the algorithm reaches in the process of data point omission. The default $d = 7$ means that every 7th data point is omitted in a given blindfolding iteration (round), of which there will be 7, so that all data points are temporarily omitted for purposes of predicting their values. The number of blindfolding rounds is always d .

Warning: In order to predict all observations, the blindfolding algorithm requires that n/d is not an integer, where n is the number of observations and d is the omission distance. The exercise dataset has 932 observations and, not being evenly divisible by 7, the default $d=7$ is acceptable.

PARTIAL LEAST SQUARES

The “Partial Least Squares” tab is identical to that discussed in the section on consistent PLS bootstrapping and the same considerations apply. The reader is referred to this section [above](#). The blindfolding example here accepts the default settings.

WEIGHTING

The “Weighting” tab is identical to that discussed in the section on consistent PLS bootstrapping and the same considerations apply. The reader is referred to this section [above](#). The blindfolding example here accepts the default settings. In this blindfolding example, no weights are used.

BLINDFOLDING

The “Blindfolding” tab appears if the “Read More!” button is pressed. Basic information about the blindfolding procedure is presented. This tab has no settings.

Output unique to blindfolding estimation

Predictive relevance (Q^2)

Q^2 is also known as Stone-Geisser Q^2 , after its authors (Stone, 1974; Geisser, 1974; for PLS context, see also Chin, 1998; Ruiz et al., 2009: 546). Applicable only to reflectively modeled endogenous factors, Q^2 greater than 0 means that the PLS-SEM model is predictive of the given endogenous variable under scrutiny. By

the same token, a Q^2 with a 0 or negative value indicates the model is irrelevant to prediction of the given endogenous factor.

As mentioned above, there are four sets of cross-validation output:

- Construct cross-validated redundancy
- Construct cross-validated communality
- Indicator cross-validated redundancy
- Indicator cross-validated communality


The “Construct” output relates to the inner model connecting the latent variables. The “Indicator” output relates to the outer model connecting the latent constructs to their indicator variables. The Q^2 statistic is found in the “redundancy” output. The “communality” output is an alternative measure of predictive relevance, discussed below.

Construct cross-validated redundancy


Construct cross-validated redundancy will usually be the blindfolding output of greatest interest since it speaks to model fit of the PLS latent variable model. In SmartPLS output, Stone-Geisser Q^2 appears as “1 – SSE/SSO” in the “Total” table of the “Construct Crossvalidated Redundancy” section, as in the figure below. For this example, Q^2 is approximately 0.35. Following Cohen (1988), .02 represents a “small” effect size, .15 represents a “medium” effect size, and .35 represents a “high” effect size. On this basis, we can say that the model is has a high degree of predictive relevance with regard to the endogenous factor Motivation.

Construct Crossvalidated Redundancy

Total

Q-squared 

	SSO	SSE	Q ² ? (=1-SSE/SSO)
Incentives	1,864.0000	1,864.0000	
Motivation	1,864.0000	1,204.6128	0.3537
SES	1,864.0000	1,864.0000	

Case1  **There is also output for each of the 7 rounds.**

	SSO	SSE	Q ² ? (=1-SSE/SSO)
Incentives	286.5902	286.5902	
Motivation	261.1720	165.9909	0.3644
SES	295.2150	295.2150	

Other cross-validation tables

The construct cross-validated communality, indicator cross-validated redundancy, and indicator cross-validated communality tables are constructed in the same way. In each case a Q^2 value is calculated as 1 minus the sum of squared error divided by the sum of squares of observed omitted values. The cutoffs for interpretation of small, medium, and high effect size remain the same as discussed above.

It will be noted that whether one is discussing constructs in the inner model or indicators in the outer model, there are two versions of Q^2 : redundancy and communality. The following comparison observations apply:

- Redundancy is only calculated for endogenous variables in the model (here, Motivation). Communality is calculate for all constructs and indicators in the model.
- Communality coefficients run higher than redundancy coefficients

- The communality calculation is done without knowledge of the path model, based only on construct (latent variable) scores.
- The redundancy calculation of Q^2 is more consistent with the PLS approach, which focuses on paths involving the endogenous variables. For this reason it is preferred by Hair et al. (2014: 183).

Construct Crossvalidated Communality			
Total			
	SSO	SSE	$Q^2 (=1-SSE/SSO)$
Incentives	1,864.0000	1,071.4315	0.4252
Motivation	1,864.0000	1,090.6371	0.4149
SES	1,864.0000	1,335.2136	0.2837

For the example data, the inner model has a high degree of predictive relevance with regard to the endogenous factor Motivation by either the redundancy or communality method.

Indicator Crossvalidated Redundancy			
Total			
	SSO	SSE	$Q^2 (=1-SSE/SSO)$
Incent1	932.0000	932.0000	
Incent2	932.0000	932.0000	
Motive1	932.0000	598.9236	0.3574
Motive2	932.0000	605.6892	0.3501
OccStat	932.0000	932.0000	
?StdEduc	932.0000	932.0000	

Indicator Crossvalidated Commuality			
Total			
	SSO	SSE	$Q^2 (=1-SSE/SSO)$
Incent1	932.0000	538.3156	0.4224
Incent2	932.0000	533.1159	0.4280
Motive1	932.0000	545.7105	0.4145
Motive2	932.0000	544.9266	0.4153
OccStat	932.0000	670.6782	0.2804
?StdEduc	932.0000	664.5353	0.2870

The tables above for the outer model connecting latent constructs to their indicators shows that here also, outer model has is has a high degree of predictive relevance with regard to the endogenous factor Motivation by either the redundancy or communality method. Nonetheless, the “Indicator Crossvalidated Commuality” table shows that the predictive relevance of the indicators of SES (OccStat and StdEduc) is only in the medium or moderate effect size range.

The effect size measure q^2

The less-used q^2 effect size measure is a third alternative statistic (in addition to redundancy and communality) which may be used to assess the predictive relevance of inner model paths to the endogenous variable. Recall [above](#) the discussion of the f^2 effect size measure, in the section on the default PLS algorithm. In the same manner that f^2 effect size was calculated based on R^2 values of models with and without an exogenous factor in the model (e.g., without SES in the Motivation model), so too similar values may be used to compute an effect size measure called q^2 , which compares Q^2 predictive relevance values discussed above for models with and without a given latent construct. As this was described above for f^2 , it is not calculated here. See Hair et al. (2014: 194-197) for a worked example. The same low/medium/high cutoff criteria based on Cohen (1988) and discussed above are used to interpret q^2 .

Confirmatory tetrad analysis (CTA)

Overview

Tetrad analysis tests the null hypothesis that the indicators for a model are reflective. If this null hypothesis is rejected, the inference is that a formative model should be used. However, PLS-CTA is a data-driven approach and a finding in support of formative modeling is trumped if there are sound theoretical reasons for thinking that reflective modeling is more appropriate.

In PLS-CTA, the model under analysis must have at least 4 indicators per latent variable (construct). The current maximum in SmartPLS 3 is 25 indicators per construct.

“Tetrad” is a Greek word for “four”. CTA examines sets of four covariances simultaneously. Given variables g , h , i , and j , the value of a tetrad equals $c_{gh}c_{ij} - c_{gi}c_{hj}$, where c is the population covariance of the subscript variables. A tetrad is said to be “vanishing” when equal to 0. Bollen & Ting (1993) demonstrated how, in a proposed structural equation model, one might determine if any of the model-implied tetrads were vanishing ones.

Confirmatory Tetrad Analysis (CTA) seeks, under PLS-SEM, to follow Bollen and Ting’s (2000; see also Ting, 2000) confirmatory method of testing model-implied vanishing tetrads (hence PLS-CTA). This method was adapted by Gudergang, Ringle, Wende, & Will (2008), using SmartPLS software, based on earlier tetrad approaches developed by Bollen and others. These authors (Bollen & Ting, 2000; Gudergang et al., 2008: 1241) outline a five-step process:

1. Form and compute all vanishing tetrads for the measurement model of a latent variable.
2. Identify model-implied vanishing tetrads.
3. Eliminate redundant model-implied vanishing tetrads.
4. Perform a statistical significance test for each vanishing tetrad.
5. Evaluate the results for all model-implied non-redundant vanishing tetrads.

While CTA-PLS generally follows the same principles and procedures as CTA-SEM, there are some differences. Because PLS does not conform to distributional

assumptions required by conventional significance testing, tetrads must be tested using bootstrap methods.

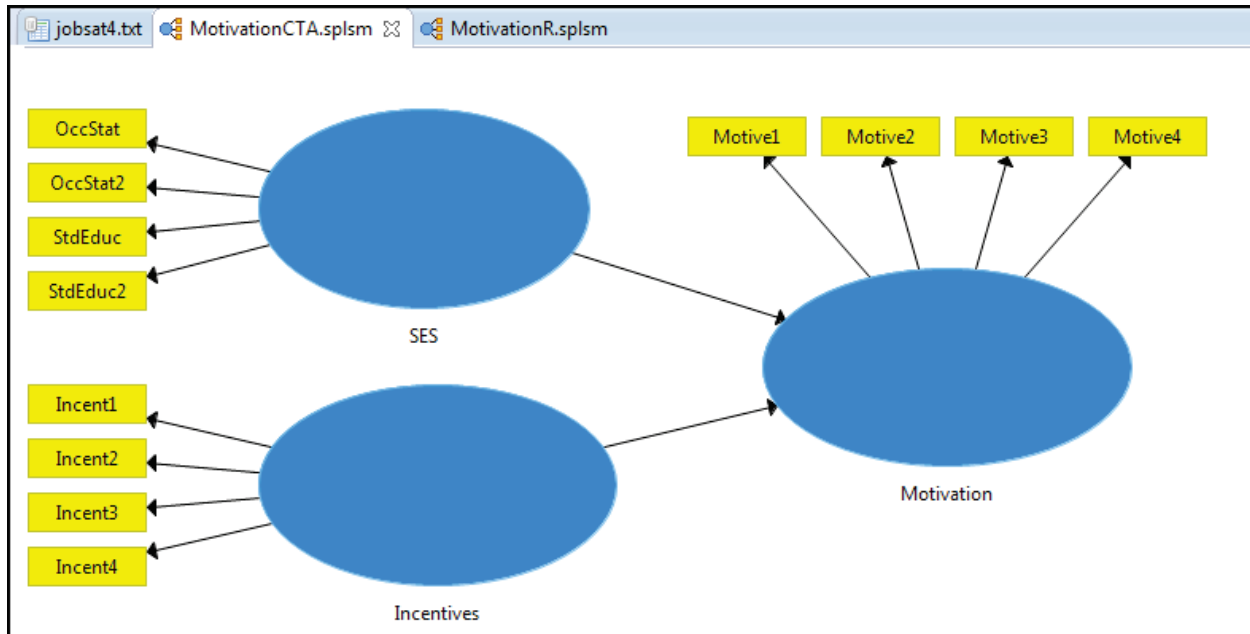
A vanishing tetrad exists when, for a set of four indicator variables, the difference between the product of the covariances of two of the variables and the product of the covariances of the other two variables in the set, yields 0. If the value of the tetrad is not significantly different from 0, then the tetrad is vanishing. However, rather than use the p value significance criterion, where significance corresponds to 0 not being within the unadjusted confidence limits, a bias correction is applied. Significance then corresponds to 0 not being within the bias-adjusted confidence limits and this is the operational test criterion.

To summarize the logic of tetrad analysis (page numbers are from Gundergan et al., 2008):

1. The null hypothesis is that a given tetrad evaluates to 0 (is vanishing) (p. 1241).
2. When a reflective model is tested, all model-implied non-redundant tetrads should vanish (p. 1239).
3. Compute and test the values of the tetrads.
4. A t-value above or below a critical value supports rejection of the null hypothesis (p. 1242), meaning that the tetrad value is significantly different from 0 and is not vanishing.
5. A t-value above or below a critical value corresponds to a significant p value ($p \leq .05$), also meaning the tetrad value is significantly different from 0 and is not vanishing.
6. Thus, when 0 is not within the bias-adjusted confidence limits, we fail to accept the null hypothesis. This usually but not always corresponds to $p \leq .05$.
7. Failure to accept the null hypotheses implies the model should be formative, not reflective.

The example model

Because PLS-CTA requires four or more indicators per construct, a new model was created as shown below, using the model-drawing methods described previously [above](#). A different dataset was also used, jobsat4.csv, with the indicator variables shown in the diagram below (see [above](#) to download).



Running confirmatory tetrad analysis

After selecting Calculate > Confirmatory Tetrad Analysis (CTA) from the SmartPLS menu, a dialog appears with two tabs. Although default settings are usually accepted, the two tabs are discussed in turn below.

1. Setup
2. Weighting

The screenshot shows the 'Setup' tab of the Confirmatory Tetrad Analysis (CTA) dialog box. The 'Weighting' tab is also visible but not selected. The 'Basic Settings' section includes the following options:

- Subsamples:** 500 (with up/down arrows)
- Processes:** 2 (with up/down arrows)
- Test Type:** One Tailed Two Tailed
- Significance Level:** 0.05

The “Weighting” tab is identical to that discussed in previous sections above and the same considerations apply. The reader is referred [above](#). The CTA example here accepts the default settings. In this CTA example, no weights are used.

The default settings for the “Setup” tab are shown in the figure above. There are four settings, all of which have been described for other procedures. The example accepts the default settings.

1. *Subsamples*: Bootstrapping, which uses multiple re-samples from the data, is used for purposes of significance testing in PLS-CTA. While the default is set to a relatively small number (500) to minimize computational time in the early stages of modeling, this should be reset to a much larger number (e.g., 5,000) for final analysis. The larger number of samples helps assure stable results.
2. *Processes*: This setting supports parallel processing. If the researcher’s computer has multiple processors, computation will be accelerated if the number of processors is specified. Do not attempt to specify a number higher than the actual number of processors on the researcher’s computer.
3. *Test Type*: The usual two-tailed significance tests are the default. See discussion [above](#).
4. *Significance Level*: The usual .05 significance level is the default cutoff for considering a result significant. See [above](#).

PLS-CTA output

PLS-CTA provides tetrad tests for the indicators for each latent construct in the original model, which was reflective. The constructs for this example were Incentives, SES, and Motivation. The table below has vanishing tetrad tests for each of these three latent constructs.

The operational decision criterion is to look at the two right-most columns in the table, which are the low and high bias-adjusted confidence limits. If 0 is not within these confidence limits, then the tetrad value is significantly different from 0, meaning that the tetrad is not vanishing. When this occurs, usually but not always the p value will be significant also ($p \leq .05$).

To uphold and retain the reflective model, ideally all non-redundant tetrads would be vanishing. This would be indicated by 0 being within the bias-adjusted confidence limits for all tetrads (and usually p also being non-significant). What if 0 is not within the bias-adjusted confidence limits but p is non-significant? This flags a marginal tetrad where bias correction was making a difference for inference. The actual decision rule, however, is governed by the bias-adjusted confidence limits, not the unadjusted p value.

For the data in this example, 0 is not within the bias-adjusted confidence limits in at least one vanishing tetrad test within each of the three latent constructs. In the example, each construct had four indicators. Four indicators yield six covariances, three tetrads, and two non-redundant tetrads. Therefore there are two vanishing tetrad tests per construct in the example output.

In a reflective model all tetrads should be vanishing, meaning that for all tests, 0 should be within the bias-corrected confidence limits. As that is not the case here, these data are better modeled formatively. Put another way, the measurement model (formative or reflective) should be selected whose assumptions are consistent with the results of the vanishing tetrads test. Here that is the formative model.

Final Results												
Incentives												
	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O /STERR)	P Values	Bias	CI Low	CI Up	Alpha adj.	z(1-alpha)	CI Low adj.	CI Up adj.
1:												
Incent1,Incent2,Incent3,Incent4	-72.6225	-72.1230	4.5394	15.9982	0.0000	0.4995	-81.0417	-63.2043	0.0250	2.2482	-82.3284	-61.9176
2:												
Incent1,Incent2,Incent4,Incent3	0.2877	0.2847	0.2839	1.0132	0.3114	-0.0029	-0.2731	0.8425	0.0250	2.2482	-0.3536	0.9230

Motivation												
	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O /STERR)	P Values	Bias	CI Low	CI Up	Alpha adj.	z(1-alpha)	CI Low adj.	CI Up adj.
1:												
Motive1,Motive2,Motive3,Motive4	-70.7761	-70.5775	5.2284	13.5367	0.0000	0.1986	-80.8500	-60.3051	0.0250	2.2482	-82.3320	-58.8231
2:												
Motive1,Motive2,Motive4,Motive3	-0.2554	-0.2675	0.2493	1.0248	0.3060	-0.0121	-0.7573	0.2222	0.0250	2.2482	-0.8279	0.2929

SES												
	Original Sample (O)	Sample Mean (M)	Standard Error (STERR)	T Statistics (O /STERR)	P Values	Bias	CI Low	CI Up	Alpha adj.	z(1-alpha)	CI Low adj.	CI Up adj.
1:												
OccStat,OccStat2,StdEduc,StdEduc2	32.9284	32.9027	3.3484	9.8342	0.0000	-0.0257	26.3242	39.4813	0.0250	2.2482	25.3751	40.4304
2:												
OccStat,OccStat2,StdEduc2,StdEduc	33.4357	33.4073	3.2934	10.1522	0.0000	-0.0284	26.9366	39.8779	0.0250	2.2482	26.0030	40.8115

Naturally, since the data and model are different for this PLS-CTA section compared to sections on other PLS algorithms, inferences derived here do not apply to other sections.

PLS-CTA and sample size

Like all significance tests, differences from the null hypothesis (here differences of tetrad values from 0) are more likely to be found significant as sample size becomes larger. As sample size becomes extremely large, eventually all differences are significant and for PLS-CTA, the researcher will always reject the reflective model.

When PLS-CTA rejects the reflective model in favor of a formative one, the researcher must ask if this is an artifact of large sample size. Partly the researcher can “eyeball” how close the lower and upper bias-adjusted confidence limits are to the 0 point. However, this author recommends the simple exploratory approach of running the analysis again for a moderate size (e.g., $n = 200$) random sample of the original data.

With a smaller sample, the researcher will find that t values in the “T Statistics” column will diminish and the likelihood of 0 being within the lower and upper bias-adjusted confidence limits will increase. If the researcher finds that 0 is now within these confidence limits for all tetrad tests, the full-sample rejection of the reflective model is an artifact of sample size and retaining the reflective model is upheld. This random subsample strategy was undertaken for the example data and although t values did diminish they did not diminish enough for 0 to be within the limits and the substantive interpretation remained the same. That is, the full-data finding that a formative model was appropriate remained upheld and the counter-hypothesis that this finding was an artifact of large sample size was rejected.

Importance-performance map analysis (IPMA)

Overview

Importance-performance map analysis (IPMA), also called importance-performance matrix analysis, adds no information about the researcher’s model apart from that already contained in the model’s path coefficients. However,

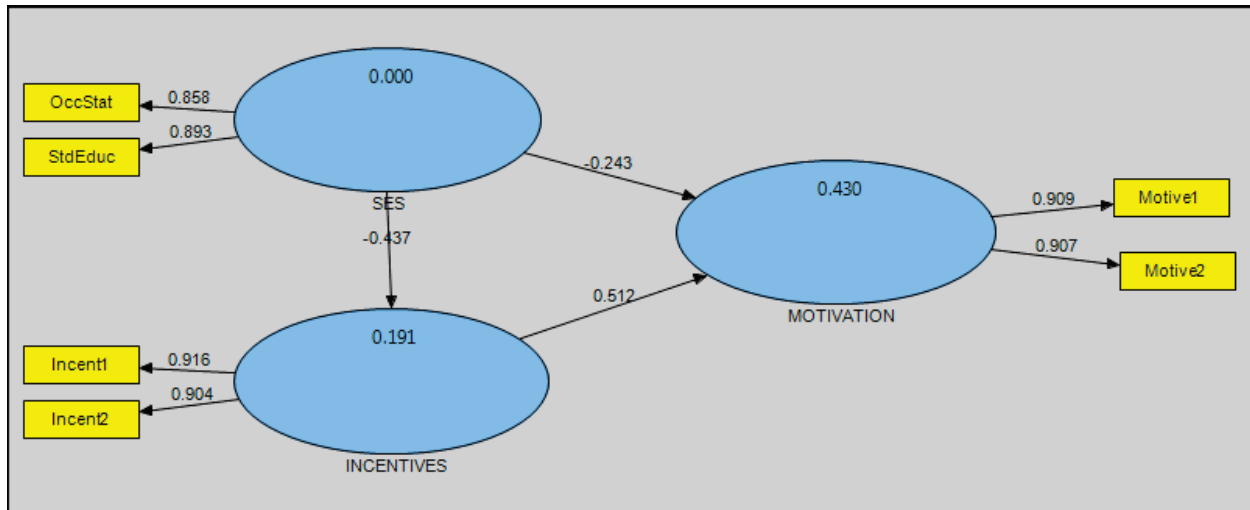
IPMA is a different way of presenting path information and this may prove insightful to the researcher. IPMA output is directed at determination of the relative importance of constructs (latent variables) in the PLS model.

As discussed [below](#), two dimensions are highlighted by IPMA analysis. Importance reflects the absolute total effect on the final endogenous variable in the path diagram (or other selected construct of interest). Performance reflects the size of latent variable scores.

SmartPLS 3 online help observes, “conclusions can be drawn on two dimensions (i.e., both importance and performance), which is particularly important in order to prioritize managerial actions. Consequently, it is preferable to primarily focus on improving the performance of those constructs that exhibit a large importance regarding their explanation of a certain target construct but, at the same time, have a relatively low performance.”

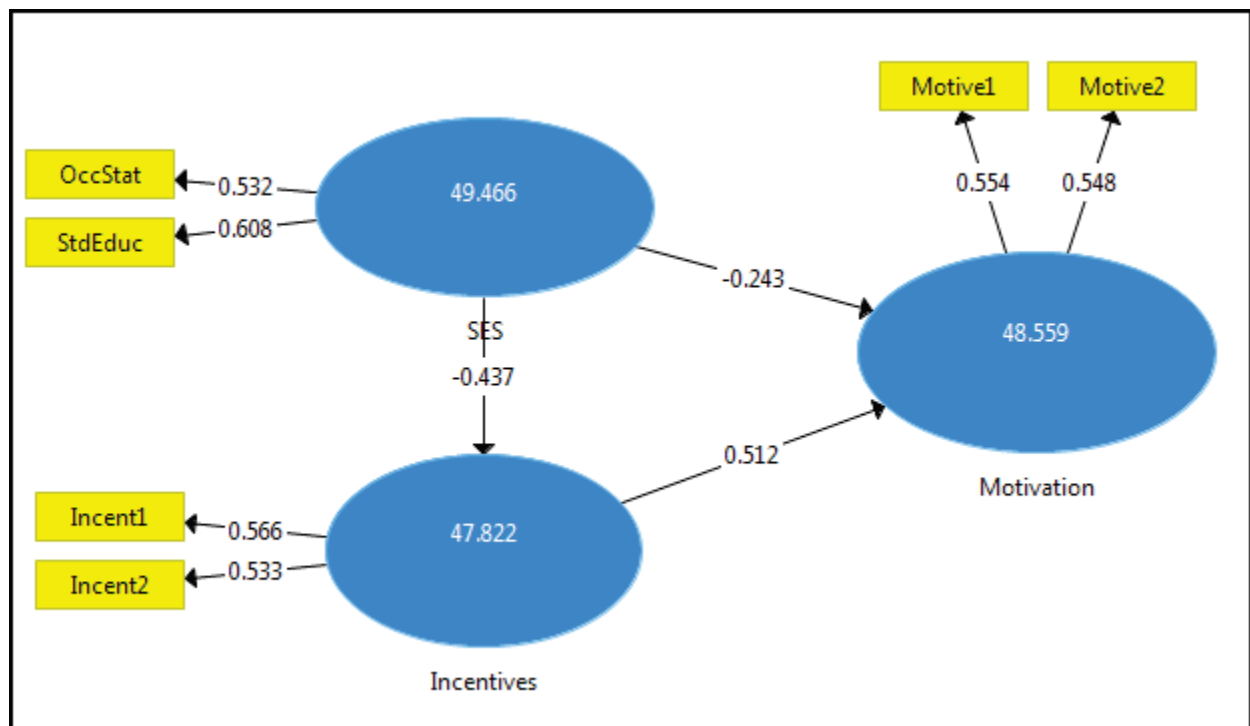
The example model

For purposes of illustration of IPMA, we adapt the previously-discussed “Motivation” model to become the “Motivation2” model by adding an arrow from SES to Incentives. (If the reader is following along, make sure the dataset is set to the original jobsat.csv). The figure below shows the Motivation model and resulting standardized structural path coefficients (inner model loadings) for the default PLS algorithm model. This is the same model as discussed [above](#) with regard to partitioning total effects. However, corresponding output for the IPMA algorithm may appear different because by default, the IPMA module displays different coefficients.



The PLS algorithm model above displays path coefficients connecting the latent constructs, the outer model paths are outer loadings, and the values inside the blue constructs are R^2 coefficients.

The IPMA algorithm model below also displays path coefficients connecting the latent constructs but the outer model paths are outer weights and the values inside the blue constructs are LV (latent variable) performance coefficients. In spite of the different appearance, the PLS and IPMA analyses are the same model for the same data. (On weights vs. loadings, see [above](#)).



Running IPMA

After selecting Calculate > Importance Performance Map Analysis (IPMA) from the SmartPLS menu, a dialog appears with three tabs. Although default settings are usually accepted, these tabs are discussed below.

1. Setup
2. Partial Least Squares
3. Weighting

The “Weighting” tab is identical to that discussed in previous sections [above](#) as is the “Partial Least Squares” tab, also discussed in a section [above](#). The CTA example here accepts the default settings under these tabs, including not using weights.

Basic Settings

Latent Variable: Motivation

PLS-IPMA Results: All Exogenous LVs
 Direct LV Predecessors

Ranges

Manifest Variable	Latent Variable	Min	Max
Incent1	Incentives	-7.414...	15.634...
Incent2	Incentives	-6.677...	13.634...
Motive1	Motivation	-7.906...	15.078...
Motive2	Motivation	-6.355...	13.553...
OccStat	SES	14.140...	28.076...
StdEduc	SES	-6.227...	12.762...

Min: / Max: / Apply to All [Reset](#)

In the IPMA setup tab there are settings for latent variable, results, and ranges.

- *Latent Variable:* Select the latent variable of interest. Here it is Motivation, which is the final endogenous variable in the model.
- *PLS-IPMA Results:* The default “All Exogenous LVs “ selection causes the importance-performance map to include all model constructs whose paths directly or indirectly lead to the latent variable of interest in the path sequence. The alternative “ Direct LV Predecessors” selection includes only model constructs which are direct predecessor constructs for the target construct of interest.
- *Ranges:* IPMA results include performance scores on a 0 – 100 scale. To correctly re-scale to a 0 – 100 basis, it is essential that the scales of the indicator (manifest) variables be input correctly. SmartPLS searches the dataset and finds minimum and maximum observed values which it assumes constitutes the range. However, this assumption may be incorrect. For instance, data may be Likert items on a 1 – 7 scale, yet the actual dataset may have values of only 3 -7. In such a case, the researcher must enter the correct actual range (1 – 7). Directionality of all variables should be the same: for all variables, the high value of the range must represent “better” or “more”. Failure to enter correct ranges will yield incorrect performance scores. Changes to provisional ranges scores are made simply by clicking on the computed value and entering another. Alternatively, minimum and maximum values may be entered at the bottom and applied to all variables.

In the example, the ranges of the Incent and Motive variables are 0 – 20; for OccStat the range is 0 – 100; the StdEduc range does not need to be reset. The changes are reflected in the figure below.

Basic Settings

Latent Variable

PLS-IPMA Results All Exogenous LVs
 Direct LV Predecessors

Ranges

Manifest Variable	Latent Variable	Min	Max
Incent1	Incentives	0.0	20.0
Incent2	Incentives	0.0	20.0
Motive1	Motivation	0.0	20.0
Motive2	Motivation	0.0	20.0
OccStat	SES	0.0	100.0
StdEduc	SES	-6.227...	12.762...

Min: / Max: / [Reset](#)

Click the “Start Calculation” button in the lower right when all settings are complete.

Overview

FIMIX-PLS (finite mixture PLS) is required when the data are not homogenous but require segmentation into groups as part of analysis (see Hahn, Johnson, Herrmann, & Huber, 2002; Ringle, Wende, & Will, 2010; Ringle, Sarstedt, & Mooi, 2010; Sarstedt, Becker, Ringle, & Schwaiger, 2011). Put another way, FIMIX is needed when unobserved heterogeneity is suspected, discussed [below](#). Failure to employ FIMIX when needed may well lead to substantive errors of interpretation of results.

FIMIX-PLS segments observations based on heterogeneity in the inner path model. As such, FIMIX-PLS can be employed to evaluate aggregate models, such as ones based on the standard procedure, to assure that aggregate results are not

influenced by unobserved heterogeneity in the inner path model estimates. See further discussion and illustration [below](#), in the section on multigroup PLS.

IPMA Output

LV index values

LV index values are the mean of the unstandardized latent variable scores. These are used, as described below, to compute performance values. Note that this, here in the IPMA module, is where in SmartPLS 3 you may obtain unstandardized latent variable scores.

LV Index Values	
	LV Index Values
Incentives	3.312
Motivation	3.304
SES	13.203

Performance values

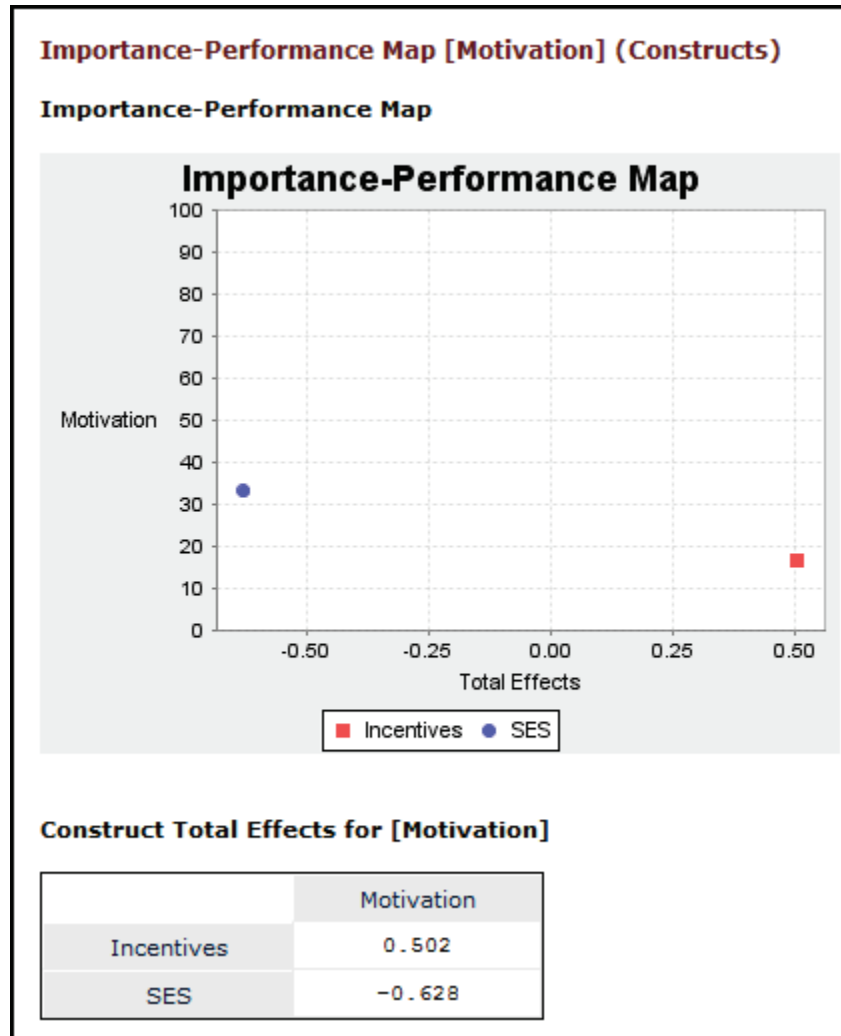
After norming to 0 – 100, the mean of the transformed latent variable scores are the performance values. Results are shown below for the Motivation model:

LV Performances	
	LV Performances
Incentives	16.558
Motivation	16.522
SES	33.030

“Importance” refers to total effects of the model, based on standardized structural (inner model) path coefficients. Total effects (and hence “Importance”) for the Motivation model is listed for the total effects of exogenous variables on the endogenous dependent variable, here the Motivation construct.

The importance-performance map

While very simple for the present case of two predictor latent variables, the graph importance-performance map becomes increasingly helpful as additional latent variables make the model more complex.



“Importance”: Measured on the X axis, a construct is more important if it has a higher absolute total effect on the construct of interest. Though in a negative direction, SES here has somewhat greater absolute importance than does INCENTIVES.

“Performance”: Measured on the Y axis, a construct has greater performance if it has higher mean latent variable scores, reflecting stronger measurement paths. Here, SES displays greater performance. Performance values are those from the “LV Performances” table [above](#).

The values in the map are also output as tables. (In SmartPLS 2, the two tables were combined in a single matrix, hence “importance-performance matrix analysis”).

Construct Total Effects for [Motivation]	
	Motivation
Incentives	0.502
SES	-0.628

Construct Performances for [Motivation]	
	Performances
Incentives	16.558
SES	33.030

For further reading, SmartPLS 3 online help recommends Hair et al. (2014) for detailed explanation of IPMA; for applications of IPMA, see Höck et al. (2010), Völckner et al. (2010) Rigdon et al. (2011), and Schloderer et al. (2014).

Finite-mixture segmentation analysis (FIMIX)

Unobserved heterogeneity

Unobserved heterogeneity means that there are one or more variables or constructs not included in the model but which account for differences in estimated coefficients. The researcher may well not even know what these unobserved variables are, much less have data for them. If unobserved variables are important, groups (subsets of data) may need to differ in PLS coefficients computed for them. That is, the model may need to differ between groups and the coefficients computed by the traditional PLS algorithm may reflect “bad

averages” across unlike groups. This in turn will lead to both Type I and Type II errors of inference.

The presence of unobserved heterogeneity may be rejected and the traditional whole-sample PLS solution may be pursued if (1) average variance explained in multi-segment models is lower than for the traditional PLS solution; and (2) PLS-FIMIX model-selection criteria for the one-segment solution shows better fit than for multi-segment solutions, for which fit deteriorates markedly (Becker et al., 2013: 686).

Under FIMIX, the researcher specifies the number of groups in advance. The general strategy of the FIMIX algorithm is to partition the dataset optimally into the given number of groups and compute separate coefficients for each group. FIMIX assigns cases to groups in a manner which optimizes the likelihood function, thereby maximizing segment-specific explained variance. The use of a maximum likelihood method, it should be noted, requires the assumption that the endogenous latent constructs have a multivariate normal distribution. That is, FIMIX-PLS is a parametric form of PLS, which in its traditional form is non-parametric.

Though further below, output is shown for the three-group solution, the strategy calls for the researcher to explore many solutions (e.g., the two-group through the ten-group solutions). Goodness-of-fit measures discussed below can be used to identify which solution is best. Since this is a data-driven strategy, the researcher also must be careful to assure that the best-solution groups make sense and have a theoretical rationale.

As with any data-driven procedure, there is the possibility that FIMIX-identified groups may reflect noise in the data, not true underlying segmentation of the dataset by unobserved variables. For this reason it is desirable to develop the model with one set of data (e.g., the even numbered cases) and validate it with another set (e.g., the odd numbered cases). Cross-validation using a hold-out validation sample is described by Becker et al. (2013: 687-688).

In summary, interpretation of PLS-SEM estimates based on the default aggregate estimation method may involve substantive error if the data are segmented such that it would be better if separate structural path models were created for each segment. If the segments are observed groups and parametric tests may be

applied, then parametric multigroup analysis may be applied, discussed [below](#). However, often there is unobserved heterogeneity – “unobserved” because the researcher does not know a priori what the groups are. As unobserved heterogeneity can bias results of default PLS, some authors recommend routine use of FIMIX-PLS to detect possible unobserved heterogeneity. Other approaches are possible, noted [below](#).

If successful in statistical and theoretical terms, finite mixture analysis serves to segment observations into groups which may be subject to different analyses, policies, marketing strategies, etc., according to the context. As such PLS-FIMIX is an alternative to cluster analysis, which also may be used to identify groups in the face of unobserved heterogeneity. See the separate Statistical Associates’ “Blue Book” volume on “Cluster Analysis.”

Comparing models with differing numbers of segments

To run a FIMIX analysis, select “Finite Mixture (FIMIX) Segmentation” from the “Calculate” button drop-down menu. The “Finite Mixture (FIMIX) Segmentation” window appears, shown below opened to the first of two tabs: Setup.

Finite Mixture (FIMIX) Segmentation

Finite mixture partial least squares (FIMIX-PLS) segmentation is a method to uncover heterogeneity by estimating the probabilities of segment memberships for coefficients for all segments.

Setup
Partial Least Squares

Basic Settings

Number of Segments

Maximum Iterations

Stop Criterion ->

Advanced Settings

Use Unstandardized Latent Variable Scores?

Estimate Regression Intercept?

Repetitions

FIMIX-PLS can be executed several times and selects the solution with the best LnL value to avoid local optima.

Number of Repetitions

The second tab, “Partial Least Squares”, provides weighting and other options for the PLS algorithm. As this was discussed [above](#), it is not discussed or illustrated here.

Since the number of segments typically is not known, the researcher must run FIMIX-PLS for 2, 3, and more segments (Ringle recommends 2 to 10; Ringle, 2006: 5). Moreover, due to random aspects of the PLS-FIMIX algorithm, for any specified number of segments, different fit values will be generated for each run. Therefore, the researcher should conduct multiple runs for each segment size, then use the mean fit values (e.g., mean AIC) when comparing numbers of segments to identify the optimal number.

After multiple runs, information theory goodness-of-fit measures are then used to select the model with the optimal number of segments. Sarstedt, Becker, Ringle,

& Schwaiger (2011: 52), based on systematic computational simulation methods and looking at 18 alternative model selection criteria, concluded that when modified AIC_3 (a variant of AIC, the Akaike Information Criterion) and CAIC (Consistent AIC) used in tandem provided the best classification performance. These authors write (p. 45), “whenever AIC_3 and CAIC indicate the same number of segments, this result meets the correct number of segments in 84% of all cases. Alternatively, a joint consideration of AIC_3 and BIC appears promising, because this combination yields the true number of segments in 82% of all cases where both criteria.”

Note that in an earlier article, Sarstedt & Ringle (2010: 1303) recommended use of CAIC as a criterion for identifying the optimal number of segments. However, reconsideration in the Sarstedt, Becker, Ringle, & Schwaiger (2011) article, based on simulation, revised this recommendation as described above. CAIC alone was found to underfit the model.

AIC_3 and CAIC values are output by default for each FIMIX-PLS run, as in the table below. As discussed above, using AIC_3 and CAIC jointly is recommended. The coefficients lack an easily-expressible intrinsic meaning. Instead they are used in model comparisons, with lower being better fit.

Example PLS-FIMIX output for one of the runs for number of segments = 3. is shown below. A variety of fit indices are output in addition to the commonly used AIC, AIC_3 , CAIC, and BIC criteria. Sarstedt et al. (2011: 44), based on their simulation study of classification performance, noted that apart from AIC_3 and CAIC as discussed above, “All other criteria (AIC, AIC_c , MDL_5 , lnL_c , NEC, ICL-BIC, AWE, CLC, and EN) exhibit very unsatisfactory success rates of 28% and lower. AIC achieved the worst performance of only 6%.”

The output below is for SmartPLS 3.2.1. Starting with version 3.2.2, SmartPLS will output a shorter list of fit and segment separability coefficients as discussed in the section which follows.

Fit Indices	
Akaike's Information Criterion - AIC	8,706.691
Bayesian Information Criteria - BIC	8,788.926
Consistent AIC - CAIC	8,805.926
Modified AIC (Factor 3) - AIC_(3)	8,723.691
Minimum Description Length (Factor 2) - MDL_(2)	8,905.160
Minimum Description Length (Factor 5) - MDL_(5)	9,253.864
Hannan Quinn Criterion - HQ	8,738.052
Entropy Statistic (Normed) - EN	0.119
Classified Likelihood Criterion - CLC	10,477.466
Integrated Completed Likelihood BIC - ICL-BIC	10,593.701
LnL	-4,336.345
E	902.388
PC	0.422
PE	0.968
NPE	0.971
NFI	0.134
C	10,477.466
LnL_C	-5,238.740
AWE	10,709.949
LP	577.865

In summary, let K be the number of proposed segments. After running FIMIX-PLS for $K = 2$ to 10, the optimal number of segments is the one with the lowest modified AIC_3 and CAIC which also has entropy of .5 or higher (entropy is discussed). below There may be no optimal solution since entropy may be low for all solutions, indicating lack of separation will undermine interpretation of segments. If segments cannot be interpreted due to low separation, indicated by low entropy, the researcher may prefer to revert to the global model using the default PLS algorithm.

Fit Indices

SmartPLS 3 now outputs a large number of fit indices in its FIMIX module. Each is discussed briefly below.

Akaike Information Criterion – AIC

AIC is a goodness-of-fit measure which adjusts model chi-square (minus 2 log likelihood) to penalize for model complexity (that is, for lack of parsimony and over-parameterization). Model chi-square is a likelihood measure and AIC is a penalized likelihood measure Model complexity is defined in terms of degrees of freedom, with higher being greater complexity. As sample size decreases, the penalty for model complexity decreases slightly. AIC will go up (higher is worse fit) approximately 2 for each parameter/arrow added to the model, penalizing for model complexity and lack of parsimony.

AIC may be used to compare models with different numbers of latent variables, not just nested models with the same latent variables but fewer arrows. That is, unlike model chi-square, AIC may be used to compare non-hierarchical as well as hierarchical (nested) models based on the same dataset, whereas model chi-square difference is used only for the nested models.

AIC is computed as $-2 \cdot \ln L + 2 \cdot N_s$, where $\ln L$ is the log-likelihood and N_s is the number of parameters for a model with S segments.

The absolute value of AIC has no intuitive value, except by comparison with another AIC, in which case the lower AIC reflects the better-fitting model.

AIC close to zero reflects good fit. It is possible to obtain AIC values < 0 . In model development, the researcher stops modifying when AIC starts rising. See Akaike (1973, 1978).

Bayesian Information Criteria – BIC

BIC is also known as Akaike's Bayesian Information Criterion (ABIC) or the Schwarz Bayesian Criterion (SBC, SBIC). *BIC* penalizes for sample size as well as model complexity. That is, as sample size increases, the *BIC* penalty increases. Compared to AIC, *BIC* more strongly favors parsimonious models with fewer parameters. In general, *BIC* has a conservative bias tending toward Type II error (thinking there is poor model fit when the relationship is real). *BIC* may be recommended when sample size is large or the number of parameters in the model is small.

BIC is computed as $-2 \cdot \ln L + \ln(N) \cdot N_s$, where $\ln L$ is the log likelihood, N is sample size, and N_s is the number of parameters in a model with S segments.

BIC is an approximation to the log of a Bayes factor for the model of interest compared to the saturated model. *BIC* came into widespread use in sociology after it was popularized by Raftery (1995) in the 1980s. Later, however, the limitations of *BIC* emerged in the literature. See Winship, ed. (1999), on controversies surrounding *BIC*. *BIC* uses sample size n to estimate the amount of information associated with a given dataset. A model based on a large n but which has little variance in its variables and/or highly collinear independents may yield misleading model fit using *BIC*. See Schwarz (1978).

Consistent AIC – CAIC

CAIC penalizes for sample size as well as model complexity (lack of parsimony). The penalty is greater than AIC but less than *BIC*. As with AIC, the lower the *CAIC* measure, the better the fit.

Modified AIC (Factor 3) – AIC₃

Modified AIC 3 was developed by Bozdogan (1994) as a version of AIC with a stronger penalty for lack of parsimony/overfitting. It penalizes by three times the number of parameters rather than by AIC's two. It is computed

as $-2 \cdot \ln L + 3 \cdot N_s$, where $\ln L$ is the log-likelihood and N_s is the number of parameters for a model with S segments.

Modified AIC (Factor 4) – AIC₄

This fit criterion will be output starting with SmartPLS 3.2.2. It adds a stronger penalty of $4 \cdot N_s$ rather than $3 \cdot N_s$.

Minimum Description Length (Factor 2) - MDL₍₂₎

MDL 3 is computed as $-2 \cdot \ln L + 3 \cdot \ln(N) - N_s$, where $\ln L$ is the log-likelihood, N is sample size, and N_s is the number of parameters for a model with S segments. See Liang, Jaszczak, & Coleman (1992). This coefficient will no longer be output starting with SmartPLS 3.2.2.

Minimum Description Length (Factor 5) - MDL₍₅₎

MDL 5 is computed as $-2 \cdot \ln L + 5 \cdot \ln(N) - N_s$, where $\ln L$ is the log-likelihood, N is sample size, and N_s is the number of parameters for a model with S segments. See Liang, Jaszczak, & Coleman (1992).

Hannan Quinn Criterion - HQ

HQ is intended to correct BIC for small samples. It does this by employing a stronger penalty term. For larger samples, HQ can be seen as a compromise between AIC's relative leniency toward adding parameters to the model and BIC's relative harshness.

Entropy Statistic (Normed) - EN

Entropy is discussed in the following section, [below](#).

Classified Likelihood Criterion - CLC

Like EN, CLC is used to gauge the separation of segments in FIMIX, but it incorporates log-likelihood fit criteria as part of its algorithm. See Biernacki and Govaert (1997); Wedel & Kamakura (2000). This coefficient will no longer be output starting with SmartPLS 3.2.2.

Integrated Completed Likelihood BIC - ICL-BIC

The integrated completed likelihood BIC is an alternative to CLC. Its algorithm also tries to balance entropy-based segmentation criteria with

BIC-based fit criteria. See Biernacki, Celeux, & Govaert, 2000. This coefficient will no longer be output starting with SmartPLS 3.2.2.

LnL

This is the log-likelihood value for the model. Minus 2 times this value is the model chi-square value. It is a measure of model error, with lower being better fit. However, it is mainly used as the basis for other measures, which adjust for model parsimony/overfitting. This coefficient will no longer be output starting with SmartPLS 3.2.2.

PC

PC is the partition coefficient, an alternative to normalized entropy when classifying observations into segments. Let p_{is} be the a-posteriori probability of observation i belonging to segment s , then $PC = p_{is}^2$ summed from 1 to N and cumulated for each segment, times the natural log of p_{is} . See Bezdek (1981). This coefficient will no longer be output starting with SmartPLS 3.2.2.

$PC = \sum_1 \sum_2 p_{is}^2 / N$, where p_{is}^2 is the squared a posteriori probability, N is sample size, S is the number of segments, the first summation is from $i=1$ to N , and the second summation is from $s = 1$ to S .

PE

PE is partition entropy, another alternative to normalized entropy when classifying observations into segments. See Bezdek (1981).

$PE = [\sum_1 \sum_2 p_{is} * \ln p_{is}] / N$, where p_{is} is the a posteriori probability, N is sample size, S is the number of segments, the first summation is from $i=1$ to N , and the second summation is from $s = 1$ to S . This coefficient will no longer be output starting with SmartPLS 3.2.2.

NFI

This is the non-fuzzy index developed by Roubens (1978). Its formula incorporates a-posteriori probabilities of an observation belonging to a particular segment. The somewhat complex formula is given in Sarstedt et al., 2011: 54. Not to be confused with the normed fit index (also NFI) used in covariance-based structural equation modeling.

LnL_C

Also labeled $\ln L_c$, this is the complete log-likelihood statistic, developed by Dempster, Laird, & Rubin (1977). This coefficient will no longer be output starting with SmartPLS 3.2.2.

AWE

AWE is the approximate weight of evidence criterion originated by Banfield & Raftery (1993).

$AWE = -2\ln L_c + 2N_s * [1.5 + \ln(N)]$. where N is sample size, S is the number of segments, N_s is the number of parameters required for a model with S segments, and $\ln L_c$ is the complete log-likelihood statistic. On $\ln L_c$, see Dempster, Laird, and Rubin (1977); Sarstedt et al. 2011: 54. This coefficient will no longer be output starting with SmartPLS 3.2.2.

E, *NPE*, *C*, and *LP* will no longer be output starting with SmartPLS 3.2.2.

There are, of course, yet other fit measures. Perhaps the most commonly cited one in the literature is GoF goodness of fit. PLS 3 does not output this for FIMIX, noting on its [website](#) that “Goodness of Fit (GoF) has been developed as an overall measure of model fit for PLS-SEM. However, as the GoF cannot reliably distinguish valid from invalid models and since its applicability is limited to certain model setups, researchers should avoid its use as a goodness of fit measure. The GoF may be useful for a PLS multi-group analysis (PLS-MGA).”

Moreover, because of its nonparametric basis, PLS is inappropriate for calculating fit measures such as found in covariance-based SEM (e.g., not CFI, RFI, NFI [normed fit index], IFI, or RMSEA). Fit measures common to PLS and covariance-based SEM include those based on information theory, such as AIC, BIC, and their variants.

Entropy

EN is the normed entropy criterion (Ramaswamy, DeSarbo, & Reibstein, 1993). Shown as "EN" in the output above, entropy is a measure of separation of segments, with 1.0 indication total separation (all observations have a 1.0 probability of being in a particular segment and a 0.0 probability of being in any

other segment). The above-mentioned simulation experiments by Sarstedt and his associates cast doubt on whether use of this measure adds utility in determining the optimal number of segments, beyond the use of AIC_3 and CAIC. However, entropy is useful as an indicator of the likelihood that the segments will be clearly defined and interpretable.

Ringle (2006: 6) suggests that entropy must be $\geq .5$ for unambiguous segmentation, not the case here for number of segments = 3 since $N = .119$. If path coefficients differ significantly across segments but the segments are not interpretable, the researcher ordinarily will prefer the default global PLS solution. For computation of entropy (EN) and further discussion, see Ramaswamy, Desarbo, Reibstein, & Robinson (1993). A normalized version of the entropy criterion is also available – NEC, the normalized entropy criterion (see Celeux & Soromenho, 1996).

Starting with SmartPLS 3.2.2, SmartPLS offered only three coefficients used for segment separability: EN, NEC, and NFI (non-fuzzy index, discussed in the previous section. The formulas for EN and NEC are shown below (Sarstedt, ecker, Ringle, & Schwaiger, 2011: 54).

- *EN (Entropy criterion, a.k.a. normed entropy criterion)*

$$EN = 1 - [\sum_1 \sum_2 p_{is} * \ln(p_{is})] / [N * \ln(S)]$$

Where p_{is} is the a-posteriori probability of observation i belonging to segment s and S is the number of segments. Let N be sample size. The first summation is from $i=1$ to N , and the second summation is from $s = 1$ to S . See Ramaswamy, DeSarbo, & Reibstein (1993).

$E(S)$ is the estimated entropy for a model with S segments.

$$E(S) = [\sum_1 \sum_2 p_{is} * \ln(p_{is})]$$

- *NEC (Normalized entropy criterion)*

$$NEC = E(S) / [\ln(S) - \ln(1)]$$

Where notation is as for EN but $\ln(S)$ is the log likelihood for a model with S segments and $\ln(1)$ is the log likelihood for a model with 1 segment.

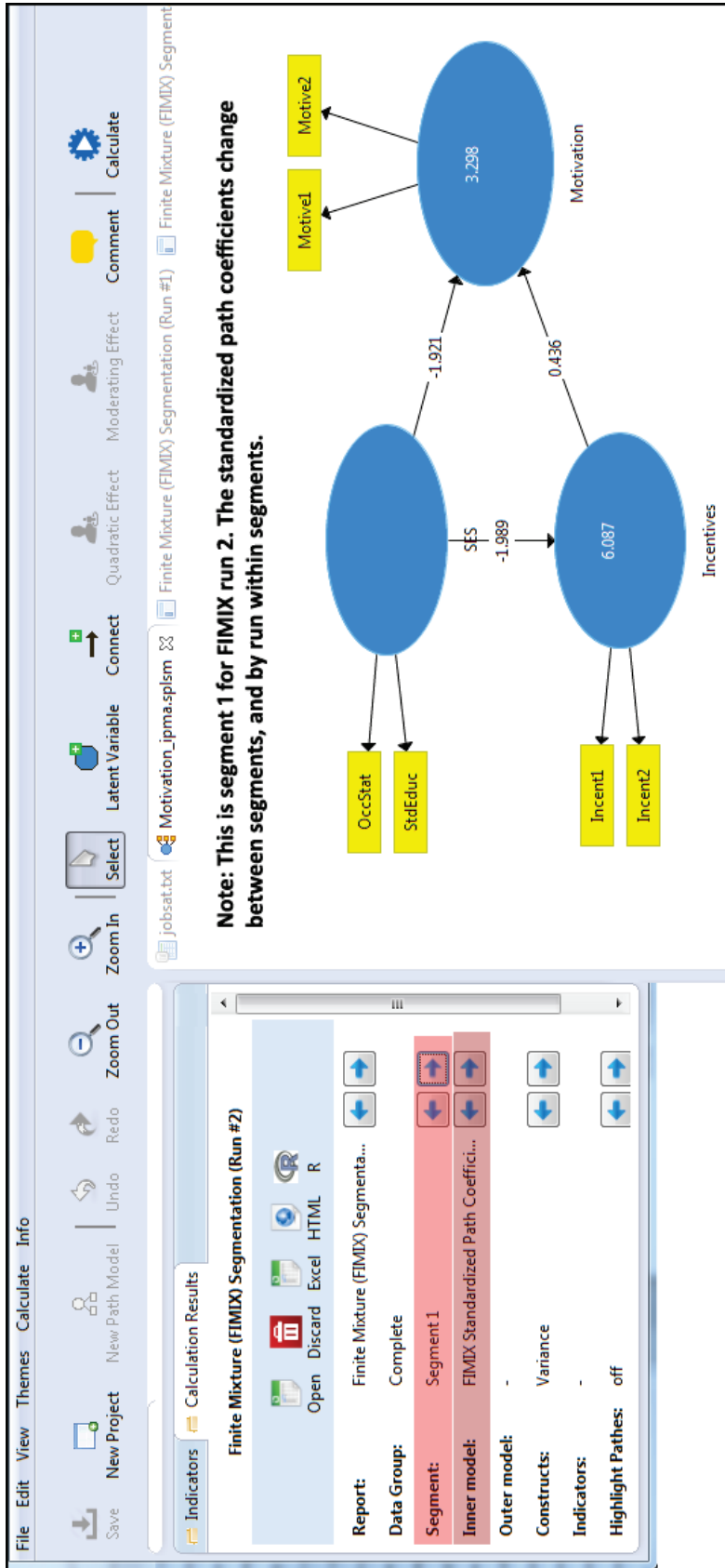
Celeux & Soromenho (1996: 203) choose S clusters if $NEC(S) < NEC(1)$; otherwise they declare no clustering structure in the data. NEC is a

parametric coefficient which assumes a Gaussian/normal distribution (which includes but is not limited to standard normal distributions where the mean is 0 and the variance is 1). They write, “our 'ad hoc' procedure to test $K = 1$ versus $K > 1$ is not theoretically based and can only be applied for Gaussian mixtures” (p. 210).

Path coefficients

Path coefficients may be displayed in standardized or unstandardized form. Using the arrow-buttons highlighted on the left in the figure below, the user may toggle among segments (here there three were requested). Path coefficients will change for each segment, reflecting somewhat different models for each segment of the population. Since coefficients will vary across runs for the same segment, the researcher may wish to average path coefficients across runs for the same segment.

In the figure below, output is shown in standardized form for segment 1, run 2. Output is not shown for other segments and runs.



The Report menu selection will also display the same coefficients in table form, shown below.

FIMIX Standardized Path Coefficients			
Segment 1			
	Incentives	Motivation	SES
Incentives		0.436	
Motivation			
SES	-1.989	-1.921	
Segment 2			
	Incentives	Motivation	SES
Incentives		0.651	
Motivation			
SES	-1.658	-0.446	
Segment 3			
	Incentives	Motivation	SES
Incentives		0.415	
Motivation			
SES	-1.659	-0.126	

- If the path coefficient differences between segments are significant and if entropy suggests the segments are interpretable, this indicates the need for different models for different groups. The researcher will report mean FIMIX path results for the optimal number of segments as determined usually using AIC₃ and CAIC as described previously.
- If the path coefficient differences are not significant and entropy is below .5, the researcher concludes that unobserved heterogeneity is not a problem and the ordinary global PLS algorithm is applied.
- If the path coefficients differ significantly but the entropy is below .5, as for the results above, unobserved heterogeneity may be affecting results but

given the variables measured in the model, the nature of the segments involved with unobserved heterogeneity is very likely to be uninterpretable. Many researchers would revert to the ordinary global PLS solution simply on the basis of low entropy. However, this situation may reflect the need for model respecification. Alternatively, if applying FIMIX to a validation dataset results in segmentation with significantly different case membership, the researcher may conclude that the segments identified by FIMIX reflect arbitrary noise in the data and the researcher may report the results of the ordinary global PLS algorithm.

T-tests of differences in path coefficients

Independent samples t-tests may be used to test the significance of differences in path coefficients between segments or between those of a segment from FIMIX-PLS and the aggregate solution using the default PLS algorithm. See Keil et al. (2000).

Testing differences may be required when considering whether to collapse a small segment into a larger one. Too-small segments may mean that the researcher has requested too many segments in the solution. Alternatively, if the number of segments is optimal but a segment is too small, it may be collapsed into other segments from which is it not significantly different (Becker et al., 2013: 686). The significance of differences between segment may be tested in multi-group analysis, as discussed [below](#), though significance testing introduces parametric assumptions (which FIMIX has anyway, by virtues of maximum likelihood methods).

Labeling the segments

PLS outputs a table of segment proportions of the sample, illustrated below. Very small segment sizes may indicate too many segments have been requested and also that all segments may not be interpretable. Here all segments are greater than 10% of the sample.

Segment Sizes			
	Segment 1	Segment 2	Segment 3
%	0.481	0.252	0.267

After selecting the optimal number of segments based on model fit measures, and after finding sufficient likely interpretability of segments using entropy, classification measures, and segment proportions, the researcher arrives at different path models for each segment. But what groups do the segments represent?

Labels for the segments must be inferred from the membership of observations in each segment. The final partition by observation table, shown below for the first 10 observations in the three-segment solution, is default output for FIMIX-PLS. Segment memberships are probabilistic and below the highest probability for each observation is shown in color (added, not part of PLS output).

Ideally, any given observation would load heavily on one and only one segment. In simple segment structure, ideally each observation would have a loading of .7 higher on just one segment, with other loadings for that observation being .30 or lower. If simple segment structure existed, segments would be easy to interpret. Conversely, the more all loadings for an observation are mid-range, the less easy is interpretation of segments. Simple segment structure is an ideal, rarely attained. Below, only observation 5 meets this ideal.

Final Partition

	Segment 1	Segment 2	Segment 3
1	0.322	0.312	0.366
2	0.598	0.192	0.210
3	0.461	0.366	0.173
4	0.503	0.313	0.185
5	0.240	0.703	0.057
6	0.505	0.214	0.281
7	0.132	0.382	0.485
8	0.595	0.148	0.257
9	0.493	0.375	0.132
10	0.108	0.259	0.633

It may be possible to infer labels for segments based on highest loading, which for the output above would group observations in segment 1 (cases 2, 3, 4, 6, 8, and 9), segment 2 (case 5), and segment 3 (cases 1, 7, and 10).

Alternatively, the researcher may find it simpler to base labeling on very highly loaded observations. Ringle (2006: 5) suggests concentrating on observations loaded at the .8 level or higher. Low [entropy](#), as for the example data above, means cross-loaded observations will be numerous and no strategy will result in credible segment labels.

Note also that labeling of segments is not required and is not always performed. See also the discussion of group assignment [below](#), in the section on PLS-POS.

Prediction-oriented segmentation (POS)

Overview

Prediction-oriented segmentation (POS, or PLS-POS) is an alternative to FIMIX as a method of treating unobserved heterogeneity in one's data. Henseler, Ringle, & Sarstedt (2016) find PLS-POS to be superior to PLS-FIMIX as a segmentation method. Like FIMIX, POS is a form of multi-group analysis in which groups are

derived through a data-driven methodology. Multi-group analysis (MGA), discussed [below](#), in contrast, typically connotes analysis in which the researcher has observed data on known groups of interest.

Unobserved heterogeneity may lead to Type I and Type II error of interpretation. Becker, Rai, Ringle, & Volckner conducted simulations showing that FIMIX and POS both perform well for reflective models, but POS performs better for formative models (Becker et al., 2013: 665-666). Where the FIMIX procedure employs parametric t-tests, the POS procedure is fully non-parametric, not assuming a normal distribution (Becker et al., 2013: 677). Where FIMIX tests unobserved heterogeneity in the structural model (the relationship among the latent constructs), POS tests unobserved heterogeneity in both the structural and the measurement model (the relationship of the indicator variables to their constructs). In general, POS conforms more to the assumptions involved in modeling unobserved heterogeneity and may be preferred for this reason.

PLS-POS uses an objective criterion for model fit, namely one of two R-square measures. The default measure uses R-square across all constructs in the model, thereby testing segmentation for both the measurement (outer) and the structural (inner) model. The alternative measure uses R-square for a target construct selected by the researcher.

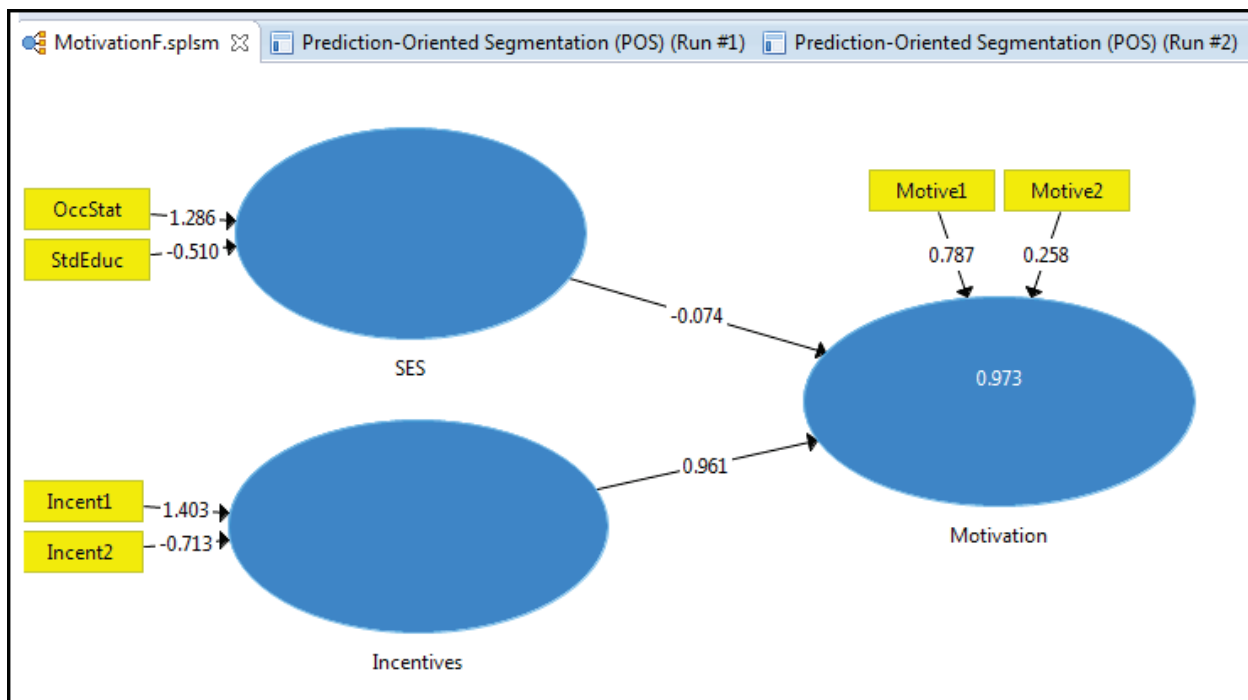
The algorithm for PLS-POS bases assignment of cases to segments on a distance measure appropriate for PLS path models. (Formulas for this complex distance measure are given in Becker et al., 2013: Appendices A5-A6). The distance measure, unique to PLS-POS, is consistent with both formative and reflective models. The distance criterion is applied over many iterations, seeking performance improvement through a process called “hill-climbing”. Although distance is used to assign cases to segments (groups), the iterative algorithm may re-assign cases to different groups as it searches for an optimal solution. The algorithm “Assigns only one observation to the closest segment and assures improvement of an objective criterion (R^2 of all endogenous latent variables) before accepting the change” (Becker et al., 2013: Appendices, A4). That is, “optimal” is defined in terms of R-squared values for the endogenous constructs in the model. It may be noted that the PLS-POS algorithm is computer-intensive and takes more time than the PLS-FIMIX solution for the same model (e.g., Becker et al. [2013: 689] report three minutes vs. ten seconds for their simulated dataset)

The presence of unobserved heterogeneity may be rejected and the traditional whole-sample PLS solution may be pursued if (1) R^2 in multi-segment models is lower than for the traditional PLS solution; and (2) PLS-POS R^2 criteria for the one-segment solution shows better fit than for multi-segment solutions, for which R^2 deteriorates markedly (Becker et al., 2013: 686).

For further details, see Becker et al. (2013) and Squillacciotti (2005).

The example model

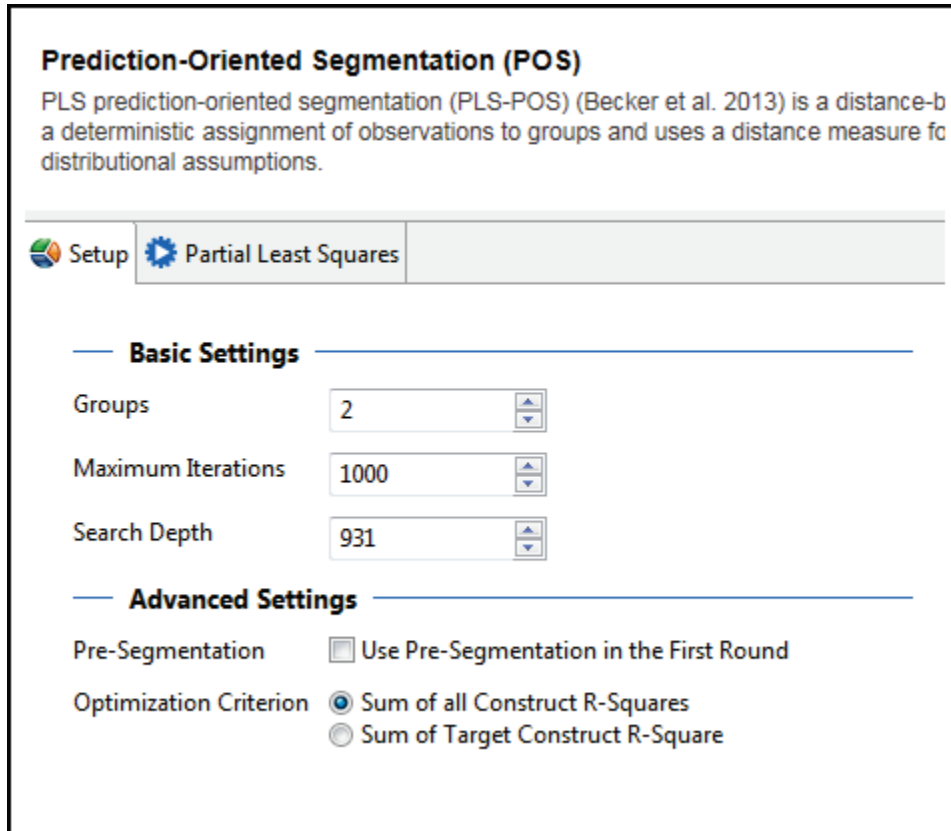
The PLS-POS example used for output discussed below is the MotivationF formative model, shown below (with path coefficients calculated by the POS algorithm). MotivationF was discussed previously [above](#).



Running POS

To run a POS analysis, select “Prediction Oriented Segmentation (POS)” from the “Calculate” button drop-down menu. The “Prediction Oriented Segmentation (POS)” window appears, shown below opened to the first of two tabs: Setup. The default values are shown (except search depth is set to sample size, 931, not the default of 1,000) and were used in the example output further below.

The second tab, “Partial Least Squares”, provides weighting and other options for the PLS algorithm. As this was discussed [above](#), it is not discussed or illustrated here.



Prediction-Oriented Segmentation (POS)

PLS prediction-oriented segmentation (PLS-POS) (Becker et al. 2013) is a distance-based deterministic assignment of observations to groups and uses a distance measure for distributional assumptions.

Setup Partial Least Squares

Basic Settings

Groups: 2

Maximum Iterations: 1000

Search Depth: 931

Advanced Settings

Pre-Segmentation: Use Pre-Segmentation in the First Round

Optimization Criterion: Sum of all Construct R-Squares
 Sum of Target Construct R-Square

Options in the “Basic Settings” and “Advanced Settings” areas are discussed below:

1. *Groups*: This specifies how many segments are to be employed in the analysis.
2. *Maximum Iterations*: POS is an iterative process. By default, the algorithm performs up to 1,000 iterations, which is sufficient in nearly all cases, but which can be overridden by the researcher.
3. *Search Depth*: The search depth is how many observations will be considered for reassignment to test if the optimization criterion is improved. The number specified may not be more than the sample size (931 in the example). In exploratory runs of the POS model, a lower search depth may be used to speed calculation. For confirmatory modeling, the sample size should be used.

4. *Pre-Segmentation*: Not to use pre-segmentation is the default. If this box is checked, a distance measure is used to pre-assign all observations to the best-fitting group (segment) and only then does the algorithm start its iterative algorithm. There is no assessment of whether pre-segmentation improves the performance of the model.
5. *Optimization Criterion*: This option sets the criterion used to assess model fit. By default, the criterion is the “Sum of All Construct R-Squares”, which is based on the sum of all R-Squares for all segments in the model. The alternative is “Sum of Target Construct R-Square”. If this is selected, the researcher must specify the target construct. The “Sum of Target Construct R-Square” is based on the sum of R-squares for this target construct (not all endogenous constructs) summed over all segments.

POS output

Overview

The iterative nature of PLS-POS means that coefficients and group assignments may vary noticeably from run to run of the model. The POS algorithm starts by splitting the sample randomly into groups (unless pre-segmentation is invoked) and then uses a distance measure to reassign observations. (PLS-FIMIX, in contrast, does not employ a distance measure). SmartPLS documentation, following Becker et al. (2013: 676), warns, “A repeated application of PLS-POS with different starting partitions is advisable to avoid local optima.” Different starting positions will occur automatically with each run of the model. Wedel & Kamakura (2000), endorsed by Becker et al. (2013: Appendixes, A6), recommend running the PLS-POS algorithm several times to attain alternative starting partitions and, finally, to select the best segmentation solution.”

Additionally, runs of the same model may be undertaken for multiple samples from the population or multiple samples from the data for purposes of assessing reliability (Becker et al., 2013: 688).

Finally, sensitivity analysis may be conducted by requesting models with differing numbers of segments, such as from 2 to 10. This also may be useful when testing some a priori assertion about the number of segments in the population (e.g., a prior assertion about the number of market segments in a marketing application).

Segment sizes

As in any classification procedure, it is desirable than no classification group be too small. When segments are not substantial in size, they may reflect outliers, “bad respondents”, over-fitting and other statistical artifacts (Becker et al., 2013: 686). One rule of thumb is that splits of 90:10 or worse are to be avoided for two-segment solutions. The “Segment Sizes:” table shows the pertinent information. In this case, the smaller of the two groups is over 11% of the total, which is not considered problematic, particularly for moderate to large samples sizes (here, $n = 931$, so the smaller segment still has 105 observations).

Segment Sizes		
Segment Sizes (Total)		
	Group1	Group2
Number:	105.0000	827.0000
Segment Sizes (Relative)		
	Group1	Group2
Percentage:	11.2661	88.7339

Too-small segments may mean that the researcher has requested too many segments in the solution. Alternatively, if the number of segments is optimal but a segment is too small, it may be collapsed into other segments from which is it not significantly different (Becker et al., 2013: 686). The significance of differences between segment may be tested in multi-group analysis, as discussed [below](#), though significance testing introduces parametric assumptions.

POS R-squared coefficients

The R-square coefficients, which were based on the default sum of R-squares for the model (though this model has only one endogenous variable), show that the level of explanation of Motivation by Incentives and SES is much higher for the smaller Segment 1 than for the larger Segment 2. However, even the latter is slightly higher than for the original sample R-square.

POS R-Squares	
Segment 1	
	R Square
Motivation	0.9735
Segment 2	
	R Square
Motivation	0.4572
Original Sample R-Squares	
	R Square
Motivation	0.4362

Original and PLS-POS path coefficients

For the structural (inner) model, standardized path coefficients are output for the original model and for each segment. Again, path coefficients are stronger for the smaller segment, Segment 1.

Original Path Coefficients			
	Incentives	Motivation	SES
Incentives		0.5144	
Motivation			
SES		-0.2481	

POS Path Coefficients			
Segment 1			
	Incentives	Motivation	SES
Incentives		0.9610	
Motivation			
SES		-0.0742	
Segment 2			
	Incentives	Motivation	SES
Incentives		0.4909	
Motivation			
SES		-0.3055	

Measurement model (outer) weights and loadings

For the measurement (outer) model, both weight and loading coefficients are output. Both are used to understand the relative importance of indicator variables vis-à-vis their constructs. Weights are used for this purpose for formative models while loadings are used for reflective models.

For reflective models, loadings are the correlations between the indicator variable and the construct. By one rule of thumb in confirmatory PLS factor analysis, loadings should be .7 or higher to confirm that indicator variables identified a priori are represented by a particular construct (Hulland, 1999: 198). However, the .7 standard is a high one and real-life data may well not meet this criterion, which is why some researchers, particularly for exploratory purposes, will use a lower level such as .4 for the central factor and .25 for other factors (Raubenheimer, 2004). Of course, loadings must be interpreted in the light of theory, not by arbitrary cutoff levels.

POS Outer Loadings**Segment 1**

	Incentives	Motivation	SES
Incent1	0.8764		
Incent2	0.3217		
Motive1		0.9863	
Motive2		0.8647	
OccStat			0.9306
?StdEduc			0.3862

Segment 2

	Incentives	Motivation	SES
Incent1	0.8807		
Incent2	0.9288		
Motive1		0.9003	
Motive2		0.9035	
OccStat			0.7203
?StdEduc			0.9643

However, for formative models (as in this example), weights represent the importance of each indicator in explaining the variance of the construct (Becker et al., 2013: 670; see Edwards & Lambert, 2007; Petter et al., 2007); Wetzels et al., 2009). It follows that the "weights" may be used to impute meanings for the formative constructs, as discussed below.

In the output below, it may be noted that the ratio of weights of Incent1 to Incent2 is approximately 2:1 for the Incentives construct in Segment 1, but the two indicator variables are much more equal in importance in Segment 2 (the larger segment). We may say that Incent1 contributes much more to the definition of "Incentives" in Segment 1 than it does in Segment 2. Likewise, a similar observation may be made with regard to Motive1 and Motive2 in defining the "Motivation" construct. StdEduc contributes much more to the definition of the "SES" construct in Segment 2. For the "SES" construct, Occstat is more important than StdEduc in Segment 1 but the reverse is true in Segment 2.

POS Outer Weights			
Segment 1			
	Incentives	Motivation	SES
Incent1	1.4029		
Incent2	-0.7134		
Motive1		0.7873	
Motive2		0.2584	
OccStat			1.2863
?StdEduc			-0.5104

Segment 2			
	Incentives	Motivation	SES
Incent1	0.4835		
Incent2	0.6181		
Motive1		0.5500	
Motive2		0.5587	
OccStat			0.3081
?StdEduc			0.8069

Group assignment

The group assignment table shows for each case in the table which segment that case was assigned to. Ideally, inference based on group assignment would enable the researcher to intuit the nature of unobserved heterogeneity accounting for segmentation. However, where the purpose is not causal analysis but is more practical, as in marketing, the demonstration that segments exist and are differentially associated with indicator variables may be valuable information.

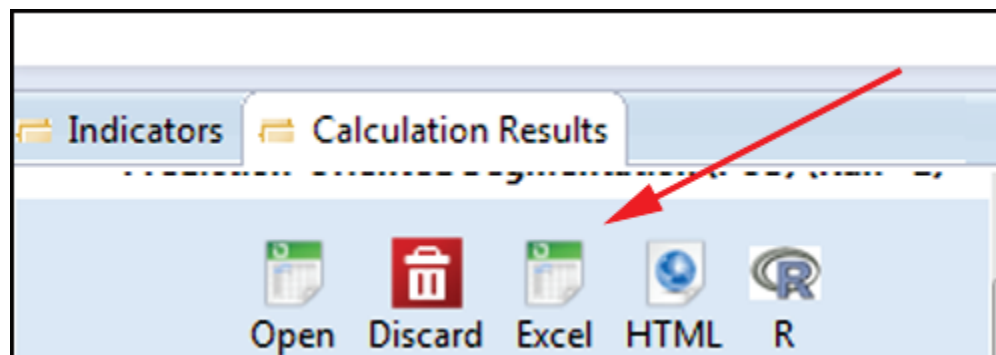
Nonetheless, Becker et al. (2013: 686) urge the researcher to determine if the segments are “plausible”, meaning that the researcher should strive to “identify theoretically reasonable variables/constructs that can represent the meaning of the plausible segments.” If this is not possible and one or more segments remain without a plausible label based on theory, Becker et al. (2013: 687) suggest that for purposes of theory-testing, “because unobserved heterogeneity can threaten the validity of conclusions based on the overall sample due to significant segment

differences, differentiable segments that are not plausible should not be part of a combined sample used to test the model/hypotheses.” Rather, segments for which a plausible, theory-based label cannot be imputed should be treated as anomalies in the process of theory development. PLS-POS “segmentation provides a mechanism to facilitate abduction* by surfacing anomalies, which then must be confronted and resolved theoretically” (Becker et al., 2013: 690). (* abduction refers to induction based on partial information).

	Group
Unit: 0	2.0000
Unit: 1	2.0000
Unit: 2	2.0000
Unit: 3	1.0000
Unit: 4	2.0000
Unit: 5	2.0000

PARTIAL OUTPUT (5 OF 931)

By selecting Excel output in the “Calculation Results” tab of the Indicators/Calculation Results area in the lower-left of the PLS interface, results can be sent to a spreadsheet.



The Excel spreadsheet, in turn, may be used to save group memberships to a file which can be imported into most statistical purposes as a variable for analysis.

MotivationF_POS.xls - Microsoft Excel

File Home Insert Page Layout Formulas Data Review View Acrobat FRED

Paste Arial 12 Bold Italic Underline Merge & Center

Clipboard Font Alignment Number

B103 Group Assignment

	B	C	D	E
1	Complete			
2	back to navigation			
3				
102				
103	Group Assignment			
105		Group		
106	Unit: 0		2.0000	
107	Unit: 1		2.0000	
108	Unit: 2		2.0000	
109	Unit: 3		1.0000	
110	Unit: 4		2.0000	
111	Unit: 5		2.0000	
112	Unit: 6		2.0000	
113	Unit: 7		2.0000	
114	Unit: 8		2.0000	
115	Unit: 9		2.0000	
116	Unit: 10		1.0000	
117	Unit: 11		2.0000	
118	Unit: 12		1.0000	
119	Unit: 13		2.0000	
120	Unit: 14		2.0000	
121	Unit: 15		2.0000	
122	Unit: 16		2.0000	
123	Unit: 17		2.0000	
124	Unit: 18		2.0000	
125	Unit: 19		2.0000	
126	Unit: 20		2.0000	
127	Unit: 21		2.0000	
128	Unit: 22		2.0000	
129	Unit: 23		2.0000	
130	Unit: 24		2.0000	
131	Unit: 25		1.0000	

Labeling the segments

Labeling the segments in PLS-POS involves the same considerations as in PLS-FIMIX. The reader is referred to the discussion [above](#) in the section on FIMIX.

Multi- group Analysis (MGA)

Overview

PLS multigroup analysis is used to determine if the PLS model significantly differs between groups. Examples of this use are:

1. Testing if segments formed by FIMIX or POS differ from each other. If no segment differs significantly in path coefficients from any other segment, a one-segment solution is warranted and the traditional PLS algorithm may be used.
2. Testing if the PLS model differs between groups formed by cluster analysis, factor analysis, multidimensional scaling, or other external statistical procedures.
3. Testing if the PLS model differs between groups for measured variables (e.g., testing if the model differs between males and females, assuming gender is a measured variable). This is the purpose illustrated in the example below.

MGA, also called parametric multigroup analysis, uses independent samples t-tests to compare paths between groups, as proposed by Kiel et al. (2000). MGA is “parametric” because significance testing requires the assumption of multivariate normal distributions, unlike traditional PLS.

Video documentation on multi-group analysis in SmartPLS 3 is provided by the publisher at <https://www.smartpls.com/documentation/pls-multigroup-analysis>.

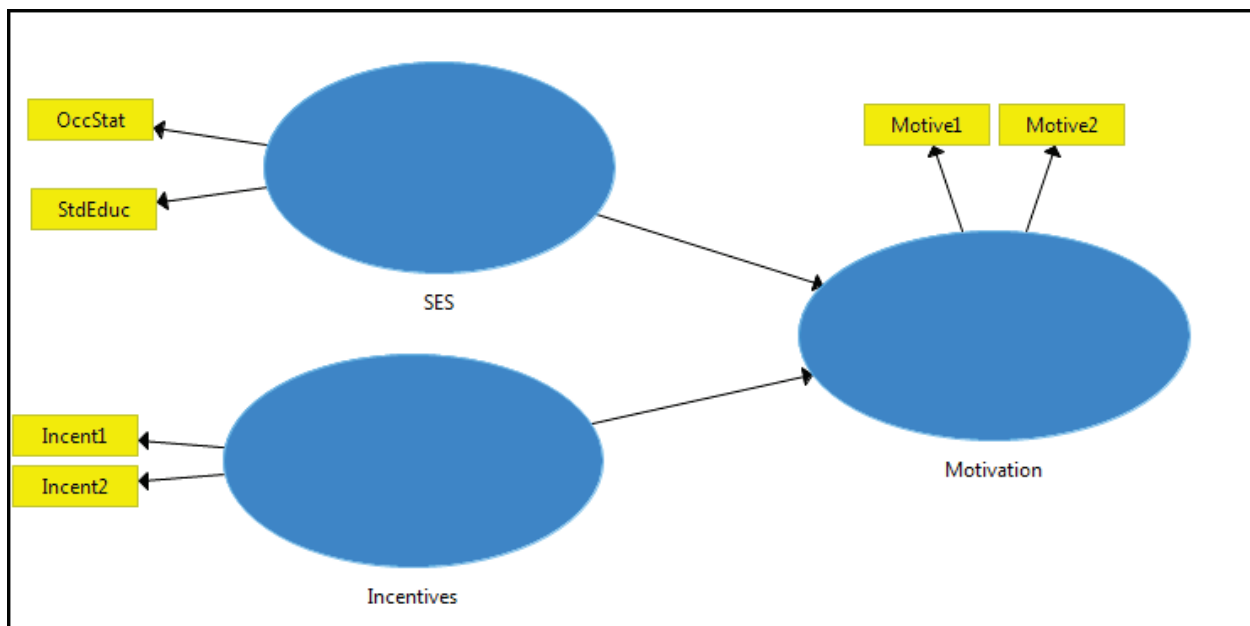
Measurement invariance

The outer model is the “measurement” model because it determines how constructs in the inner model are measured. Put another way, the outer model determines the meaning of the constructs in the inner model.

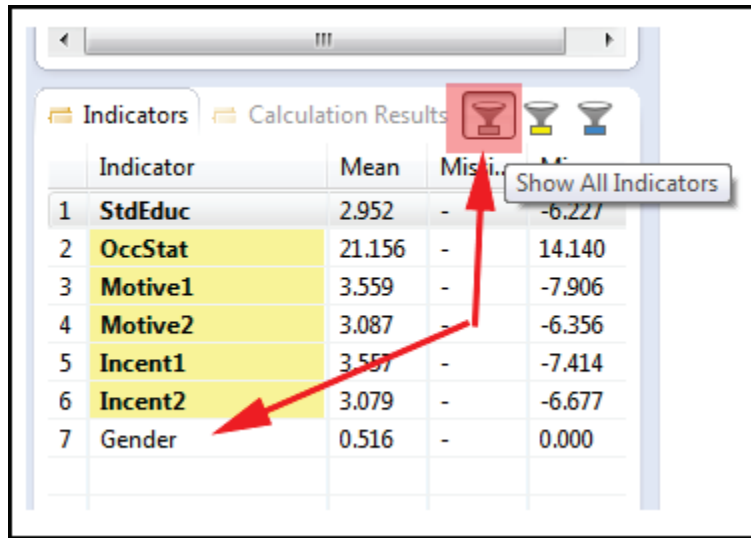
The issue of “measurement invariance” arises in multigroup analysis (see [below](#)), in which the researcher seeks to determine if the model is the same or different between groups (e.g., between males and females). This comparison of models makes logical sense only if the inner model constructs are measured the same in each group and thus have the same meaning. That is, establishing measurement invariance is a necessary prerequisite for performing multigroup analysis. In SmartPLS, measurement invariance is tested using the MICOM procedure described [below](#) in the section on the “Permutation” algorithm.

The example model

For purposes of illustrating MGA, we use the same Motivation model discussed for traditional PLS [above](#). The model is reproduced in the figure below. It is the same as MotivationR, which is reflectively modeled and which was discussed [above](#).



This time, however, we will use Gender as basis for multigroup comparison. As Gender is not part of the model, click the “Show all Indicators” button in the lower-right panel of the PLS interface, Indicators tab, as illustrated below. Gender appears in the variable list.



	Indicator	Mean	Misli.	M
1	StdEduc	2.952	-	-6.227
2	OccStat	21.156	-	14.140
3	Motive1	3.559	-	-7.906
4	Motive2	3.087	-	-6.356
5	Incent1	3.557	-	-7.414
6	Incent2	3.079	-	-6.677
7	Gender	0.516	-	0.000

Defining groups

Prior to running MGA, it is necessary to define groups. Double-click on the desired data file (here, jobsat), causing the data view to appear on the right. Then click the “Generate Data Groups” button/icon as illustrated below.

The screenshot shows the SmartPLS software interface. The 'Project Explorer' on the left displays a tree view of the project structure, with 'jobsat [932 records]' selected. A red arrow labeled '1' points to this file. The 'Generate Data Groups' button in the top toolbar is highlighted in red, with a red arrow labeled '2' pointing to it. The 'Indicators' table on the right shows a list of variables with their statistics.

Indicator	Mean	Missi...	Min	Max
1 StdEduc	2.952	-	-6.227	12.763
2 OccStat	21.156	-	14.140	28.076
3 Motive1	3.559	-	-7.906	15.078
4 Motive2	3.087	-	-6.356	13.553
5 Incent1	3.557	-	-7.414	15.635
6 Incent2	3.079	-	-6.677	13.634
7 Gender	0.516	-	0.000	1.000

1. Double-click the jobsat data file to get the data view of jobsat.txt.

2. Click the "Generate Data Groups" icon to define groups.

In the "Generate Data Groups" page shown below, you may:

1. Optionally change the prefix for group names. The default prefix is "GROUP_". This example accepts the default name.
2. Enter the indicator (observed variable) name in the "Group column 0:" box, using the drop-down list of possible indicators in the current dataset. For this example, Gender is selected, labeled "Gender (2 unique values)".
3. Optionally add up to two additional indicators to be used when forming groups (left blank in this example).
4. Optionally change the "Minimum cases" value from its default value of 10. Groups will be formed only if as large or larger than the "Minimum cases" value. The default was accepted in this example.
5. Click the OK button (lower right, not shown) to go to data view of jobsat.txt.

Generate Data Groups

This option allows you to define groups of data for carrying out group-specific analyses. You need to define a variable in your set of data. This grouping variable should have numbers to determine the group membership of each observation (e.g., 1, 2, and 3). The dialog uses the name of the selected variable to name the group. For example, "age_" produces group names of "age_1", "age_2", and "age_3" in the results report. The user can change the prefix for the automatic naming of groups.

Generate Data Groups

Name prefix:

Group Columns

Group column 0:

Group column 1:

Group column 2:

Prune groups

Total: 2

Minimum cases: 10

Click OK on this page to get to this page:

The screenshot shows the SmartPLS software interface. The 'Generate Data Groups' dialog is open in the foreground, with the 'Name prefix' set to 'GROUP_' and 'Group column 0' set to 'Gender (2 unique values)'. The 'Prune groups' section shows a total of 2 groups and a minimum of 10 cases. In the background, the 'Project Explorer' shows a folder named 'jobsat [932 records]' which is highlighted with a red arrow. The 'Generate Data Groups' dialog also shows a preview of the resulting data groups: 'GROUP_Gender(0,0)' with 451 records and 'GROUP_Gender(1,0)' with 481 records.

In data view of jobsat.txt, open the “Data Groups” tab if not already open. This tab shows for this example that there are two Gender groups of 451 and 481 records respectively.

If the cursor is hovered to the right of the two groups, the “Delete” and “Edit” buttons appear. Clicking the “Edit” button leads to the “Configure Data Group” window, where groups may be renamed. Below, GROUP_0 is renamed “Male”. Not shown, GROUP_1 is renamed “Female”.

Name	Records		
GROUP_Gender(0.0)	451	Delete	Edit
GROUP_Gender(1.0)	481		

Configure Data Group

Group Name:

Group Terms

Gender equals

Group names change in data view:

Name	Records
Female	481
Male	451

Running MGA

After defining groups, highlight the MotivationR project in the Project Explorer (the upper left pane in the SmartPLS interface) and click the “Calculate” icon at the far right of the menu bar at the top. Select “Multi-Group Analysis (MGA)”, giving the MGA “Setup” tab dialog below. Check “Male” to assign Groups A to males. Similarly, check “Female” for Groups B, as shown below.

The screenshot shows the MGA Setup dialog box with the following configuration:

Group	Gender	Cases	Selected
Groups A	Female	481 cases	<input type="checkbox"/>
	Male	451 cases	<input checked="" type="checkbox"/>
Groups B	Female	481 cases	<input checked="" type="checkbox"/>
	Male	451 cases	<input type="checkbox"/>

As the PLS solution does not follow a known distribution, bootstrapped significance is the available option. The “Bootstrapping” tab is the tab which gives parameters for significance testing. It was also illustrated and discussed [above](#) and in the section on estimation with bootstrapping [above](#). For this example, the only change from the defaults is to reset “Subsamples” from the default 500 to a much larger number (5,000) more suitable for confirmatory analysis.

The “Weighting” tab is also the same as discussed [above](#). For this example, the defaults are accepted.

After assigning groups and filling out the tabs as desired, click the “Start Calculation” button in the lower right. Bootstrapped standard errors and significance levels take a while to compute (about two minutes for this small dataset with two groups).

Multi-Group Analysis (MGA)

The multi-group analysis allows to test if pre-defined data groups have significant differences in their group-specific parameter estimates (e.g., outer weights, outer loadings and path coefficients). SmartPLS provides outcomes of three different approaches that are based on bootstrapping results from every group.

[Read more!](#)

Setup
Partial Least Squares
Bootstrapping
Weighting

Basic Settings

Select Groups

The selected groups will be assessed for significant differences in the parameter estimates (e.g., outer weights, outer loadings and path coefficients).
All data groups selected under Group A will be compared against all data groups selected under Group B.

Groups A

Select All

Female	481 cases
Male	451 cases

Female Male

Groups B

Select All

Female	481 cases
Male	451 cases

Female Male

After Calculation:

[Open Full Report](#)

[Close](#)

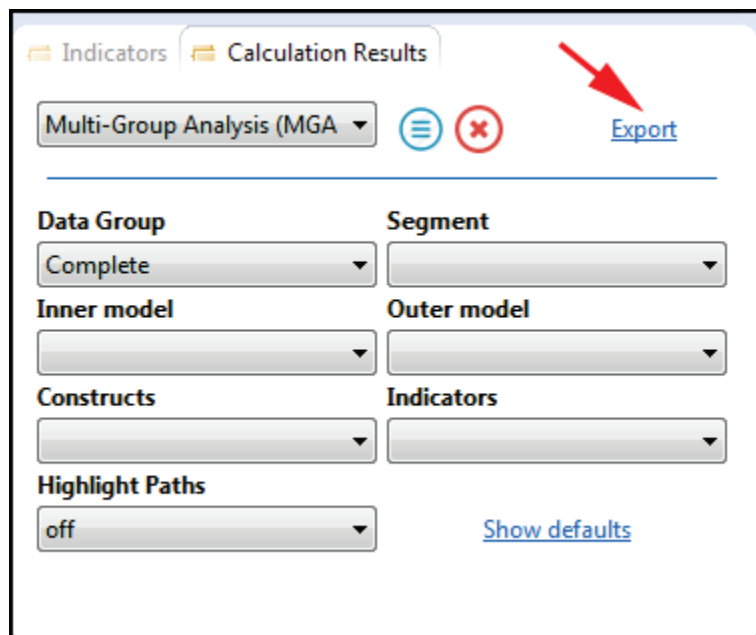
[Start Calculation](#)



Multi-group output

Overview

Since the procedure just outlined runs the traditional PLS algorithm, but with groups, the basic report is the same as for that algorithm, discussed [above](#) and not treated here. However, the report (shown below) now has columns for “Male” and “Female” in addition to “Complete”. This figure is the top of the report saved by clicking the “Export” button shown below, then selecting “HTML” (Excel and R export is also available) under the “Calculation Results” tab for MGA output in the output options pane in the lower left of the PLS interface.



(Note the figures above and below are for SmartPLS 3.23. Earlier versions had a separate “HTML” button in the corresponding figure above, and had separate “Complete”, “Male”, and “Female” links in the report table of contents below.)

Report (MotivationR.splsm)

Please cite the use of SmartPLS: Ringl
<http://www.smartpls.com>.

Content**Complete****Final Results***Path Coefficients* [show](#)*Indirect Effects* [show](#)*Total Effects* [show](#)*Outer Loadings* [show](#)*Outer Weights* [show](#)**Quality Criteria***R Square* [show](#)*Average Variance Extracted (AVE)* [show](#)*Composite Reliability* [show](#)*Cronbach's Alpha* [show](#)**Interim Results***Path Coefficients (Samples)* [show](#)*Indirect Effects (Samples)* [show](#)*Total Effects (Samples)* [show](#)*Outer Loadings (Samples)* [show](#)*Outer Weights (Samples)* [show](#)**Base Data***Setting* [show](#)*Inner Model* [show](#)*Outer Model* [show](#)*Indicator Data (Original)* [show](#)*Indicator Data (Groups)* [show](#)

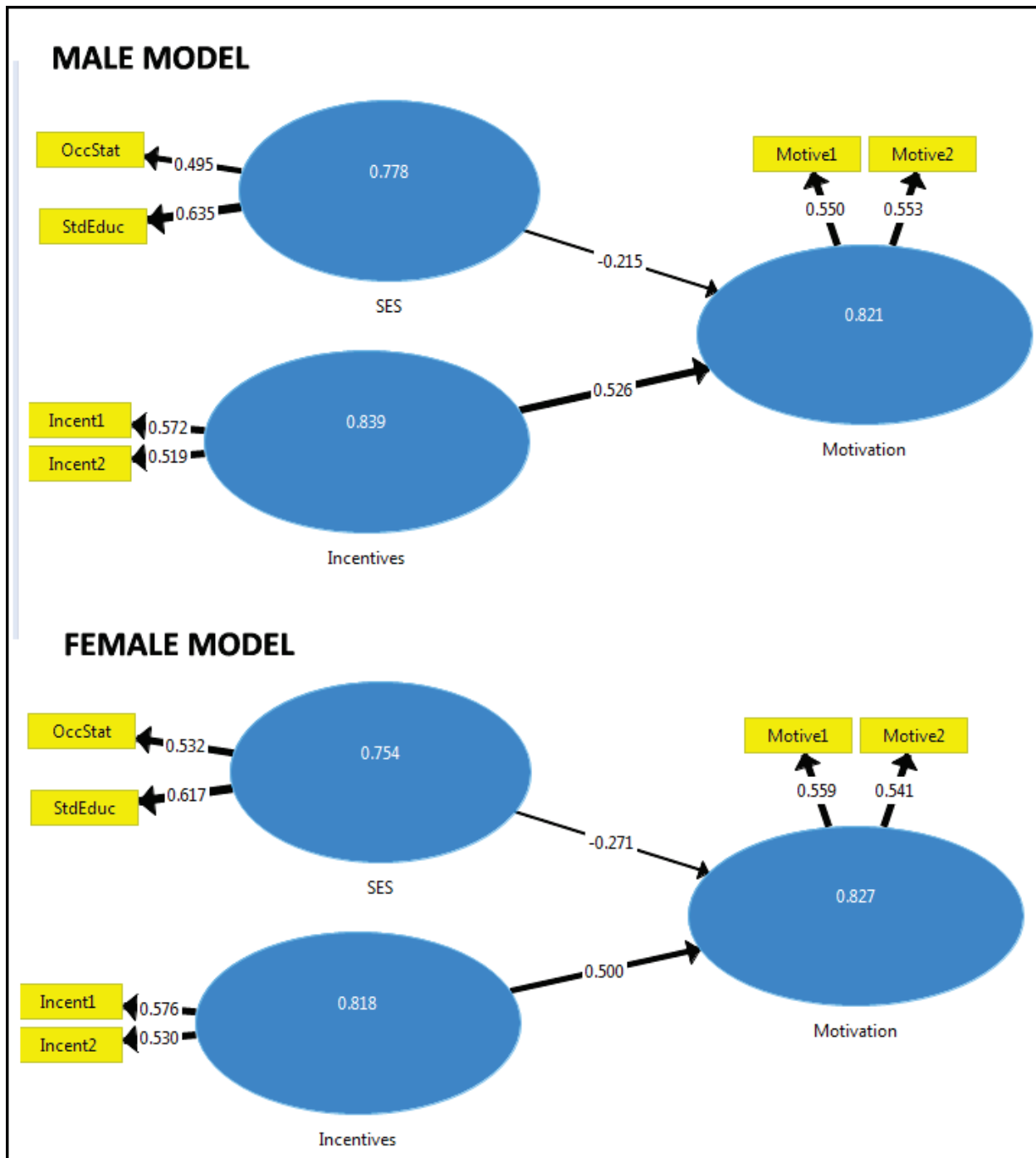
The report provides path coefficients separately for the Female and Male groups, along with bootstrap-estimated standard deviations, t-values, and significance p-values as well as confidence intervals. While the standardized path coefficients in the structural (inner) model are higher for Males than for Females, is this difference significant? The bootstrap t-test answers this question in the output section below on confidence intervals. Note that for the path from Incentives to Motivation, the confidence intervals overlap (Female, from 0.4249 lower to 0.5611 upper; Male 0.4553 lower to 0.5932 upper). The confidence intervals for the path from SES to Motivation also overlap. Overlapping confidence intervals mean that at the .05 significance level, we fail to reject the null hypotheses that there is no difference in path coefficients between the Male and Female samples.

In summary, for the example data, all paths in the structural model (the path from Incentives to Motivation and the path from SES to Motivation) are significant for both Males and Females, as shown in the p-Values columns. The same inference may be taken by noting that 0 is not within the confidence limits of Males or Females in the “Confidence Intervals” columns.

Path Coefficients										
Bootstrapping Results										
	Path Coefficients Original (Female)	Path Coefficients Original (Male)	Path Coefficients Mean (Female)	Path Coefficients Mean (Male)	STDEV (Female)	STDEV (Male)	t-Values (Female)	t-Values (Male)	p-Values (Female)	p-Values (Male)
Incentives -> Motivation	0.4996	0.5261	0.4988	0.5252	0.0340	0.0359	14.6972	14.6447	0.0000	0.0000
SES -> Motivation	-0.2707	-0.2154	-0.2722	-0.2162	0.0359	0.0410	7.5505	5.2537	0.0000	0.0000

Confidence Intervals (Bias Corrected)				
	2.5% (Female)	97.5% (Female)	2.5% (Male)	97.5% (Male)
Incentives -> Motivation	0.4249	0.5611	0.4553	0.5932
SES -> Motivation	-0.3414	-0.1989	-0.2576	-0.1438

The differences between the Male and Female models may also be viewed graphically.



The figure above displays path coefficients and average variance extracted for the Male and Female models, using absolute highlighting for paths. We can see that

the models are similar in path weights, reflected in path widths. However, the numeric values of the path coefficients differ somewhat.

Testing for segment difference

By using t-tests, MGA reintroduces distributional assumptions into PLS, which otherwise is a distribution-free procedure. Note also that when sample size is large, even small differences in coefficients may test as significant. Therefore, inspection of the distance between coefficients is still recommended, particularly if [entropy](#) is low, indicating that segments may not be interpretable.

The “Bootstrapping Results” table in the “Path Coefficients” section of Smart-PLS output report the Male and Female path coefficients, means, standard errors, t-values, and p-values, as shown in the figure below. The exact coefficients will vary from run to run of the MGA model.

The difference between Male and Female path coefficients is subject to three tests. These significance tests by default use the .05 significance level. The three methods of testing the significance of path differences are:

1. *PLS-MGA*: This non-parametric significance test finds a difference to be significant if the p-value is smaller than 0.05 or larger than 0.95 for the difference of group-specific path coefficients. This method (see Henseler et al., 2009) is an extension of the original nonparametric Henseler's MGA method as described, for example, by Sarstedt et al., 2011, and is the most commonly used test.
2. *Parametric Test*: This is a similar method but is parametric, assuming that groups have equal variances.
3. *Welch-Satterthwait Test*: This is an alternative parametric test, assuming unequal variances between groups.

For further discussion, see Sarstedt et al. (2011). Hair et al. (2014: 247-255) present the manual approach, including formulas and a worked example.

Examining the p-value columns, the difference is not significant by any of the tests. We may say that the same PLS structural path model applies to both Males and Females.

PLS-MGA		
	Path Coefficients-diff (Male - Female)	p-Value(Male vs Female)
Incentives -> Motivation	0.0265	0.2987
SES -> Motivation	0.0553	0.1577

Parametric Test			
	Path Coefficients-diff (Male - Female)	t-Value(Male vs Female)	p-Value(Male vs Female)
Incentives -> Motivation	0.0265	0.5372	0.5913
SES -> Motivation	0.0553	1.0196	0.3082

Welch-Satterthwait Test			
	Path Coefficients-diff (Male - Female)	t-Value(Male vs Female)	p-Value(Male vs Female)
Incentives -> Motivation	0.0265	0.5368	0.5917
SES -> Motivation	0.0553	1.0163	0.3100

Other group comparisons. SmartPLS outputs similar tables, not shown here, for comparing and testing the difference by group for outer (measurement) weights, outer loadings, indirect effects, total effects, R-square, average variance extracted (AVE), composite reliability, and Cronbach's alpha as well as for path coefficients). For the example data, there is no significant difference by gender on any of these coefficients.

Bonferroni adjustment

Note that when there are multiple t-tests rather than just one, the computed probability level of significance is too liberal and may involve incurring Type I errors (false positives). That is, the nominal .05 level used by the researcher as a cut-off will be too high and requires adjustment. One common, albeit conservative, adjustment is the Bonferroni adjustment for multiple independent tests. The Bonferroni adjustment calls for reducing the alpha significant level by the number of tests used as a denominator. For instance, if .05 alpha is desired for 5 independent t-tests, then $.05/5 = .01$ should be the required computed level to achieve an underlying real level of .05.

The permutation algorithm. As discussed in the section below, the permutation algorithm provides a different approach to measuring inter-group differences.

Permutation algorithm (MICOM)

Overview

The permutation algorithm may be used to compare groups. Additionally, the algorithm may be used to implement the PLS-SEM measurement invariance assessment procedure (MICOM) described by Henseler, Ringle, & Sarstedt's (2015). MICOM is used to show if significant inter-group differences are due to inter-group differences in constructs (e.g., SES) when assessing composite models (composite models are discussed [above](#)). For further exposition, see Dibbern & Chin (2005) and Ringle, Wende, and Becker (2015).

It is assumed that the researcher has already created groups, as discussed above in the multi-group analysis section. By default, 1,000 random samples are drawn from each group (without replacement), though for stability of results, 5,000 is recommended for the final analysis run.

When this option is selected in the "Calculate" button menu, output includes both PLS multigroup analysis using the permutation test, and includes MICOM results used for assessing measurement invariance.

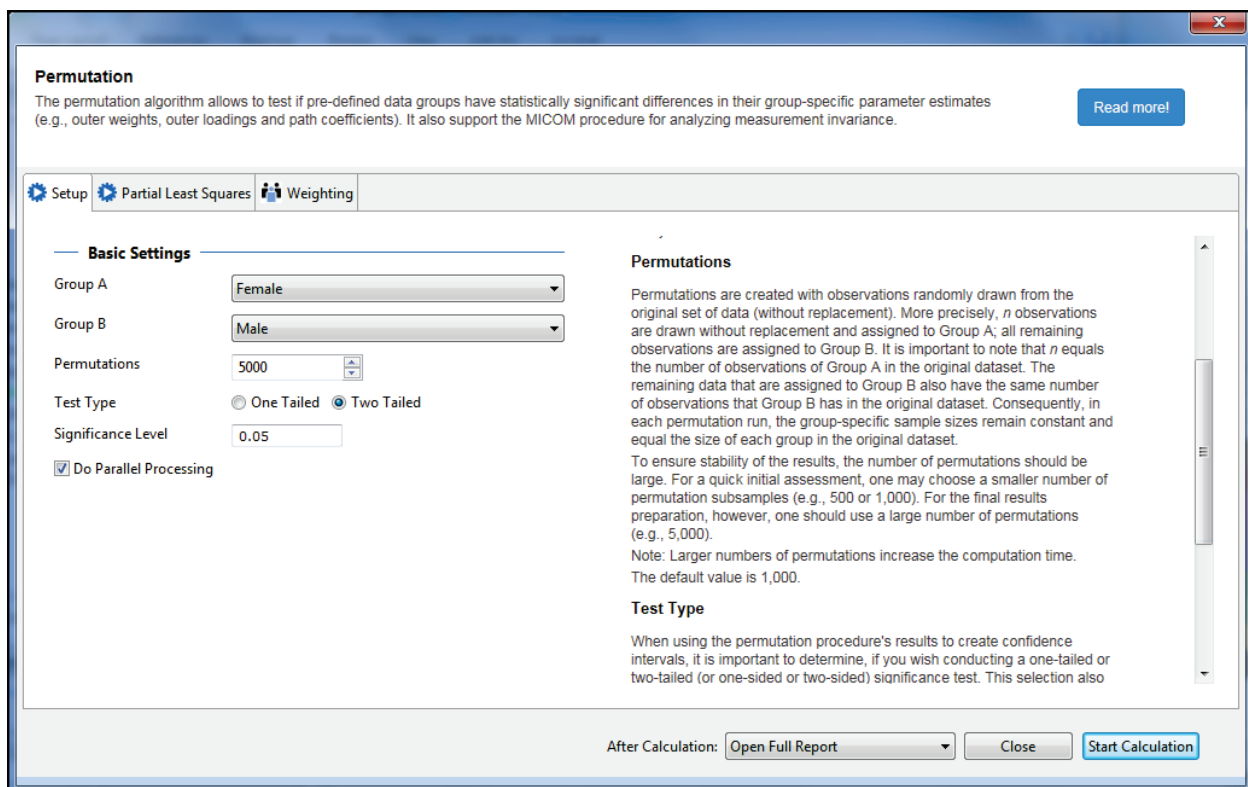
The example model

In this section, the MotivationF.splsm model described [above](#) is used. MotivationF has the same variables as in the section on multigroup analysis.

Running the permutation algorithm

To run the permutation algorithm with the example data, highlight the MotivationR project in the Project Explorer (the upper left pane in the SmartPLS interface) and click the “Calculate” icon at the far right of the menu bar at the top. Select “Permutation”.

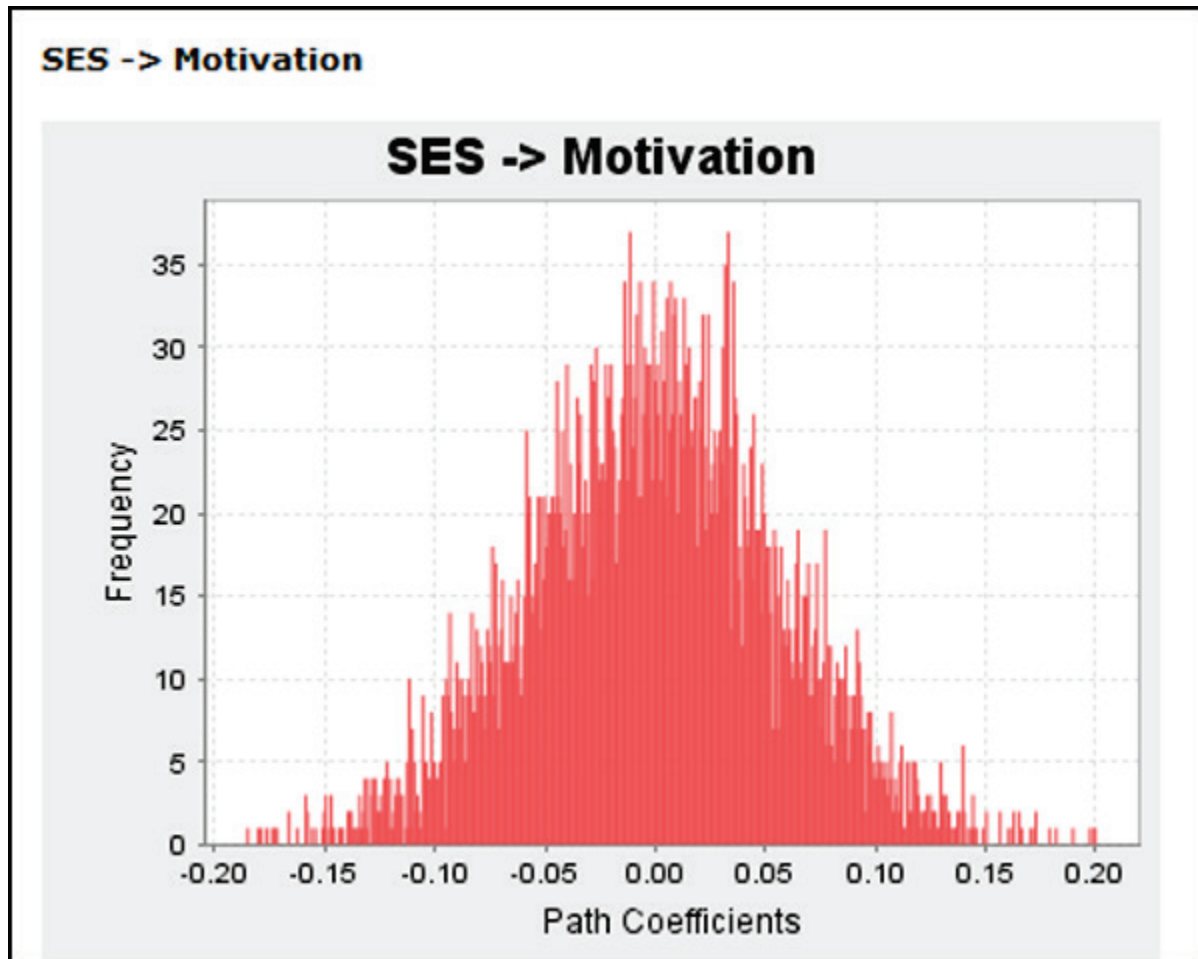
The “Permutation” window shown below appears. Set Group A and Group B to previously-defined groups (here, Female and Male). Optionally reset the number of permutations from the default of 1,000 to 5,000 for greater stability of results. The default settings of .05 alpha significance for two-tailed tests are normally accepted. Click the “Start Calculation” button to run the analysis.



The “Partial Least Squares” and “Weighting” tab defaults were accepted for this example. These tabs are the same as described previously [above](#).

Permutation algorithm output

The permutation process is illustrated in histograms of the permutation sample results for any given path coefficient, such as the histogram below for the path from SES to Motivation.



Permutation-based significance test results for the PLS model comparing the Female and Male groups are shown in the output below. Similar output, not shown, contains corresponding tests for outer loadings, outer weights, indirect effects, total effects, R-Square, average variance extracted (AVE), composite reliability, Cronbach's alpha. MICOM results are discussed below.

Path Coefficients							
	Path Coefficients Original (Female)	Path Coefficients Original (Male)	Path Coefficients Original Difference (Female - Male)	Path Coefficients Permutation Mean Difference (Female - Male)	2.5%	97.5%	Permutation p-Values
Incentives -> Motivation	0.5011	0.5277	-0.0266	-0.0002	-0.0989	0.1009	0.6231
SES -> Motivation	-0.2745	-0.2232	-0.0512	0.0002	-0.1075	0.1094	0.3699

The permutation test results confirm no significant difference between Female and Male groups for the structural (inner) model, as all “Permutation p-values” in the far right column are above the .05 cutoff.

Measurement invariance (MICOM) tests

The measurement invariance of composite models (MICOM) procedure is designed to test that the measurement (outer) model is the same between groups. Since the indicators in the outer model determine the meaning of the constructs in the structural (inner) model, lack of measurement invariance means that even though the constructs for, say, the “Female” and “Male” groups carry the same labels, this is deceptive because the constructs measure different things. MGA tests make sense only if there is measurement invariance, meaning only if the inner model constructs measure the same things.

MICOM therefore is a logically necessary step prior to conducting multi-group analysis (MGA). Hult et al. (2008: 1028) thus note that “failure to establish data equivalence is a potential source of measurement error (i.e., discrepancies of what is intended to be measured and what is actually measured), which accentuates the precision of estimators, reduces the power of statistical tests of hypotheses, and provides misleading results.”

MICOM is detailed in Jörg Henseler, Christian M. Ringle, & Marko Sarstedt, “Testing measurement invariance of composites using partial least squares” (forthcoming in *International Marketing Review* (2015), available [here](#)).

In SmartPLS, MICOM tests are part of the output of the “Permutation” algorithm. The MICOM procedure, the output of which is shown in the figure below, is a three-step process, analyzing:

1. *Configural invariance*. Configural invariance exists when the model in each group has the same number of constructs in the inner model and the same indicators in the outer model. Configural invariance also requires that an indicator in one group be coded in the same manner as in another group (e.g., dummy coding), that data treatment be the same (e.g., standardization or missing values treatment), and that algorithmic options and settings be the same. SmartPLS online documentation states, “Running MICOM in SmartPLS usually automatically establishes configural invariance.” Statistical output does not apply to this step and is not shown.

2. *Compositional invariance*: “Step 2” is a test of the invariance of indicator weights for measurement (outer) paths between groups. Taking the example data, a vector of indicator weights for men and another vector of corresponding indicator weights for women may be computed as a measure of difference in measurement models between groups. If there is compositional invariance, scores created by the indicator weights for the observed groups should correlate perfectly with scores created by the indicator weights vectors for pooled data. The permutation algorithm does this by creating two groups of the same size as the observed groups, but populating them with randomly sampled observations (sampling without replacement) from the pooled data. MICOM output displays “Permutation p-values” which test if item loadings in the outer model are invariant across groups. If not significant, as in the example below, the observed correlation of indicator vectors do not differ significantly from that for same-size groups populated randomly from the pooled data, showing that the indicator vectors are not different from each other either. Specifically, the algorithm tests the null hypothesis that correlation, c , in the original (Female and Male) data equals one. If c is smaller than the 5%-quantile of the distribution of c in the permutations for pooled data, the hypothesis of compositional invariance is rejected. A finding of non-significance means that compositional invariance may be assumed. This will happen when the correlations are not significantly lower than 1.0, as for the example data below.

3. *Scalar invariance (equality of composite means and variances)*: “Step 3” tests for scalar invariance in a manner analogous to that described for Step 2, detailed in Henseler, Ringle, & Sarstedt (2016). MICOM output shows “Permutation p-value” tests for intergroup differences in means and variances for each of the inner model constructs. For the example output shown further below, all are non-significant.

If Steps 2 and 3 both return findings of non-significance there is “full measurement invariance”. If only Step 2 returns findings of non-significance, there is “partial measurement invariance”. The following actions may ensue:

- With full measurement invariance, pooling the data is warranted and MGA may be unnecessary. Henseler, Ringle, & Sarstedt (2016) somewhat more

leniently recommend pooling only if most structural effects are invariant. Note that pooling will increase statistical power.

- If there is compositional invariance, the researcher may proceed with MGA for purposes of comparing models in the sense of comparing structural paths across groups. Henseler, Ringle, & Sarstedt (2016) recommend interrupting MICOM analysis when Step 2 upholds compositional invariance in order to run MGA to determine if structural invariance exists, prior to interpreting results for Step 3.
- Requiring scalar invariance (Step 3) also – full measurement invariance – is a quite stringent and conservative requirement, though necessary if means are to be compared across groups or if data are to be pooled. More leniently, Steenkamp & Baumgartner (1998) suggest that sufficient scalar invariance exists if at least two indicators of a construct have equal loadings and/or intercepts across groups.
- Even more stringent and conservative would be requiring equal error variance and therefore this level of invariance is typically not sought.

For the example data, there is full measurement invariance.

Type I and Type II error

Note that the statistical power of the MICOM procedure is unknown, meaning that the risk of Type II error (false negatives) is unknown. Also, when more than two groups are compared the number of tests increases exponentially, inflating risk of Type I error unless some penalty adjustment (e.g., see discussion of Bonferroni adjustment [above](#)) is applied, though doing so in too stringent a manner may increase the risk of Type II error. Future simulation research and sensitivity analysis may throw light on these issues. For now it may be observed that while Type II risk is unknown, power increases and risk decreases as sample size increases, making MICOM more reliable for larger samples.

MICOM

Step 2

	Original Correlation	Correlation Permutation Mean	5.0%	Permutation p-Values
Incentives	0.9998	0.9948	0.9798	0.8418
Motivation	0.9993	0.9961	0.9849	0.6733
SES	0.9934	0.9926	0.9720	0.3553

Step 3

	Mean - Original Difference (Female - Male)	Mean - Permutation Mean Difference (Female - Male)	2.5%	97.5%	Permutation p-Values	Variance - Original Difference (Female - Male)	Variance - Permutation Mean Difference (Female - Male)	2.5%	97.5%	Permutation p-Values
Incentives	0.0180	-0.0001	-0.1260	0.1248	0.7814	0.0452	0.0001	-0.1812	0.1851	0.8406
Motivation	-0.0292	0.0000	-0.1325	0.1248	0.6527	-0.0548	0.0002	-0.1877	0.1915	0.7574
SES	0.0492	0.0019	-0.1241	0.1266	0.4679	-0.0969	-0.0019	-0.1706	0.1767	0.5559

PLS regression modeling with SmartPLS

PLS regression: SmartPLS vs SPSS or SAS

Output in SmartPLS regression is quite different from that in SPSS or SAS due to fundamental differences of approach. SmartPLS requires explicit specification of latent constructs prior to analysis. In the model below, two constructs are stipulated, one for predictors and one for response variables. In PLS regression in SPSS and SAS there is no requirement to specify the number of latent constructs or dimensions a priori nor to associate indicator variables with particular dimensions. Rather, the researcher can accept the default number of dimensions.

Even if the researcher constrains the model to the same number of dimensions as in the SmartPLS solution, the factors computed by SPSS or SAS will be data-driven dimensions rather than the theory-driven dimensions required by SmartPLS modeling. In SAS and SPSS, the same constructs explain both the predictor and the response indicators, whereas in SmartPLS regression models there are separate constructs for the predictors and the response indicators. Therefore the coefficients will be different and have a different meanings, and model fit will differ as well. Most SmartPLS users would rarely perform PLS regression modeling at all. Rather they would perform PLS-SEM modeling as described above, specifying the number of exogenous and endogenous factors in advance and associating specified indicators with each, along with structural arrows connecting factors as suggested by theory. SPSS and SAS do not support PLS-SEM modeling.

PLS regression: SPSS vs. SAS

Due to different algorithms and different options, the factors created by SPSS and SAS differ in composition and meaning, although for each all factors cumulatively explain 100% of the variance in the measured predictor and response variables. SPSS defaults to 4 and SAS to 5 factor solutions. SPSS handles nominal and ordinal dependent indicators as categorical whereas SAS assumes all dependent indicators are continuous. SPSS and SAS exhibit differences which lead to different path coefficients and different model fit for many PLS regression models.

Example

In this section a set of two response variables (happy, life) are predicted from a set of three predictor variables (race, age, prestg80), coded as follows:

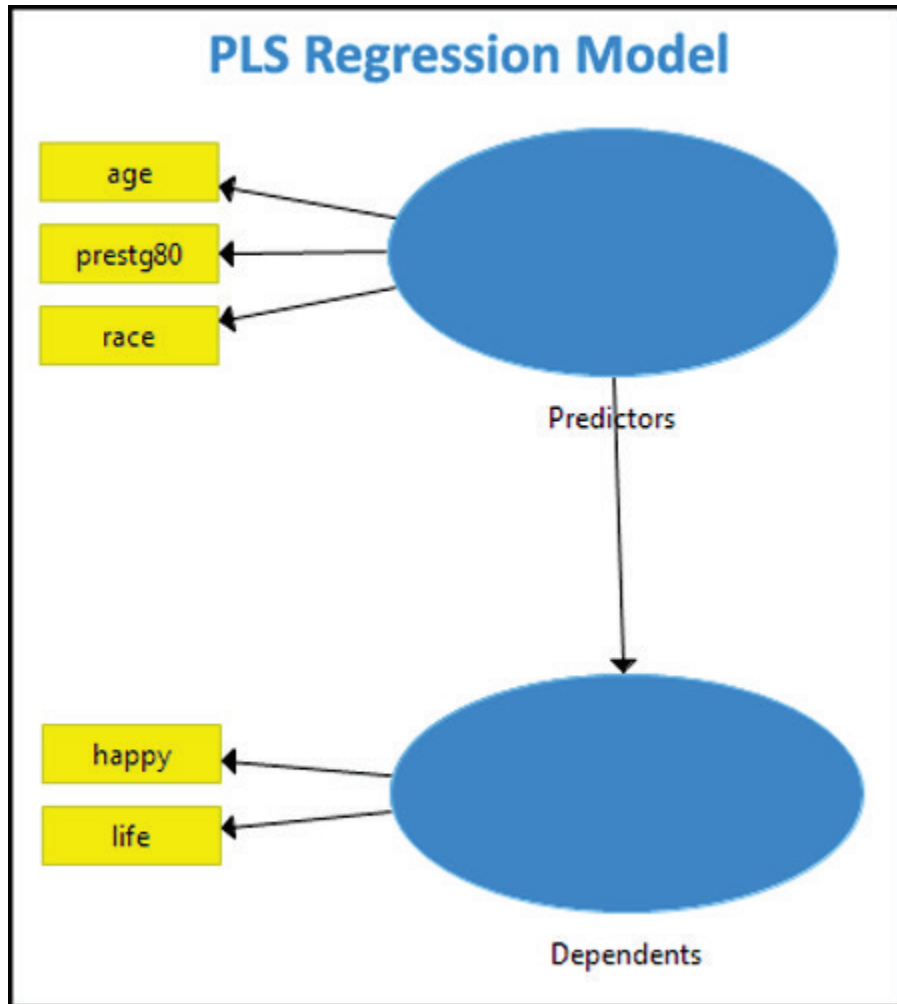
- happy: General happiness, 1=Very Happy, 2=Pretty Happy, 3=Not Too Happy; a categorical variable
- life: Is life exciting or dull?, 1=Exciting, 2=Routine, 3=Dull; a categorical variable
- race: Race of respondent, 1=White, 2=Black, 3=Other; a categorical variable
- age: Age of respondent; a continuous variable
- prestg80: Occupational prestige of respondent; a continuous variable

Data were from the SPSS sample file, 1991 U.S. General Social Survey.sav, but with multiple imputation of missing values since SmartPLS wants a dataset without missing values. The resulting dataset was labeled HappyLife.csv and is available [above](#).

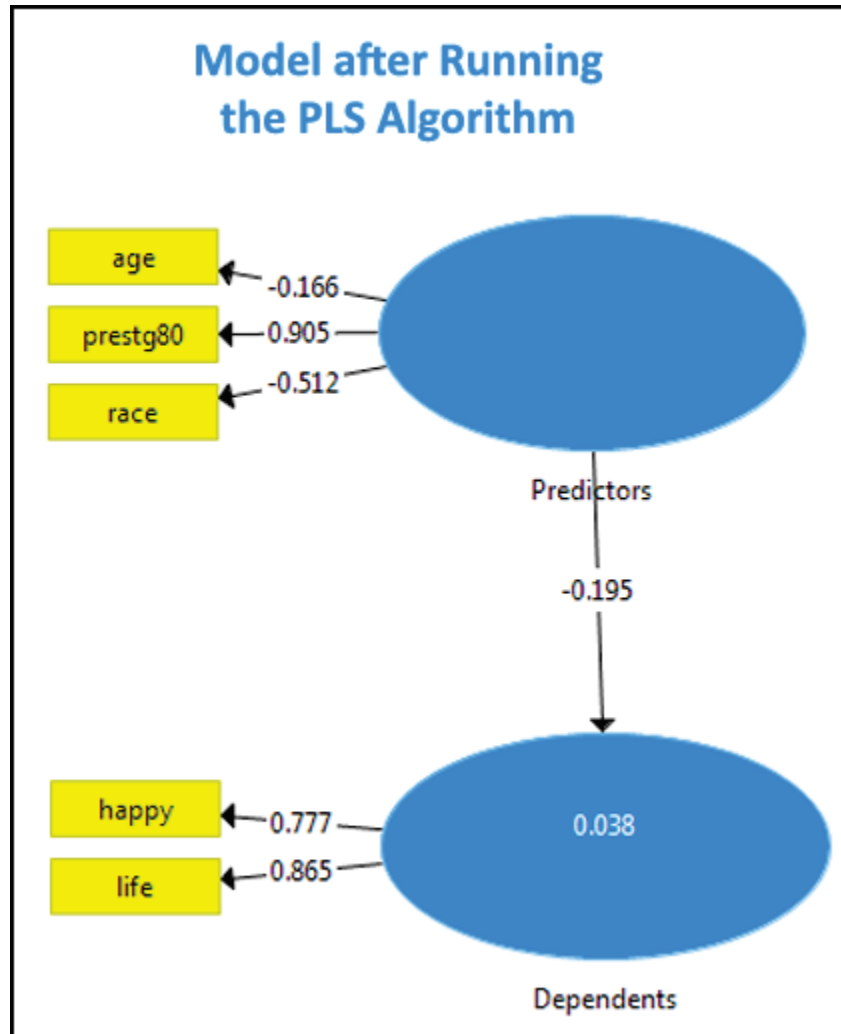
Data input and model creation. Same as described [above](#) for SmartPLS path modeling.

Creating a simple regression model in SmartPLS

In this example a simple regression model is created in which race age, and occupational prestige predict happy and life attitudes. In the usual type of PLS regression model there are two factors, one for the predictor variables and one for the response variables. All measured predictor variables are indicators for the predictor factor and all measured dependent variables are indicators for the dependent factor. The graphical model is shown below.



When the model is run by selecting Calculate > PLS Algorithm, from the SmartPLS menu, path coefficients appear near the measurement and structural arrows in the model. If desired, the R-squared value may be displayed within the dependent factor (ellipse) is the R-squared value for the dependent factor, which indicates a weak model for these data.

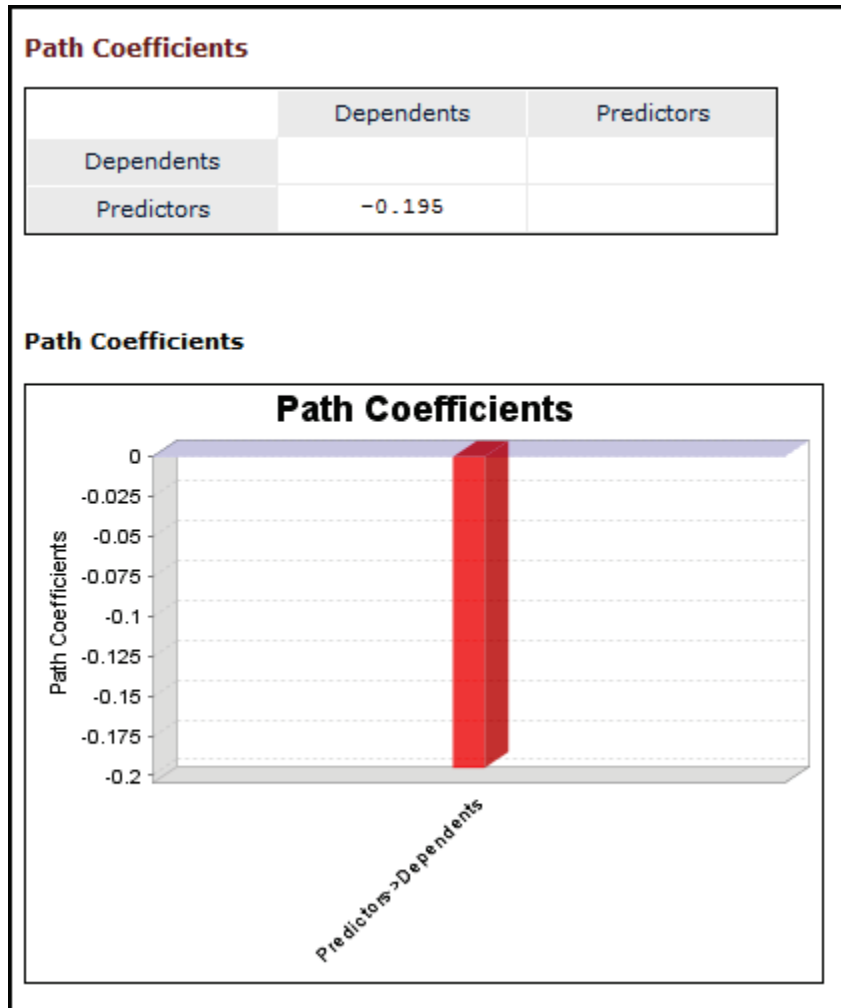


SmartPLS output for PLS-regression

Statistical output parallels that displayed and discussed [above](#) for PLS-SEM modeling in SmartPLS. Only partial output corresponding to the graphical model above is illustrated below.

Path coefficient

In a PLS regression model there is only one path, from the construct for the predictors to that for the dependents. SmartPLS output is shown below.



The histogram output is interesting in path models, where there are multiple paths in the structural (inner) model, but is trivial here. Below, such histograms are not displayed. The path coefficient is the same as that displayed in the completed path diagram above.

Outer loadings and weights

Path output for the measurement (outer) model may be displayed as loadings or weights, shown below. Path “loadings” are those shown by default in the completed path diagram above and are what is usually meant by “path coefficients” in reflective PLS models, as in the current example. See the previous discussion [above](#) regarding the choice between indicator loadings and weights.

Outer Loadings		
	Dependents	Predictors
age		-0.166
happy	0.777	
life	0.865	
prestg80		0.905
race		-0.512

Outer Weights		
	Dependents	Predictors
age		-0.212
happy	0.537	
life	0.674	
prestg80		0.845
race		-0.391

Model fit/quality criteria

To assess model fit, SmartPLS outputs the following coefficients in the default PLS algorithm:

[R Square](#)

[f Square](#)

[Average Variance Extracted \(AVE\)](#)

[Composite Reliability](#)

[Cronbach's Alpha](#)

[Discriminant Validity](#)

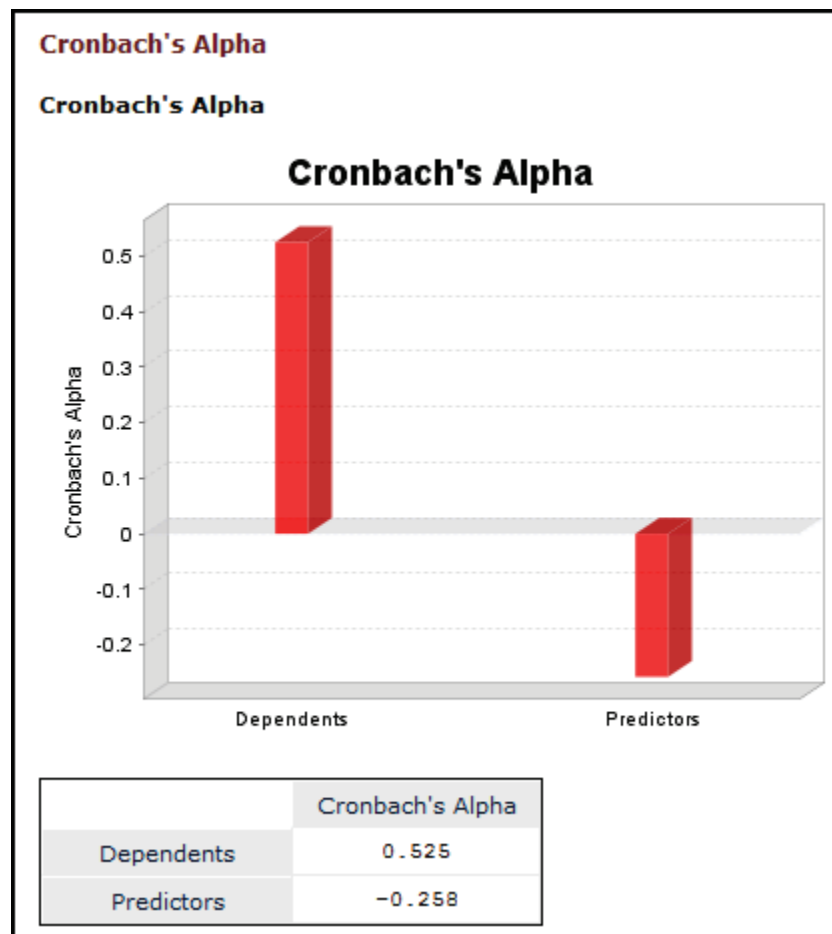
[Collinearity Statistic \(VIF\)](#)

[SRMR](#)

These coefficients were discussed in a previous section [above](#)., or click on specific links in the list above.

Cronbach's alpha

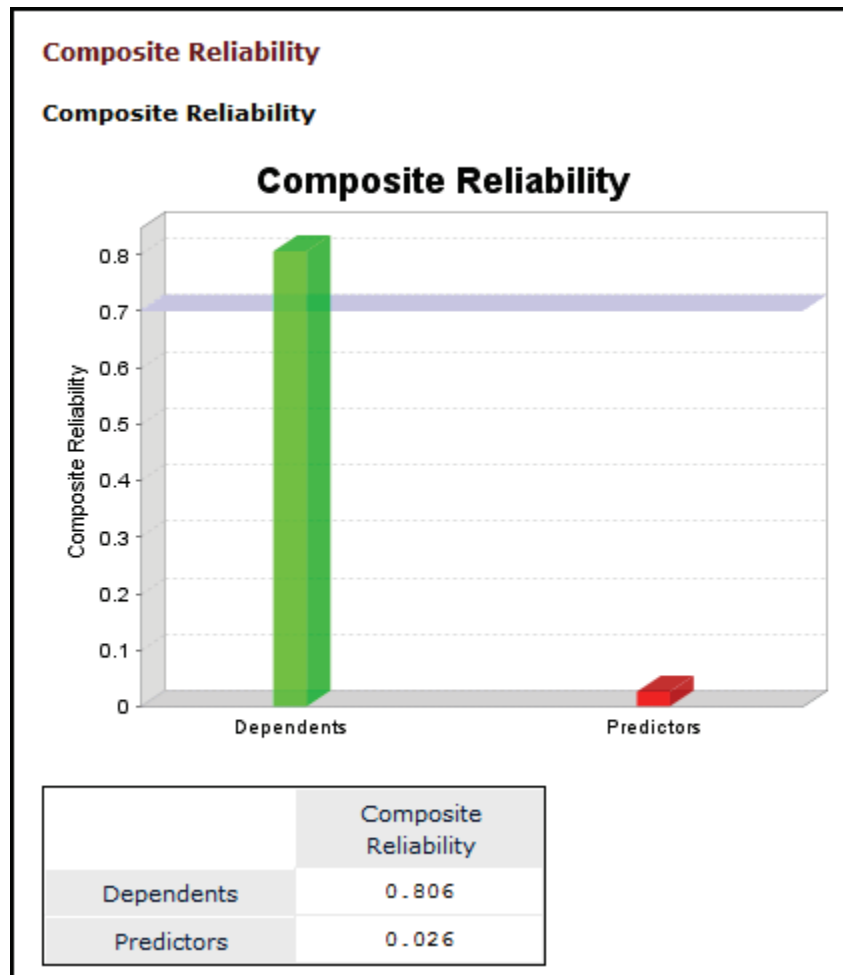
Although fit and quality measures were discussed previously above, Cronbach's alpha output is shown as an illustration below. Cronbach's alpha is a common measure of convergent validity, measuring the internal consistency of constructs. By common rule of thumb, .60 or higher is adequate reliability for exploratory purposes, .70 or higher is adequate for confirmatory purposes, and .80 or higher is good for confirmatory purposes. Here Cronbach's alpha is below .60, a sign that the indicators for the "Predictors" construct and for the "Dependents" construct do not cohere well. This implies the constructs are multi-dimensional rather than unidimensional. Multidimensionality is one reason that the R-squared between the two constructs is low. In this example.



Composite reliability

Composite reliability is a somewhat more lenient convergent validity criterion often favored by PLS researchers. It uses the same cutoffs as for Cronbach's

alpha. For the current example, this reliability measure shows good reliability for the “Dependents” construct but poor reliability for the “Predictors” construct.



Other output

SmartPLS produces a variety of other output not illustrated here:

- Indirect Effects
- Total Effects
- Latent Variable Scores
- Residuals
- Stop Criterion Changes
- Base Data
- Setting
- Inner Model
- Outer Model

Indicator Data (Original)
Indicator Data (Standardized)
Indicator Data (Correlations)

PLS regression modeling with SPSS

Overview

SPSS added PLS starting with version 16, in 2007. It implements PLS regression (projection to latent structure regression), not full PLS path modeling as described above for SmartPLS. In the menu system it is found under Analyze > Regression > Partial Least Squares.

The PLS algorithm extracts a latent factors (technically, components since principal components analysis is used) for the set of independent variables and for the set of dependent variables, such that explanation of the covariance between the two latent variables is maximized. Using multiple regression for scale variables, a classification algorithm for categorical variables, or a mixed model, the dependent variable or variables is predicted.

SPSS recommends PLS regression as “particularly useful when predictor variables are highly correlated or when the number of predictors exceeds the number of cases” (from SPSS online help for PLS).

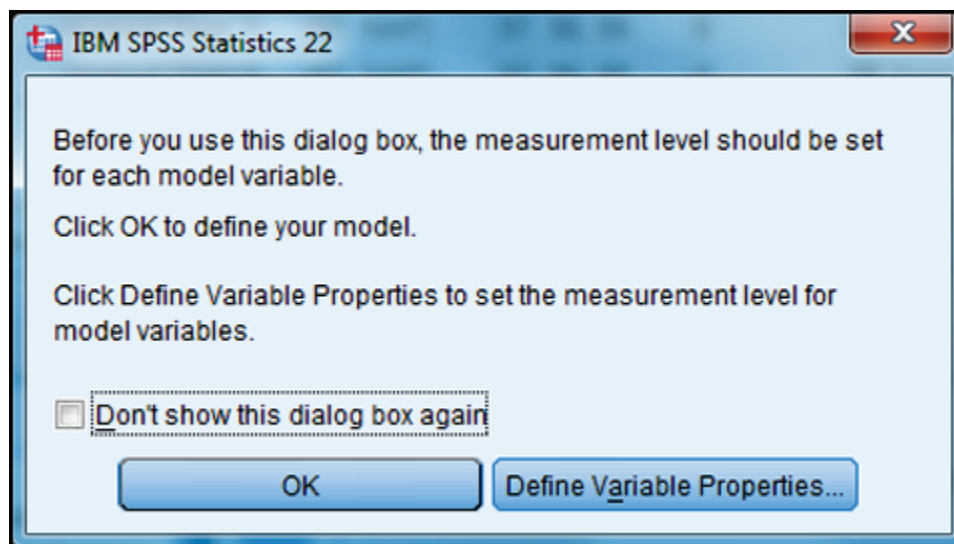
Python runtime environment. SPSS PLS is an extension which requires the Python Extension Module be installed separately. Further information about installing the PLS module for SPSS is found in the FAQ section [below](#).

SPSS example

Data for the example used in this section was the SPSS sample file, 1991 U.S. General Social Survey.sav, available [above](#). The dependent and independent variables may be continuous (interval, scale) or categorical (nominal or ordinal, which are treated equivalently). In variable view in the SPSS worksheet, the researcher should make sure that the variables to be used in the model are at the desired and proper level. For the example data as downloaded here, the levels are as follows:

age	scale
prestig80	scale
race	nominal
happy	ordinal
life	ordinal

If the researcher is uncertain about data levels, when PLS is first run in SPSS, the window below appears. If “Define Variable Properties” is clicked, SPSS will analyze the data distribution of specified variables and will suggest the appropriate data level.



Also note that in the main SPSS window for PLS, show [below](#), in the “Variables” tab, the researcher may highlight and right-click any variable to set its data level on a temporary basis (for the current session).

For these data, a set of two response variables (happy, life) are predicted from a set of three predictor variables (race, age, prestig80), coded as follows:

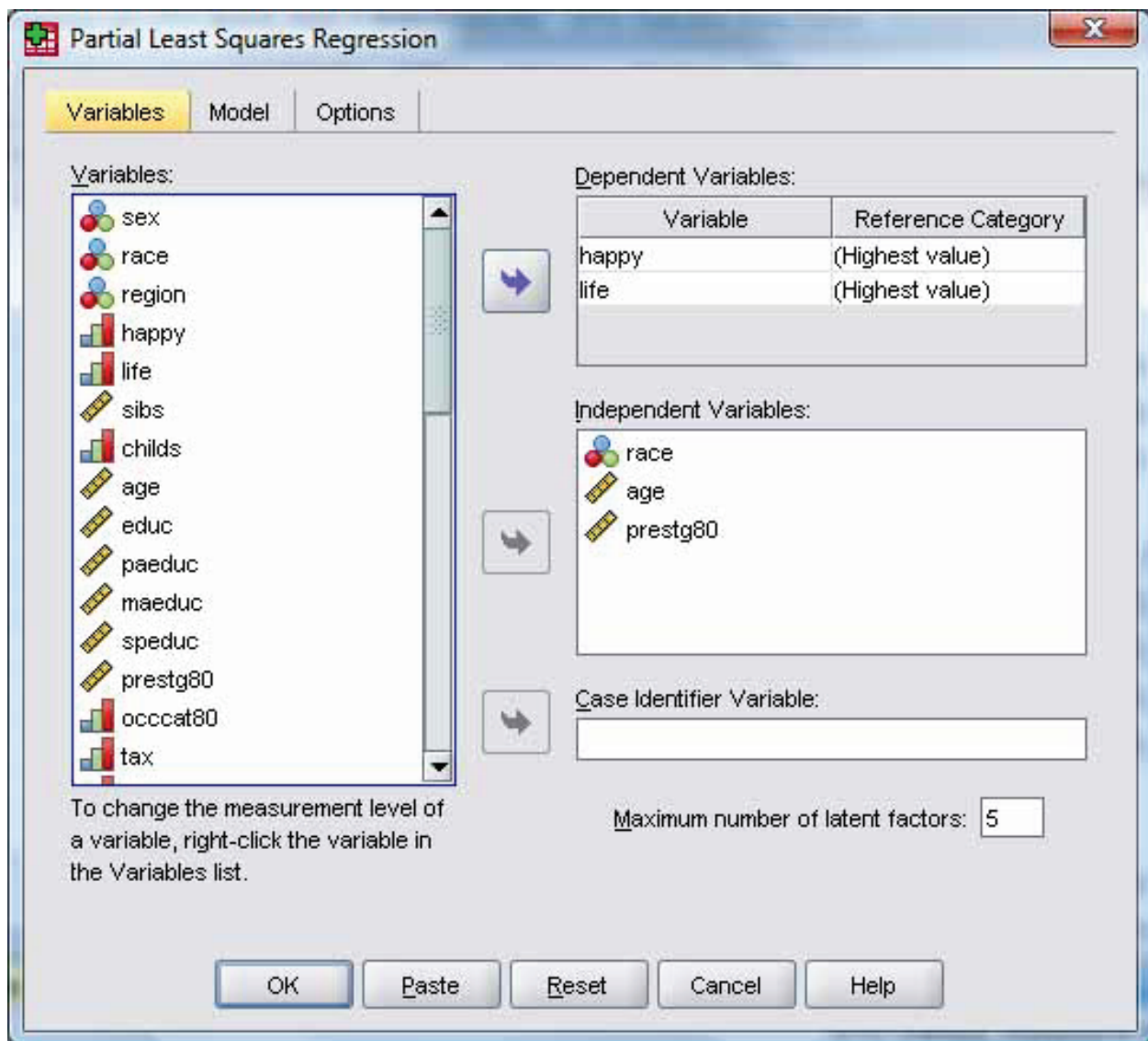
- happy: General happiness, 1=Very Happy, 2=Pretty Happy, 3=Not Too Happy; a categorical variable
- life: Is life exciting or dull?, 1=Exciting, 2=Routine, 3=Dull; a categorical variable
- race: Race of respondent, 1=White, 2=Black, 3=Other; a categorical variable
- age: Age of respondent; a continuous variable

- prestg80: Occupational prestige of respondent; a continuous variable

SPSS input

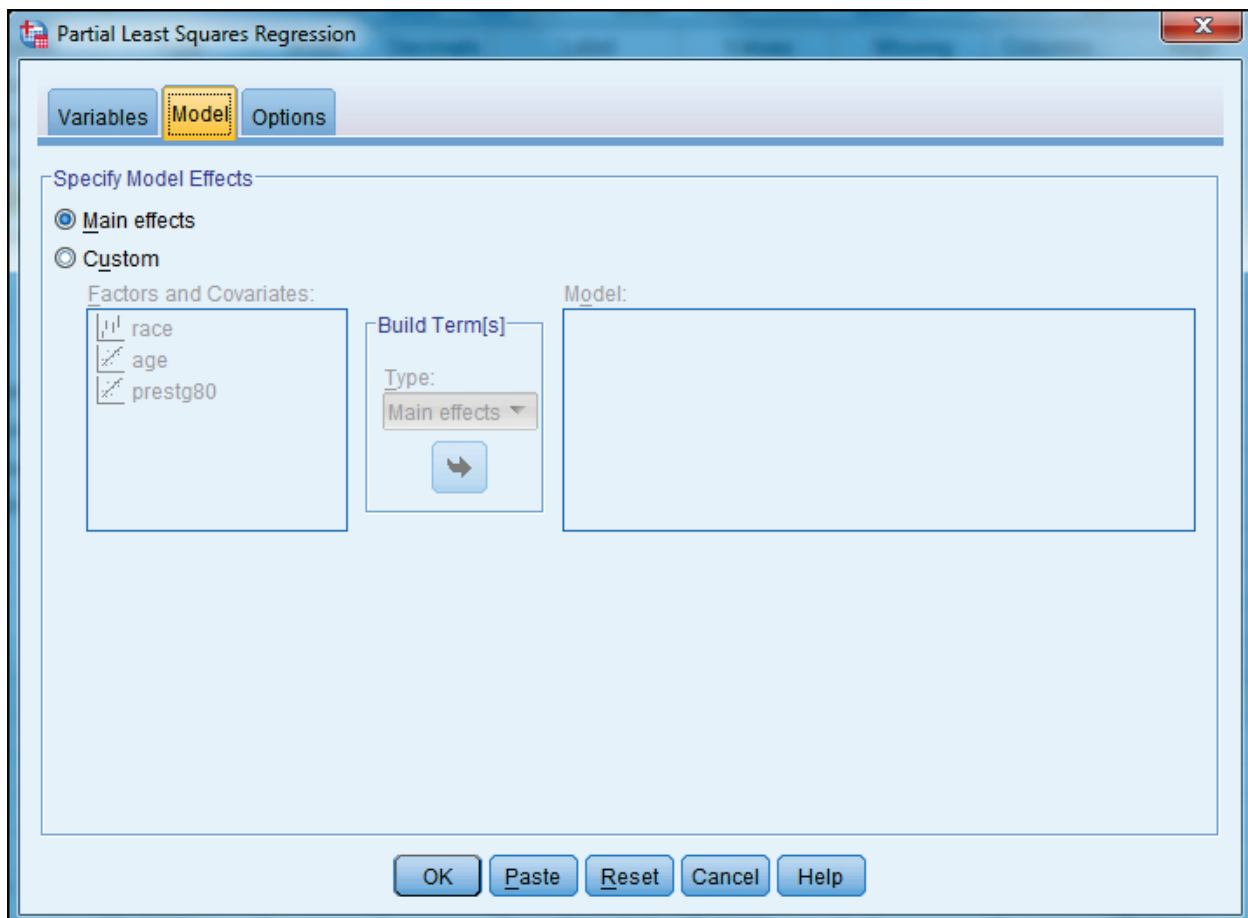
Prior to running SPSS's PLS module, load the dataset described above (1991 U.S. General Social Survey.sav) and, if needed, specify the data levels of variables to be employed as described above.

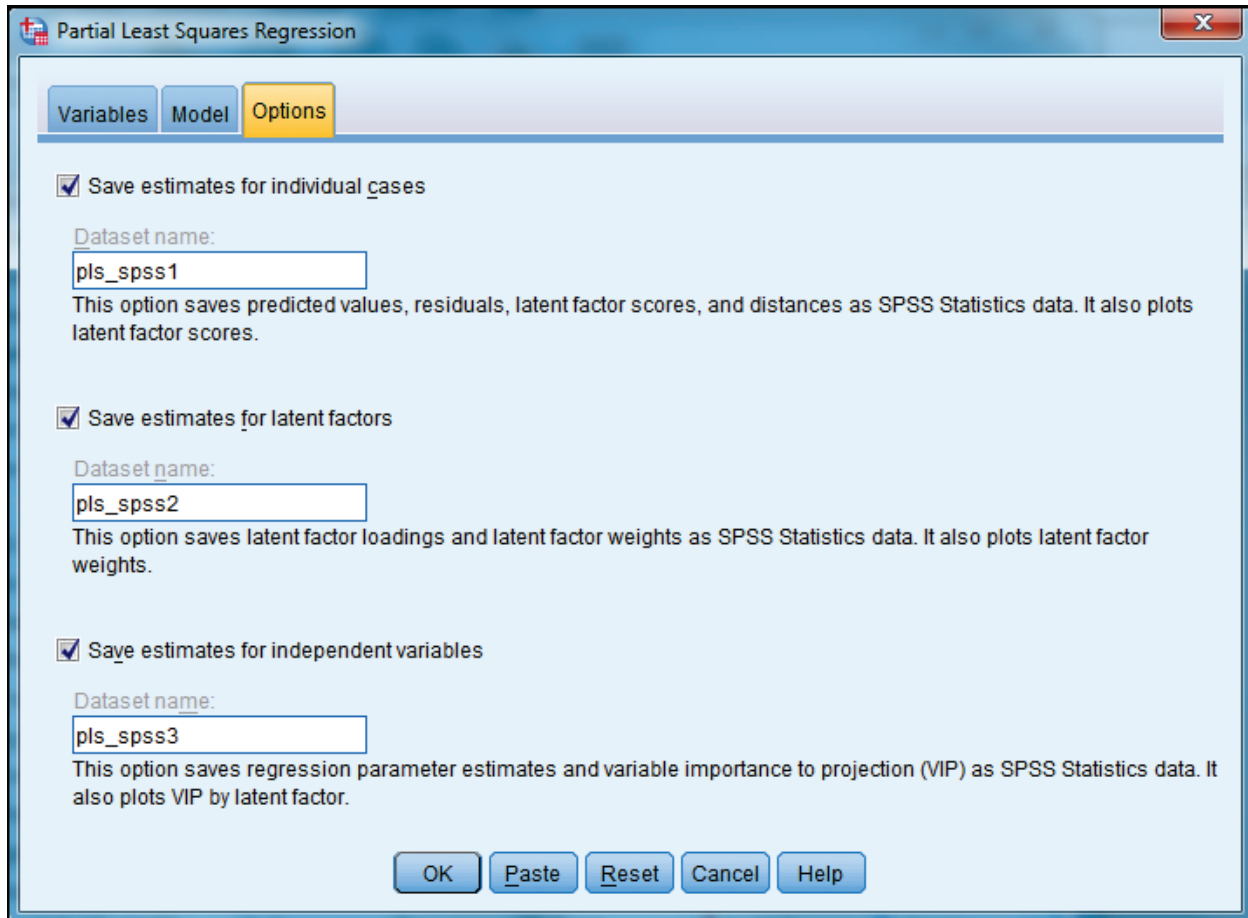
After the SPSS PLS module is installed, select Analyze > Regression > Partial Least Squares to bring up the dialog below.



Under the “Variables” tab, drag the dependent and independent variables to their respective locations as shown in the figure above. SPSS can tell the data level of each and marks each independent variable with symbols shown in the illustration (a ruler symbol for continuous, a bar chart for ordinal, and three circles for nominal variables). For the dependent variables, which here are ordinal, the default is for the highest level to be the reference level. The reference level may be changed by highlighting one of the dependent variables (e.g., happy), yielding other reference level options.

The Model and Options tabs are also illustrated below. In this example the default settings are accepted under the Model Tab. The default for the Options tab is nothing checked, but here checks were added so as to obtain output described below in the “SPSS output” section.





The three options above are:

Save estimates for individual cases. Saves predicted values, residuals, distance to latent factor model, and latent factor scores by case (observation). This option also plots latent factor scores.

Save estimates for latent factors. Saves latent factor loadings and latent factor weights and plots latent factor weights.

Save estimates for independent variables. Saves regression parameter estimates and variable importance to projection (VIP). This option also plots VIP by latent factor.

SPSS output

Proportion of variance explained by latent factors

This section of the output lists latent factors by rows (here, there are 4). The "cumulative X variance" is the percent of variance in the X variables (the predictors) accounted for by the latent factors. Four factors were necessary to explain 100% of the variance in the dependent variable. The "cumulative Y variance" is the percent of variance in the Y variables (the dependent variables) accounted for by the latent factors.

A well-fitting model would explain most of the variation in both the X and Y variables, which is not the case in this example. The cumulative R-square is interpreted as in regression. "Adjusted R-square" penalizes for model complexity (increasing number of factors). The more a factor explains in the variation of the X variables, the more it well reflects the observed values of the set of independent variables. The more a factor explains of the variation in the Y variables, the more powerful it is in explaining the variation in a new sample of dependent values, which is why the "Cumulative Y Variance" equates to "R-Square" in the table below.

Latent Factors	Statistics				
	X Variance	Cumulative X Variance	Y Variance	Cumulative Y Variance (R-square)	Adjusted R-square
1	.334	.334	.011	.011	.010
2	.274	.608	.004	.015	.013
3	.358	.966	.002	.017	.014
4	.034	1.000	.000	.017	.013

PRESS (predicted error sum of squares)

Not shown above, but when cross-validation is requested, the variance explained table will also contain a column for the PRESS statistic, first proposed by Allen (1974). In the "Proportion of Variance Explained" table above, the lowest PRESS statistic flags the row with the best-fitting model. That is, the row with the lowest PRESS statistics shows the optimal number of useful latent factors.

However, when PRESS statistic values differ only by very small amounts, on parsimony grounds the researcher may opt to re-run the model requesting the number of factors for the row corresponding to the fewest factors for the set of rows all comparably small on the PRESS statistic. That is, PRESS tends to be higher for more complex models (ex., more factors), just as R^2 is. An adjusted PRESS statistic to compensate for potential bias has been proposed (Hastie & Tibshirani, 1990) but is not incorporated in SPSS or SAS output. Nonetheless, the researcher should be aware of the parsimony issue.

The PRESS statistic is computed using a leave-one-out method. Using a jackknife technique, the dependent variable can be predicted using the full dataset and for the dataset leaving out a given case. This can be done for all cases, leaving one out each time. The difference in estimates of the dependent variable between the full dataset and the leave-one-out dataset for the given case is the PRESS residual for that case. The sum of these squared residuals is the PRESS statistic. All other things equal, the lower the PRESS statistic, the better the model in terms of prediction, where prediction is defined as prediction to the leave-one-out data. In actual software calculation, formulae have been developed not requiring an iterative procedure to arrive at the PRESS statistic (see, for ex., Tarpey, 2000).

Latent component weights and loadings

Loadings and weights both indicate how much each independent variable contributes to the axis representing the four factors (technically, components) shown in the four columns of the table below. The sign indicates the direction of the correlation. The "weights" are X-loadings, representing the directions of the lines for each independent in X-space. Weights are used to plot the position of independent and dependent variables in factor space, as illustrated [below](#). The "loadings" are X-weights, representing the correlation of X variables with the Y-scores.

Typically, X-weights and X-loadings are similar in sign. Loadings, as in principal components factor analysis, are used to impute meanings for the components (ex., Component 1 is heavily associated with occupational prestige). By one rule of thumb in confirmatory PLS factor analysis, loadings should be .7 or higher to confirm that independent variables identified a priori are represented by a particular factor (Hulland, 1999: 198).

However, the .7 standard is a high one and real-life data may well not meet this criterion, which is why some researchers, particularly for exploratory purposes, will use a lower level such as .4 for the central factor and .25 for other factors (Raubenheimer, 2004). In any event, factor loadings must be interpreted in the light of theory, not by arbitrary cutoff levels. If factors can be convincingly labeled, then one may use R-square contributions from the proportion of variance explained table above to assign relative importance to, say, occupational prestige (factor 1) vs. race (factor 4). To the extent that variables are cross-loaded, such comparisons may be unwarranted or misleading.

Weights				
Variables	Latent Factors			
	1	2	3	4
[race=White]	.212	-.108	.544	.711
[race=Black]	-.163	.177	-.600	.707
age	-.019	-.973	-.397	-.005
prestg80	.963	.142	-.571	.000
[happy=Very Happy]	.101	-.066	-.026	.015
[happy=Pretty Happy]	-.043	.053	.056	.019
[life=Exciting]	.128	.080	-.027	.050
[life=Routine]	-.101	-.030	.021	-.049

Loadings				
Variables	Latent Factors			
	1	2	3	4
[race=White]	.433	-.281	.660	.730
[race=Black]	-.435	.276	-.665	.681
age	-7.813E-5	-.933	-.232	.036
prestg80	.869	.090	-.262	-.045
[happy=Very Happy]	.449	-.508	-.590	.185
[happy=Pretty Happy]	-.376	.559	.611	-.073
[life=Exciting]	.594	.524	-.438	.738
[life=Routine]	-.584	-.505	.445	-.732

Variable importance in the projection (VIP) for the independent variables

VIP coefficients reflect the relative importance of each X variable for each X factor in the model. VIP coefficients thus represent the importance of each X variable in fitting both the X- and Y-scores, since the Y-scores are predicted from the X-scores. As a rule of thumb advanced by Wold (1994), the researcher may wish to drop from the model any independent variable which (a) has a small VIP ($< .8$) on

all factors, and (b) also has a regression coefficient (see "parameter estimates" below) small in absolute size. Here, race is a candidate for deletion.

Variables	Latent Factors			
	1	2	3	4
[race=White]	.425	.384	.505	.524
[race=Black]	.325	.333	.499	.518
age	.037	.973	.956	.951
prestg80	1.927	1.675	1.628	1.619

Cumulative Variable Importance

Regression parameter estimates by dependent variable

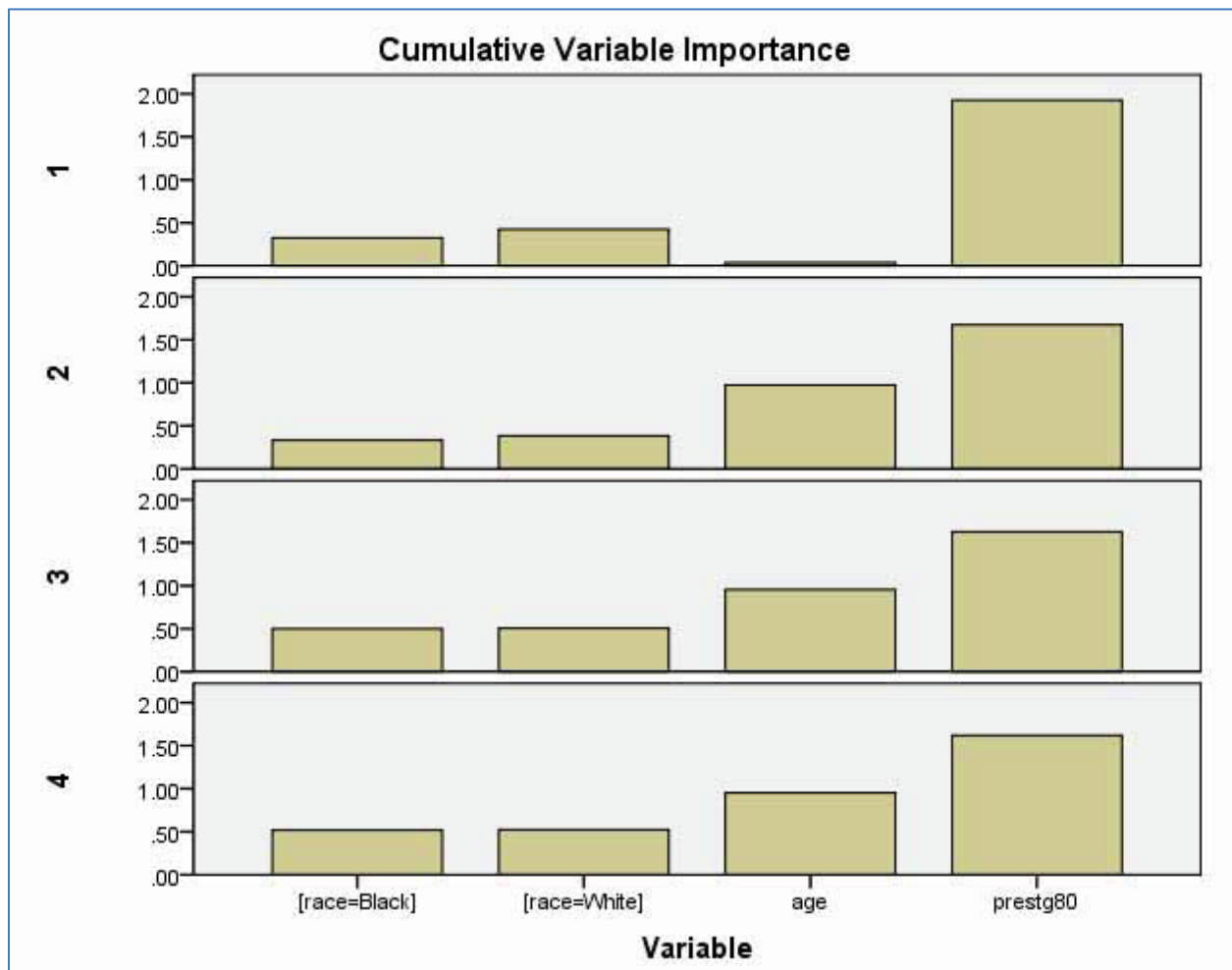
In the example below, the dependents had three levels. Level 3 is treated by default as the reference category, which is why the table below does not have columns for Happy=3="Not too happy" or Life=3="Dull". The parameter estimates are the regression coefficients used in conjunction with the independent variables, which are both categorical and covariate variables, to predict the dependent variables. The sign of the coefficient indicates the direction of the effect. For instance, below, being white rather than other race (the reference category for race) is associated positively with being very or pretty happy compared to not too happy, and with finding life to be exciting rather than dull. Being white rather than other race is negatively associated with finding life routine compared to dull.

Independent Variables	Dependent Variables			
	[happy=Very Happy]	[happy=Pretty Happy]	[life=Exciting]	[life=Routine]
(Constant)	.040	.753	.249	.716
[race=White]	.033	.041	.055	-.059
[race=Black]	-.003	-.006	.069	-.056
age	.002	-.002	-.002	.001
prestg80	.004	-.002	.006	-.004

Charts/plots

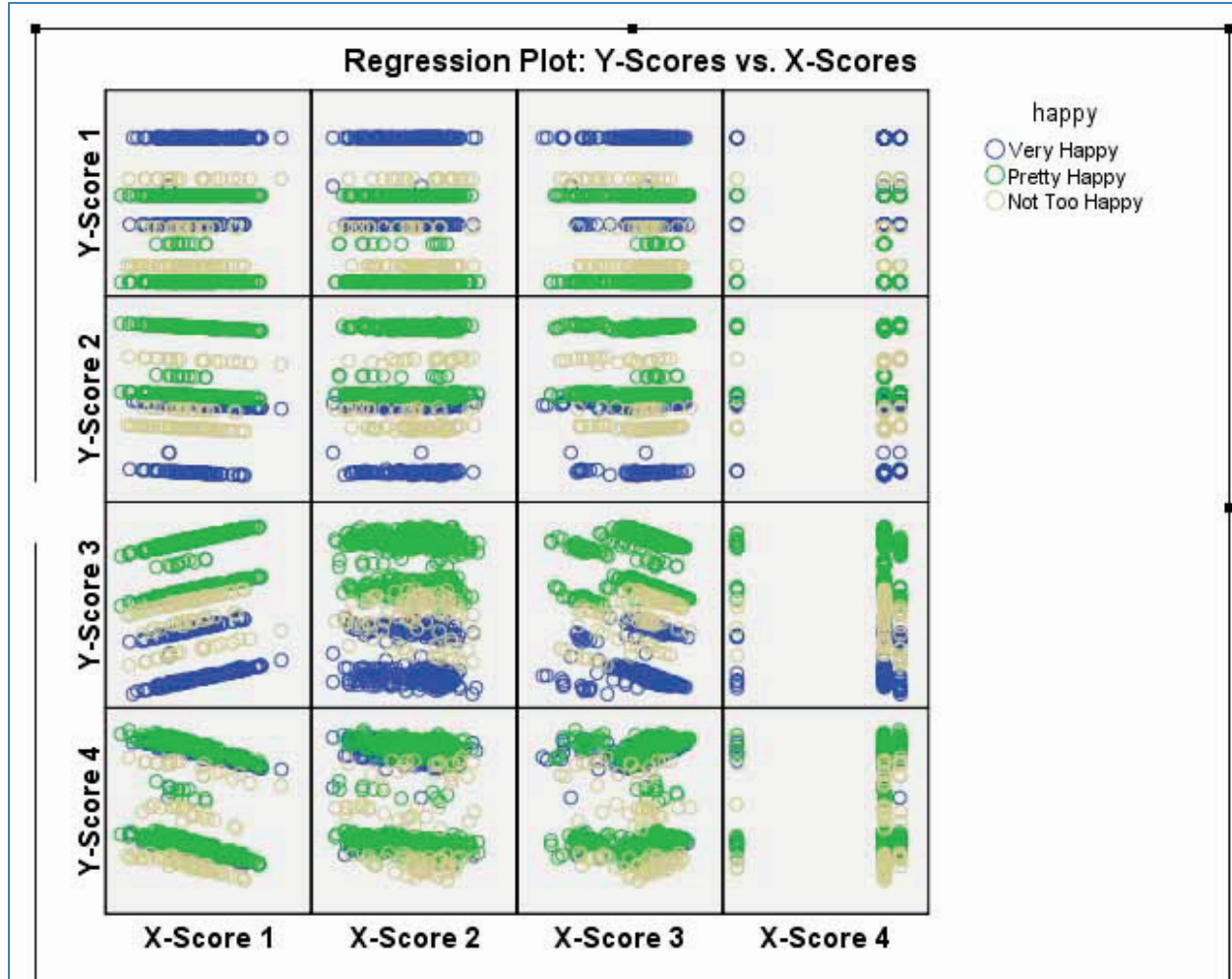
In SPSS, the following plots are available.

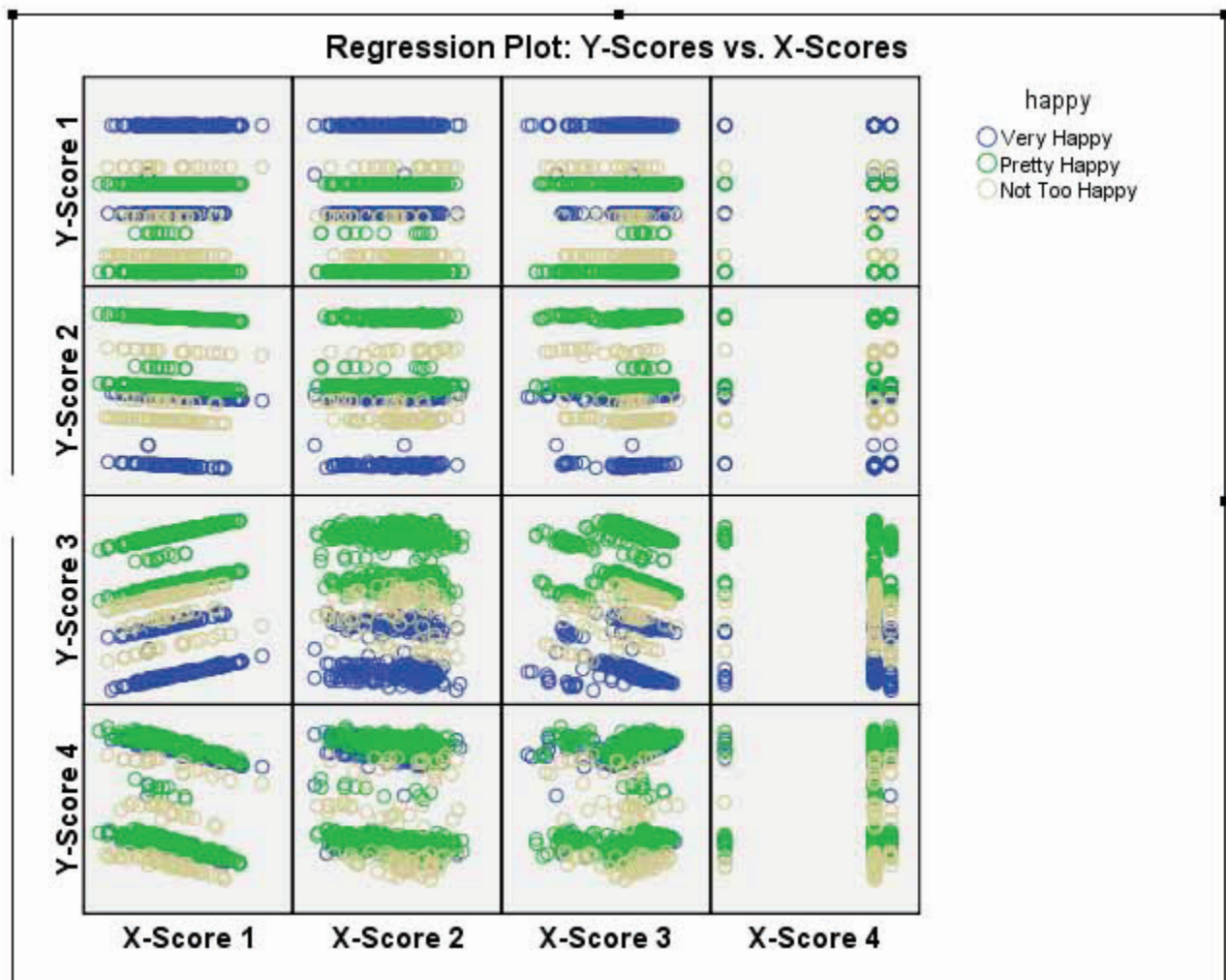
Plots of variable importance to projection (VIP) by latent factor: This plot simply reproduces in graphic form the cumulative VIP scores from the "Variable importance in projection" table above. For this example, occupational prestige is the most important predictor for all four factors used to predict the response variables.



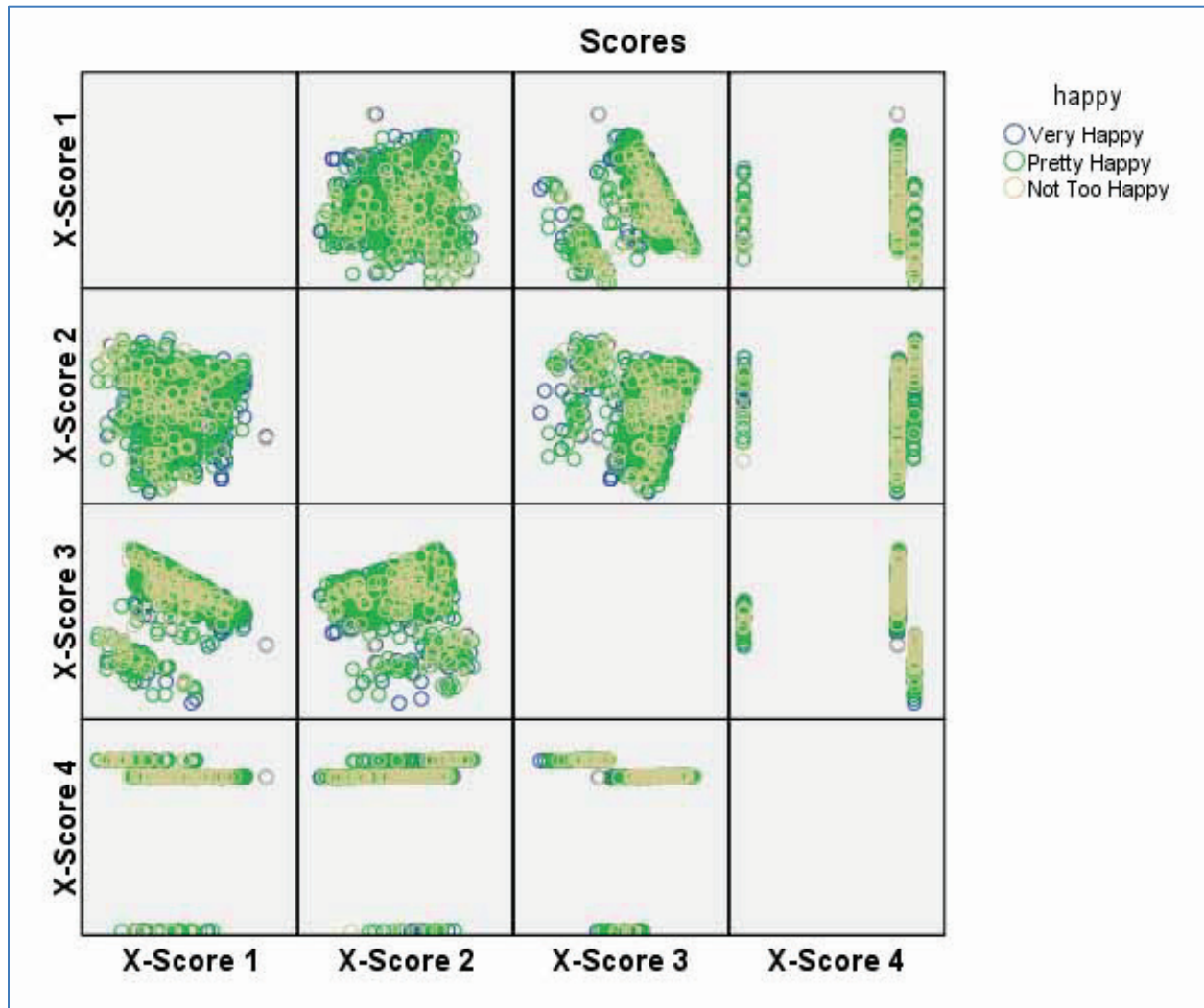
Plots of latent factor scores: In this plot matrix, the X and Y scores for each factor are plotted against each other for the three levels of the first dependent variable, Happy. These plots show the direction toward which each PLS X-factor is projecting with respect to the Y factors. For instance, in the example below, the X-

scores for factor 1 are associated with increasing values on Y-scores for factor 3, but with decreasing Y-scores for factor 4. Overall, however, the prevalence of horizontal lines in the plot matrix reflects a weak model, with a low percent of variance explained.



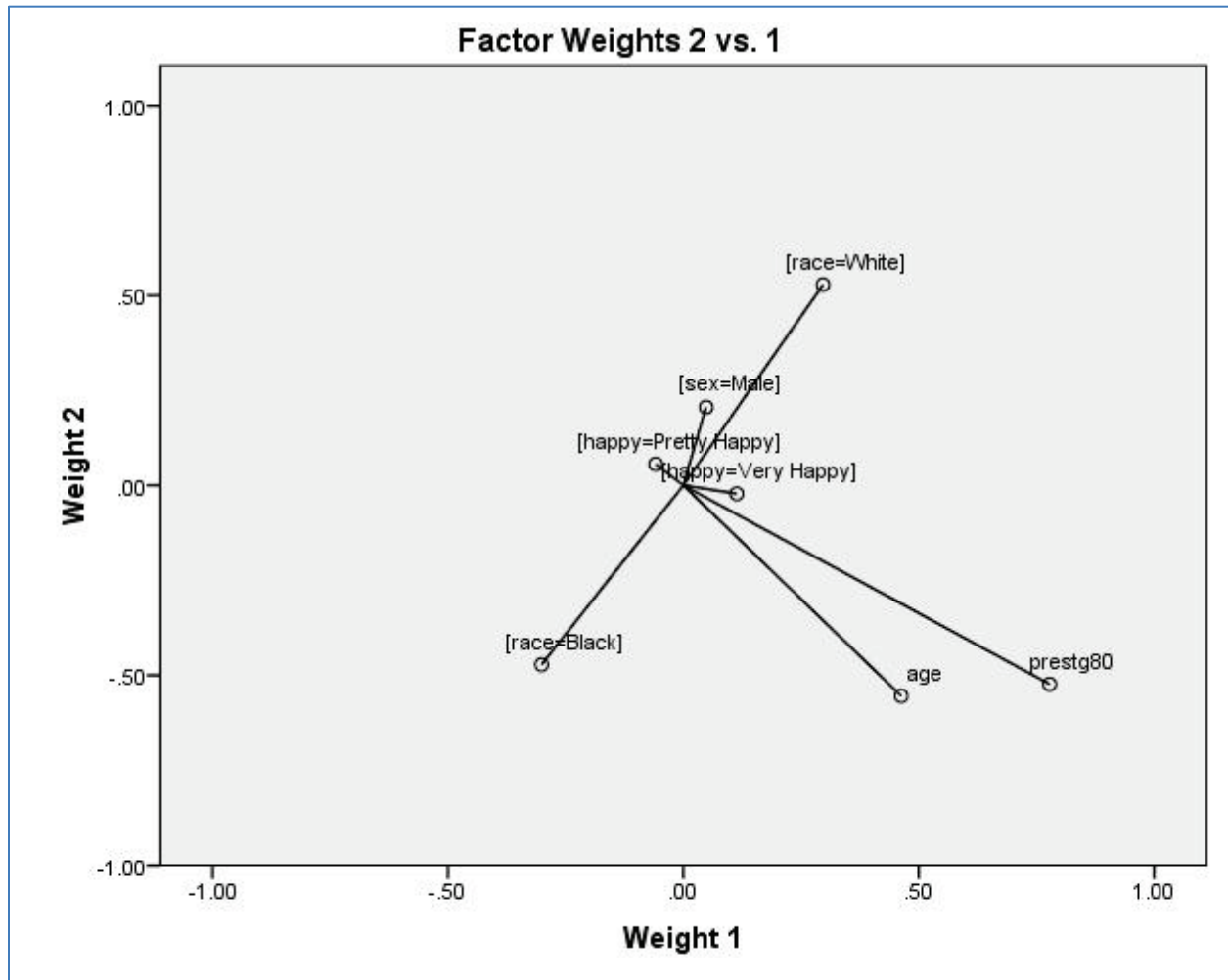


It is also possible to plot X scores from one PLS factor against the X scores for a different PLS factor. In the example below, X-scores for factor 1 are negatively related to X-scores for factor 3, but are largely unrelated to those for factor 2.



Plots of latent factor weights

In SPSS, these are plotted for the first three latent factors. Variables located near the 0,0 mark contribute little to model fit. Variables further from the origin contribute more to differentiating the X factors (dimensions). Variables which contribute little on the X factors which explain the bulk of the variance in Y are variables which the researcher may wish to drop from the model; dropping them may improve the Y-variance explained. The plot for factor 1 vs. 2 is shown below, but there are also plots for the other possible pairs of factors among the first three.



Residual and normal quantile plots

Based on saved residual values, these are a means for identifying outlier observations. Residual plots and normal quantile plots also help identify non-normality and heteroscedasticity of error terms. A cloud-like residual plot with most cases in the middle third of the plot indicates heteroscedasticity and normality assumptions are not violated. In the case of normal quantile plots, points on a straight line indicate the normality assumption is not violated.

Saving variables

Clicking the "Options" tab in the SPSS PLS main dialog allows the user to save variables to a SPSS dataset. The dataset name should be unique or the file will be overwritten. One may save predicted values, residuals, distance to latent factor model, latent factor scores, latent factor loadings, latent factor weights,

regression parameter estimates and variable importance to projection (VIP) coefficients.

PLS regression modeling using SAS

Overview

SAS statistical software implements PLS regression under PROC PLS. In PROC PLS one set of latent factors is extracted for the set of manifest independent variables and another set of latent factors is extracted simultaneously for the set of manifest response (dependent) variables. The extraction process is based on decomposition of a crossproduct matrix involving both the independent and response variables. The X-scores of the independent latent variables are used to predict the Y-scores or the response latent variable(s), and these predicted Y scores are used to predict the manifest response variables. The X- and Y- scores are selected by PLS so that the relationship of successive pairs of X and Y scores is as strong as possible.

Though SAS was constrained in the example below to computer the same number of factors (4) as SPSS, the factors are entirely different, having in common only the fact that cumulatively all four explain 100% of the variance in the measured predictor and response indicators. See the discussion [above](#) about differences between SPSS and SAS. The factors in SmartPLS, SPSS, and SAS PLS regression models are not comparable in meaning or coefficients even though all seek to calculate parameter estimates for the same indicators using the same data.

For the same regression models, SAS online help recommends use of PROC CALIS as more efficient than its PROC PLS regression procedure. This follows the common preference among statisticians for causal modeling using covariance-based structural equation models (SEM) over variance-based modeling represented by PLS. PROC CALIS is discussed in the separate Statistical Associates “Blue Book” volume on “Structural Equation Modeling.”

Further discussion of PLS regression is found in the SPSS section [above](#).

SAS example

The same example data is used here for the SAS example as for SPSS. In this model the independent variable set includes age, race, and prestg80. The dependent variable set includes happy and life.

The data file is labeled USGSS1991.sas7bdat and is available [above](#). See also the discussion [above](#) of differences among SAS, SPSS, and SmartPLS implementations of PLS regression modeling.

SAS syntax

The syntax below contains the code entered into SAS's Editor window to run the model in this section. Text with slash and asterisk symbols constitute comments not implemented by SAS. Note SAS has numerous additional options not illustrated here.

```
LIBNAME in "C:\Docs\David\Statistical Associates\Current\data";
    /* LIBNAME declares the data directory and calls it 'in' */
    /* LIBNAME calls this folder 'in' but you can have a different name */
ODS HTML; /*turn on html output*/
ODS GRAPHICS ON; /*turn on ods graphics*/
TITLE "PROC PLS EXAMPLE" JUSTIFY=CENTER; /* Optional title on each page */
PROC PLS DATA=in.USGSS1991 DETAILS CENSCALE PLOTS (UNPACK)=(CORRLOAD (TRACE=OFF) VIP
XYScores DIAGNOSTICS);
    /* Use USGSS1991.sas7bdat in the in directory */
    /* DETAILS lists details of the fitted model for each factor */
    /* CENSCALE lists centering & scaling information */
    /* PLOTS = gives correlation loadings plot, variable importance plot, and */
    /* X-Scores vs. Y-Scores plot */
    /* DIAGNOSTICS IN the PLOTS option list gives residual plots */
    /* A CV=SPLIT(2) option could have requested cross-validation using */
    /* every 2nd case */
    /* A NFAC= option would set the number of factors to a specific number; */
    /* otherwise it is the number of predictors */
    /* A MISSING=EM option could request data imputation of missing values */
    /* using expectation maximization */
CLASS race;
    /* CLASS declares categorical predictors. */
    /* The ordinal dependent variables must be treated as interval */
MODEL happy life = race age prestg80 / SOLUTION;
    /* The syntax is MODEL response-variables = predictor-effects /<options >; */
    /* By default, data are centered and no intercept is needed */
    /* Add INTERCEPT as an option to use raw data with an intercept */
    /* SOLUTION lists final coefficients */
RUN;
ODS GRAPHICS OFF;
ODS HTML CLOSE;
```

Note that by default, SAS centers and scales both the predictor and response variables. If values are already centered around 0 or a target value, then the NOCENTER option should be used in the PROC PLS statement. If values are all on the same or comparable scale, then the NOSCALE option may be used in the PROC PLS statement to suppress scaling.

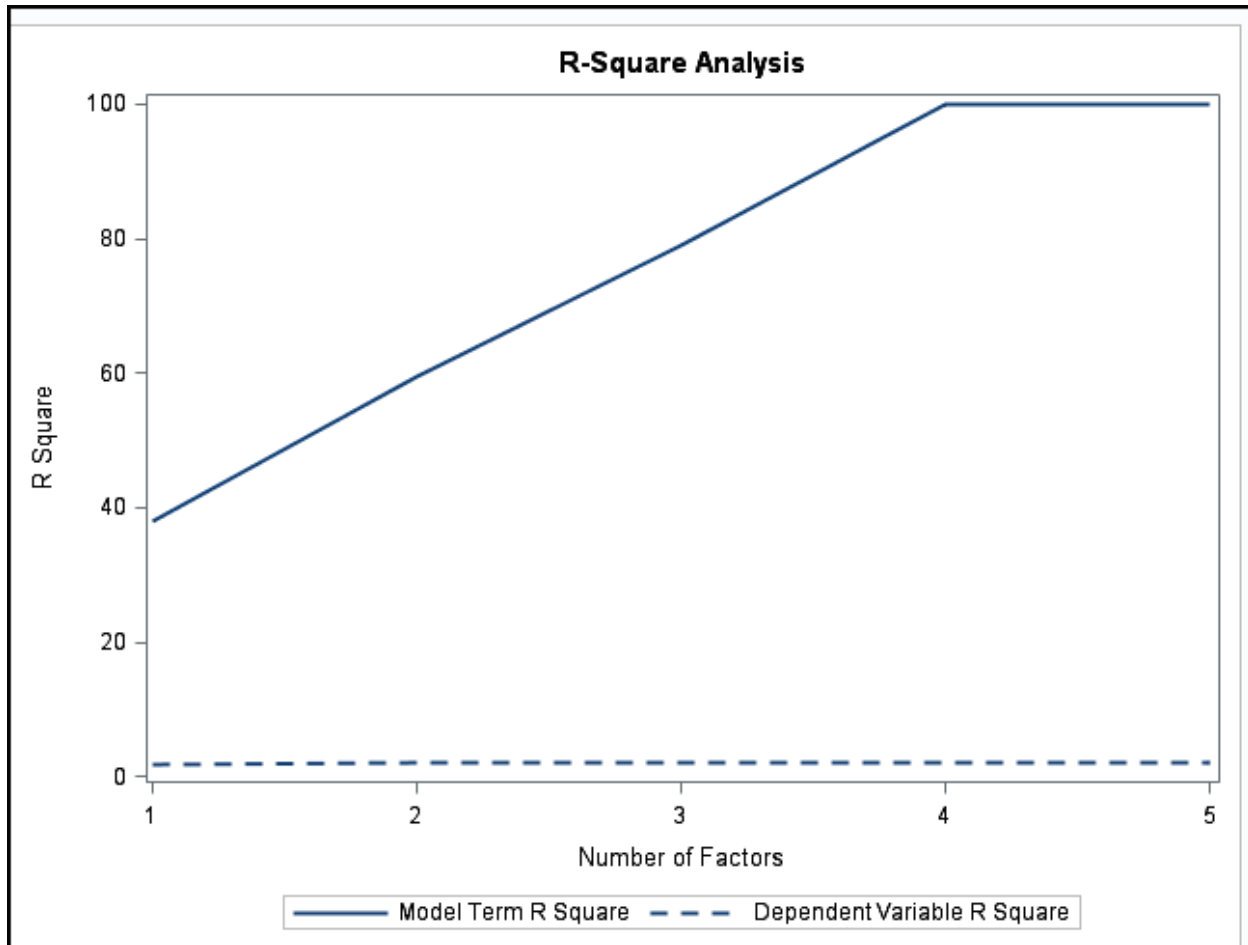
SAS output

R-square analysis

R-square analysis provides an indication of model fit. Unless a NFAC- option specifies fewer, SAS will extract as many factors as there are predictor variables (5 in this example). Below, 79% of the predictor variables are explained by the first three factors and 100% by the first four. However, on the dependent variable side (for which the manifest variables are life and happy), only about 2% is explained even on the last factor.

Percent Variation Accounted for by Partial Least Squares Factors				
Number of Extracted Factors	Model Effects		Dependent Variables	
	Current	Total	Current	Total
1	37.8957	37.8957	1.6754	1.6754
2	21.6258	59.5216	0.4039	2.0793
3	19.4924	79.0140	0.0343	2.1136
4	20.9860	100.0000	0.0006	2.1142
5	0.0000	100.0000	0.0000	2.1142

The “R-Square Analysis” plot shows the cumulative percent of variance explained by each factor. This contains the same data as the table above, but in graphic form. The R-squared for the dependent variables hugs the X axis, reflecting a very weak model.

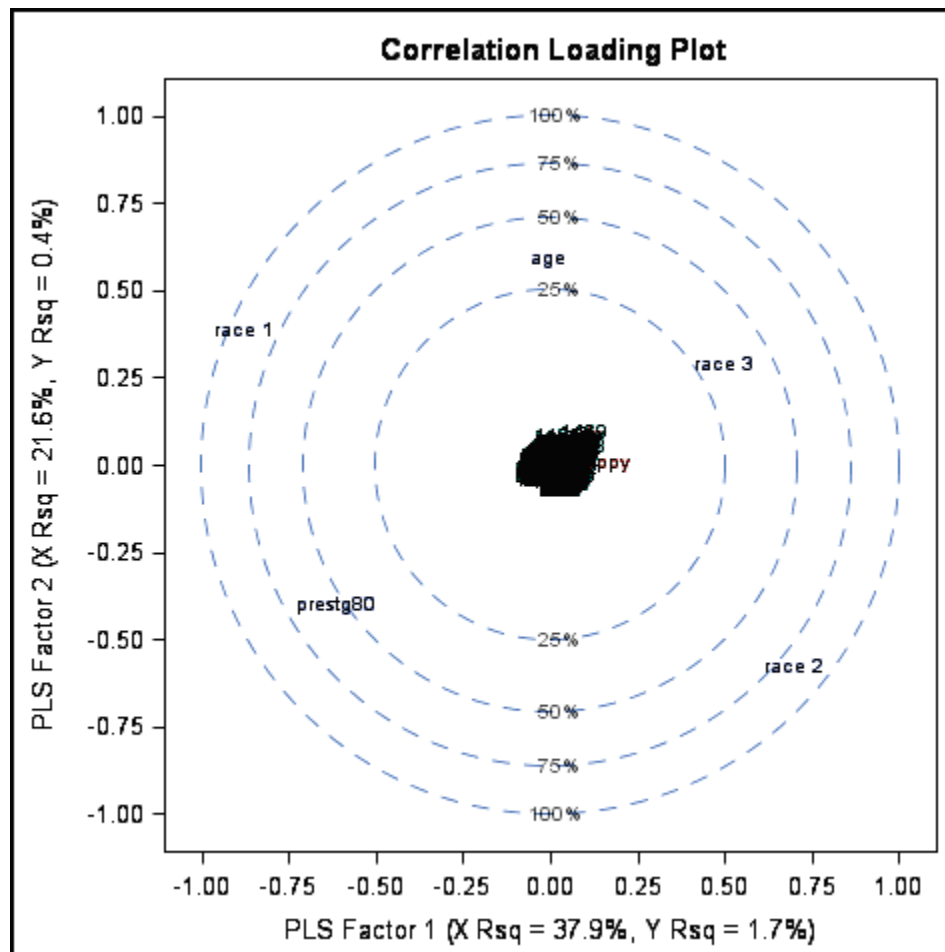


Correlation loading plot

By default, SAS generates the plot below if ODS graphics are turned on. For the first two factors it shows the location in factor space of all covariates (recall happy and life are treated as covariates) and of all levels of categorical predictor variables. It reflects the loadings of both predictor and response variables scaled so distance from the origin corresponds to percentage of variation in the variable explained by the PLS factor model.

The concentric circles display the percentages explained, with further from the origin being higher percent explained by the model. Predictor effects closer to the origin are less well explained by the factors. The dependent manifest variables, happy and life, are close to the origin because this is a weak model. The axes display the R-squared values of each factor in explaining the X (predictor) and Y (response) indicators and it can be seen that the R-squared values for the Y (response) variables are very weak in this model. Note that the PLOTS= option in

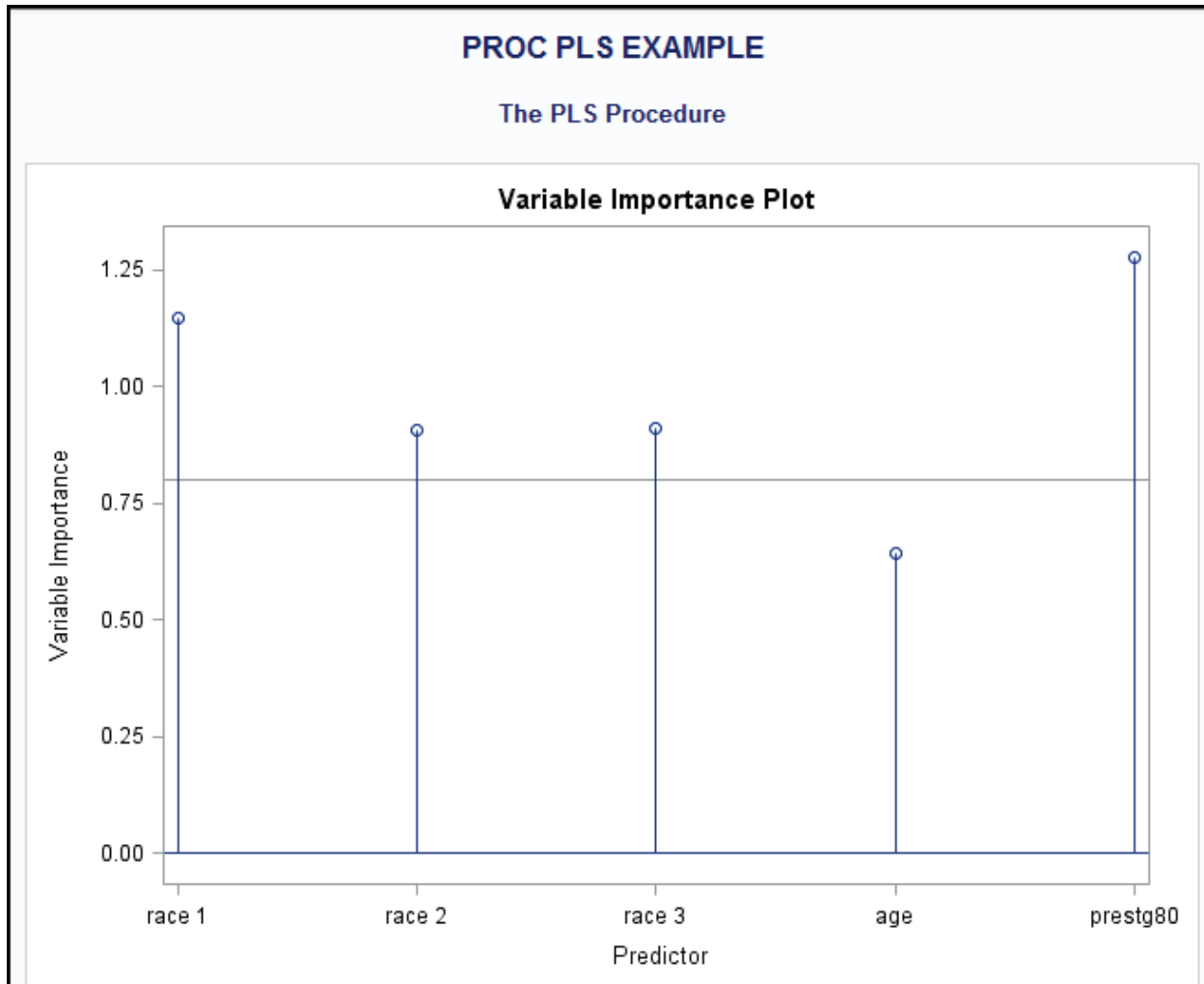
the PROC PLS statement has the capability to generate a large number of other plots not illustrated here.



Corresponding tables of model effect loadings, model effect weights, and dependent variable weights are also output but not shown here.

Variable Importance Plot

The variable importance plot (VIP) shows the relative importance of each of the continuous predictor variables and each level of the categorical predictor variables. Here it is seen that in the weak model, `prestg80` has the greatest effect on the set of dependent variables (`happy`, `life`), followed by `race1` (black), with `age` having the least effect.

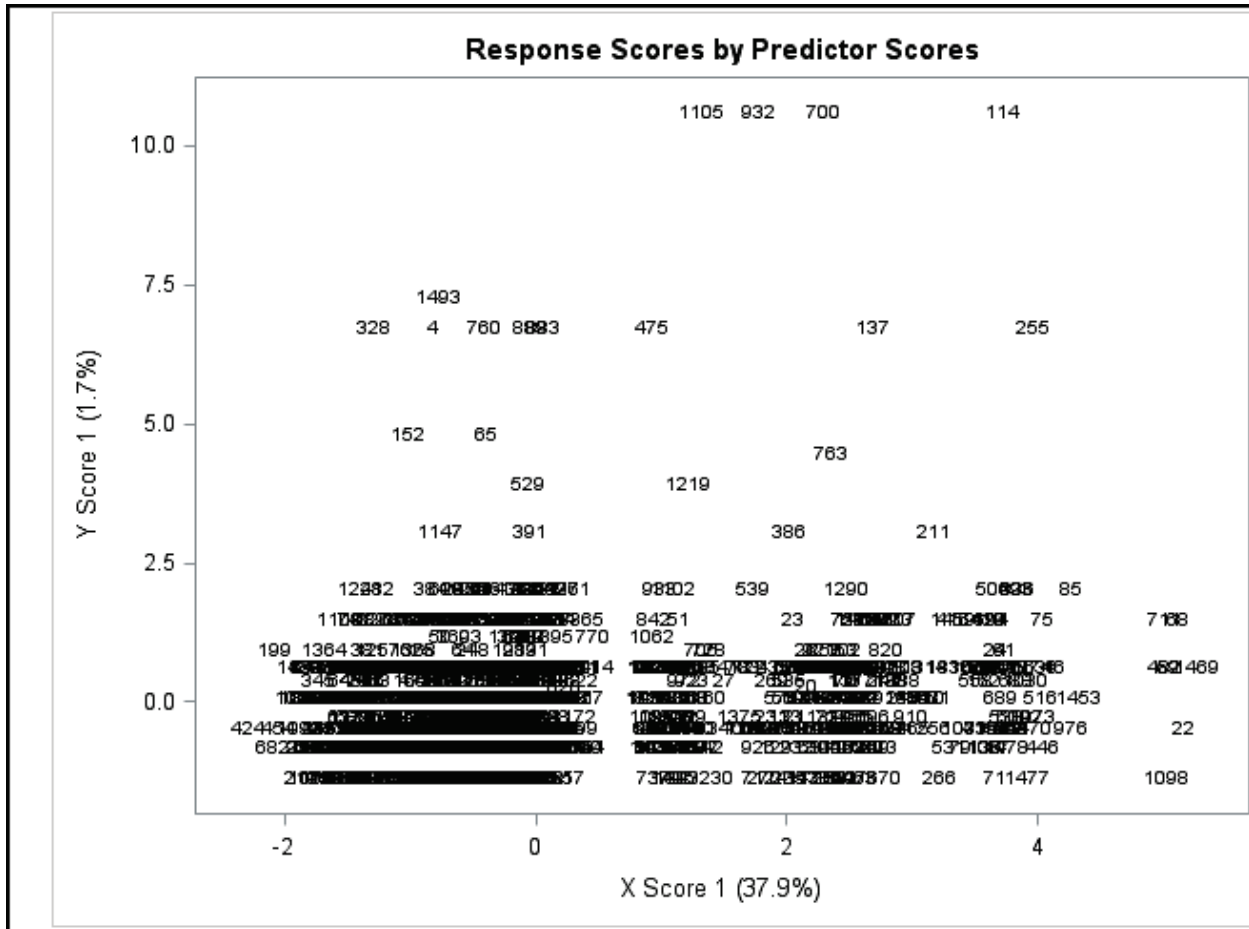


The VIP plot reflects the contribution of each predictor variable to PLS model fit, for both the predictor and response sets. Values on the Y axis are the “Variable Importance for Projection” statistic developed by Herman Wold (1994) to summarize these contributions. Wold in Umetrics (1995) stated that a value less than 0.8 was "small". This is which a horizontal guideline is displayed at the 0,8 mark of the Y axis. Here, age is the only variable with small effect by Wold’s definition.

Response scores by predictor scores plots

Response scores by predictor scores plots, also called X-Y score plots, show model fit and also show outliers.

In the figure below, relative lack of model fit is shown by the dot pattern not forming an ascending pattern with higher X axis values roughly corresponding to higher Y axis values. As there is no ascending trend, it is difficult to speak of outliers to it. However, the observation numbers floating in the upper half of the figure are exceptions to the prevailing horizontal pattern in the lower portion of the figure.

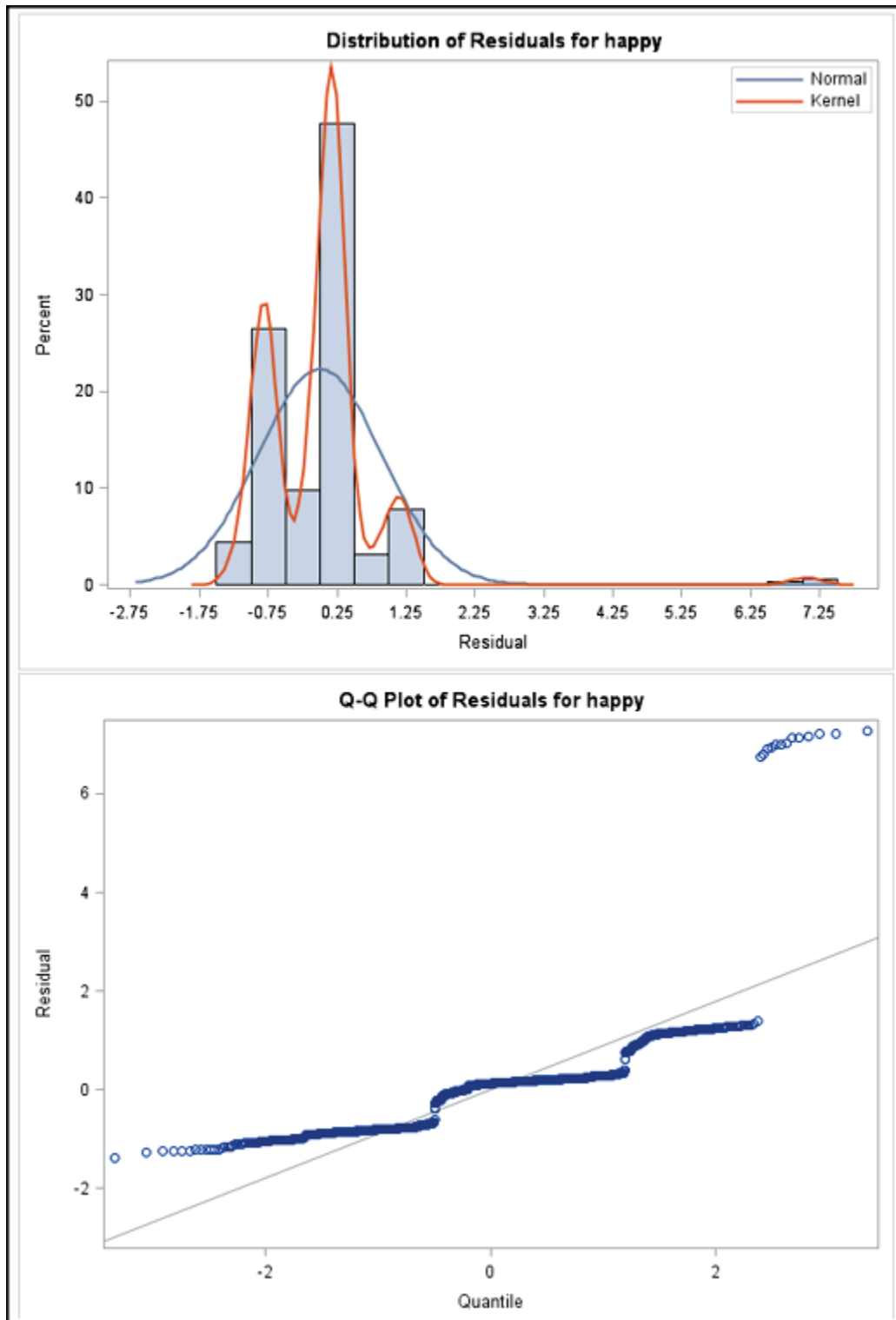


Note that the figure above plots X-Y scores for Factor 1, always the most important factor in the model. However, there are similar figures for the remaining factors and these may well show different patterns.

Residuals plots

The DIAGNOSTICS specification in the PLOTS= option of the PROC PLS statement produces a variety of residuals plots, of which only two are depicted below, both dealing with predicting the manifest dependent variable “happy”.

The “Distribution of Residuals” plot in the upper portion of the figure ideally should be normally distributed but bimodally deviates from normal. It should be normal because most estimates should be close to “right on”, making for



residuals close to zero, with declining absolute residuals on either side. The Q-Q plot in the lower half of the figure below confirms that residuals are not normally distributed since the pattern does not closely follow the ascending line shown.

Parameter estimates

If the SOLUTION option is used in the MODEL statement, SAS outputs parameter estimates for the centered and uncentered data. These are the coefficients used to predict the raw (Y) response variables based on the raw (X) predictor variables. Unlike estimates in regression models, the error distribution is unknown and so no significance tests are presented. The parameter estimates, therefore, are often treated as an “internal” computational result of little interest to the researcher.

Parameter Estimates		
	happy	life
Intercept	2.147430215	1.243685561
race 1	-0.125625351	-0.077820833
race 2	0.082327858	-0.019467584
race 3	0.251936565	0.418463426
age	-0.000283844	0.003967464
prestg80	-0.004686420	-0.006637346

Parameter Estimates for Centered and Scaled Data		
	happy	life
Intercept	0.0000000000	0.0000000000
race 1	-.0518046106	-.0260014384
race 2	0.0310707395	-.0059528812
race 3	0.0492730672	0.0663111068
age	-.0056337973	0.0638034757
prestg80	-.0854921604	-.0981047128

Summary

From the PLS output above, the researcher would conclude that contrary to the belief of some, life/happiness values do not closely associate with age, race, and occupational status as a set of determinants, for the example data drawn from a U.S. national sample in 1991.

PLS regression modeling using Stata

Overview

Though neither PLS-SEM or PLS-regression is part of the official version of Stata, Adrian Mander of the University of Cambridge has made available an extension called “plssas.” It is available from <http://fmwww.bc.edu/RePEc/bocode/p> or Stata users may type “help pls” at the command line.

The `plssas` module simulates implementation of PLS regression in SAS. Specifically, it creates “.sas” program code for a PLS regression, runs SAS in the

background, and converts SAS output datasets to comma-delimited .csv files. The Windows version of SAS is required.

The syntax is `plssas [varlist] [, options] – for example, plssas, y(income14 jobstat14 x(educ14 GPA) exe(C:\SAS\sas.exe)`. In this syntax, `y()` contains the list of outcome variables and `x()` contains the list of predictors. The `exe()` term contains the path to the SAS executable program file.

Upon running `plssas`, the following comma-separated values files are created:

- yweights.csv
- xweights.csv
- xload.csv
- xeff.csv
- pest.csv
- perc.csv
- csp.csv
- codedcoef.csv
- out.csv

In addition a file labeled “temp.sas” is created, containing the SAS syntax to assemble output into a file labeled “temp.csv”, which can be imported into SAS.

As `plssas` module implements only a subset of SAS PLS commands and as it requires the user to have SAS, implementation of PLS regression directly in SAS may well be preferred. For this reason, implementation of `plssas` in Stata is not treated further here.

Assumptions

Robustness

In general, PLS is robust in the face of missing values, model misspecification, and violation of the usual statistical assumptions of latent variable modeling (Cassel et al., 1999, 2000). Although conventional PLS is quite robust, note various authors have advanced versions of “robust PLS” not discussed here (cf., Yin, Wang, & Yang, 2014).

Specifically with regard to robustness of bootstrapped significance testing in PLS, McIntosh, Edwards, & Antonakis (2014: 229) note, “the bootstrapped confidence

intervals demonstrated by Henseler et al. appear reasonably robust to violations of normality and divergence between analytical and bootstrap sampling distributions, at least for the relatively simple models examined by Henseler et al. Future simulation work is needed that considers more complex models, different sample sizes, and additional violations of assumptions to determine when this approach might break down.” (Referring to Henseler et al., 2014).

Parametric v. non-parametric

Traditional PLS is usually described as a distribution-free approach to regression and path modeling, unlike structural equation modeling using the usual maximum likelihood estimation method, which assumes multivariate normality (see Lohmoller, 1989: 31; Awang, Afthanorhan, & Asri, 2015). It is possible to use PLS path modeling with highly skewed data (Bagozzi and Yi, 1994). PLS-FIMIX, which does use maximum likelihood estimation, is parametric and is the exception among PLS algorithms. However, the multi-group analysis/permutation approach, which has superseded PLS-FIMIX, is non-parametric.

Reinartz, Haenlein, & Henseler (2009: 332), in a simulation study, found covariance-based SEM to be “extremely robust with respect to violations of its underlying distributional assumptions”, making selection of PLS-SEM over covariance-based SEM questionable if done on the grounds that PLS-SEM is non-parametric.

Note that while PLS itself is distribution free, adjunct use of t-tests and other parametric statistics may reintroduce distributional assumptions. However, Marcoulides and Saunders (2006, p. vi) have noted that even moderate non-normality of data will require a markedly larger sample size in PLS, even if indicators are highly reliable. Based on simulation studies, Qureshi & Compeau (2009) found neither PLS nor SEM could consistently detect differences across groups when the dependent variable was highly skewed or kurtotic, though both PLS and SEM detected inter-group differences in other paths in the model not involving the dependent. However, Hsu, Chen, & Hsieh (2006), using simulation studies to compare PLS, SEM, and neural networks for moderate skewness, found that "all of the SEM techniques are quite robust against the skewness scenario" (pp. 368-369).

Treating traditional PLS as nonparametric refers to its use without parametric tests of significance. However, apart from questions of significance, as in other procedures, distributions affect effect size. Two variables from different distributions have a maximum correlation less than 1.0, whereas two variables from the same distribution (ex., normal) have a maximum correlation of 1.0. That is, if two variables come from different distributions (e.g., bimodal versus normal) and are optimally matched in order (ex., ascending order), the correlation will be less than 1.0. If the researcher's definition of "perfect association" between two variables is optimal matching given the distributions, then PLS (and other techniques) assumes the same distribution and, for most situations, that same distribution will be the normal distribution. If the researcher's definition of "perfect association" between two variables is unconditional, then the "same distributions" consideration does not apply.

Independent observations

Some authors state that observations need not be independent in PLS (see Lohmoller, 1989: 31; Chin & Newsted, 1999; Urbach & Ahlemann, 2010), apparently based on the statement by Herman Wold (1980: 70) that, "Being distribution-free, PLS estimation imposes no restrictions on the format or on the data." However, being distribution-free does not mean data independence can be ignored or that use of repeated measures data is not problematic. Ignoring the assumption of independence is a form of measurement error and since PLS is relatively robust in the face of measurement error, in this sense only is it true that PLS does not require independent observations. Wold in his 1980 article did not state PLS handles repeated measures data in spite of him being cited to the contrary. More to the point, PLS is a single-level form of analysis, not a form of multilevel analysis. If there is some grouping variable that might be handled via multilevel analysis (ex., time, for repeated measures), and if it has a limited number of levels, it may be possible to handle it within PLS by creating separate factors for each level (ex., time1, time2, time3). Note, though, that PLS is less powerful than covariance-based structural equation modeling for such repeated measures models since SEM can model correlated residual error and PLS cannot.

Data level

In SmartPLS path modeling, continuous (metric) indicator variables are assumed since the iterative algorithm uses OLS regression. Binary indicator variables are acceptable in reflective models but violate regression assumptions in formative models since the binary indicator serves as a dependent variable in such models.

However, as PLS-SEM is robust against measurement error, use of binary variables in formative models is widely accepted. For the same reason, use of ordinal indicators is commonly accepted (Henseler, Ringle, & Sarstedt, 2012: 266). In SmartPLS nominal variables must be implemented as a series of dummy variables, or a nominal variable can be the grouping variable for [multigroup PLS](#). *Neusrel* software, however, supports PLS-SEM modeling even with nominal variables.

Dependent and independent manifest variables may be any level (nominal, ordinal, or interval) in SPSS PLS-regression. In SAS PLS-regression, independent indicators may be of any level but dependent indicators are treated as interval.

Unobserved homogeneity

This assumption refers to the problem of "unobserved heterogeneity in the global model". Like other procedures, coefficients generated by traditional PLS may be misleading averages when subgroups differ significantly in the ways in which the independent variables relate to the response variables. Also, unobserved heterogeneity may lead to results without plausible interpretation and to low goodness of fit measures. Finite mixture PLS (FIMIX-PLS) or prediction-oriented segmentation (PLS-POS) should be used to test for significant segmentation and if found significant, should be used to generate models for the multiple segments provided the segments are interpretable (see the discussion of [entropy](#) as an interpretability measure for FIMIX).

Becker et. al. (2013: 684), based on extensive simulation analysis, determined, "we can conclude that the use of either PLS-POS or FIMIX-PLS is better for reducing biases in parameter estimates and avoiding inferential errors than ignoring unobserved heterogeneity in PLS path models. A notable exception is when there is low structural model heterogeneity and high formative measurement model heterogeneity: in this condition, FIMIX-PLS produces results that are even more biased than those resulting from ignoring heterogeneity and

estimating the model at the overall sample level. PLS-POS shows very good performance in uncovering heterogeneity for path models involving formative measures and is significantly better than FIMIX-PLS, which shows unfavorable performance when there is heterogeneity in formative measures. However, FIMIX-PLS becomes more effective when there is high multicollinearity in the formative measures, while PLS-POS consistently performs well.”

Alternatively, some authors use cluster analysis to segment the sample prior to using PLS, then create one global (traditional PLS) model per cluster. See the separate Statistical Associates “Blue Book” volume on “Cluster Analysis”. This approach, however, requires that the variables associated with heterogeneity be measured indicators or interactions among measured indicators.

Linearity

PLS output may be distorted due to nonlinear data relationships using SmartPLS, SPSS, or SAS. PLS-SEM modeling using Neusrel handles nonlinearities.

Outliers

As with other procedures, PLS results may be distorted due to the presence of outliers.

Residuals

Residuals should be uncorrelated with independent variables and should be random normal, as in other predictive procedures.

Appropriate sample size

Along with robustness, handling small samples is another reason why PLS is sometimes preferred over structural equation modeling. However, while PLS can be computed even for very small samples (ex., <20) or even when cases are fewer than the number of indicator variables, reliance on small samples can yield flawed results. Ed Rigdon (2014) has noted, “ Yes, PLS will produce parameter estimates when n is very low, and the bootstrapping approach will produce estimates of sampling variability when n is low, but you have to ask what those estimates are

really worth. They won't cross-validate, and the out-of-sample performance of those numbers will be extremely poor. “

Some authors (ex., Barclay, Higgins, & Thompson, 1995; Chin, 1998) recommend PLS users follow a similar "rule of 10" guideline as SEM users: at least 10 cases per measured variable for the larger of (1) the number of indicators in the largest latent factor block, or (2) the largest number of incoming causal arrows for any latent variable in the model. Note, however, that appropriate sample size choice is more complex than any rule of thumb. The appropriate size depends in part both on the degree that factor structure is well defined (ex., are weights $> .70$) and how small are the path coefficients the researcher seeks to establish (prove different from 0; ex., a much larger sample is needed to establish path coefficients of .1 than .7). The “rule of 10” may yield sample size with inadequate statistical power.

The larger the sample, the more reliable the PLS estimates. Thus, Hui and Wold (1982) in simulation studies found that the average absolute error rates of PLS estimates diminished as sample size increased. Small sample sizes (ex., < 20) will not suffice to establish weak path coefficients (ex., $\leq .2$); sample sizes equivalent to those commonly found in SEM (ex., 150-200) are needed (see Chin & Newsted, 1999).

Simulation studies.

- Marcoulides & Saunders (2006), based on simulation studies, have published a table (p. vii) addressing the question of "what sample sizes would be needed to achieve a sufficient level of power, say equal to .80 (considered by most researchers as acceptable power) to reject the hypothesis that the factor correlation in the population is zero." Their Monte Carlo results show that while, indeed, PLS estimates may be reliable for very small samples (ex., 17), this is true only when factor loadings are large and the researcher is examining high factor correlations. On the other hand, their experiments suggested, for example, that using indicators with 0.7 factor loadings and examining factor correlations of .2, a sample of size 1,261 would be required to achieve the .80 power level. A sample size of 98 was sufficient for loadings equal or greater than .6 when establishing correlations equal or greater than .4. A sample size of 23 was sufficient for

loadings equal or greater than .7 when establishing correlations equal or greater than .6.

- Qureshi & Compeau (2009) also used Monte Carlo simulation to research related issues. They found PLS better than SEM when data were normally distributed, with a small sample size and correlated exogenous variables. They also found, however, that with large sample sizes and normally distributed data, both approaches consistently detected differences across groups. Neither PLS nor covariance-based SEM performed well for datasets where the dependent was non-normal, though for smaller samples at moderate effect sizes, PLS outperformed SEM in detecting intergroup differences in other paths in the model (paths not involving the dependent).
- Reinartz, Haenlein, & Henseler (2009) likewise used Monte Carlo simulation found that for smaller samples (ex., 100), PLS-SEM achieved acceptable levels of statistical power. For larger samples (ex., 250), however, covariance-based SEM was clearly better than PLS-SEM in terms of parameter accuracy and consistency. For any size sample, PLS-SEM had greater power than covariance-based SEM and thus might be preferred for purposes of model-trimming in theory development as Type II error would be lower.
- Henseler, Dijkstra, Sarstedt, et al. (2014), based on simulation studies, found that PLS-SEM generally required sample sizes similar to traditional SEM, though PLS-SEM could converge in the face of small samples when traditional SEM could not. They note (p. 198), “With regard to statistical power, it can be expected that covariance-based SEM, as a full information estimator, will most of the time deliver smaller standard errors than limited information estimators such as PLS.” Smaller standard errors correspond to greater statistical power.

Missing values

While PLS has been found to be robust in the face of missing values (Cassel et al., 1999, 2000), accuracy will be increased in PLS or any procedure if values are imputed rather than the default taken (listwise deletion of cases with missing values). As a rule of thumb, imputation of a variable is often called for when more than 5% of its values are missing. If too missing values are too numerous, however, the variable should simply be dropped from analysis. Hair et al. (2014:

55) suggest “too numerous” is greater than 15%, but researchers vary on the appropriate cutoff.

SmartPLS software only offers listwise deletion or mean substitution, a procedure generally derogated. It is better to impute data in a major statistical package outside of SmartPLS. See the separate Statistical Associates “Blue Book” volume on “Missing Value Analysis and Data Imputation.”

Model specification

Like almost all multivariate procedures, PLS results may differ markedly if previously-omitted important causal variables are added to the model, though PLS is less sensitive to inclusion of spurious causal variables correlated with indicator variables. Note that modeling a factor as reflective when in reality it is formative, or vice versa, is a misspecification form of measurement error. Jarvis, MacKenzie, & Podsakoff (2003) found this to be one of the most common measurement errors in PLS research. Formative and reflective models are discussed [above](#).

With regard to robustness against model misspecification, Henseler, Dijkstra, Sarstedt et al. (2014) write, “Full-information approaches” (like covariance-based SEM – DG) “often suffer ... because model misspecification in a subpart of a model can have detrimental effects on the rest of the model (Antonakis, Bendahan, Jacquart, & Lalive, 2010). In contrast, limited information methods are more robust to misspecification and are therefore useful for the analysis of initially formulated but misspecified models (Gerbing & Hamilton, 1994). Consequently, there are good reasons to prefer PLS as a limited-information approach over full-information approaches when the correctness of all parts of a model cannot be ensured.”

Appropriate model fit assessment

As discussed [above](#), model fit assessment in PLS-SEM differs for formative models as compared to reflective models. In particular, using composite reliability, Cronbach’s alpha, and AVE for assessing fit of formative models is not appropriate. Hair et al. (2012) has found this to be a widespread error in reporting PLS-SEM models.

Recursivity

Most PLS-SEM software, including *SmartPLS*, assume a recursive model. That is, there cannot be any circular feedback loops in the model. *Neusrel*, discussed [below](#), supports non-recursive PLS-SEM models.

Multicollinearity

Perfect multicollinearity within a set of indicators for a factor prevents a solution and requires dropping the redundant indicator.

High multicollinearity among the indicators is generally not a problem. Gustafsson & Johnson (2004) found PLS to be resilient in the face of multicollinearity. . Note, however, that this does not mean that multicollinearity just "goes away." Multicollinearity of the factor indicators in the measurement model (the outer model) is still problematic for high correlations between indicators for one factor and indicators for another. To the extent this type of multicollinearity exists, PLS will lack a simple factor structure and the factor cross-loadings will mean PLS factors will be difficult to label, interpret, and distinguish. For multicollinearity of indicators within the set for a single factor, the researcher should check the content of the items to make sure that high correlation is not due to some artifact such as non-substantive word variations of items.

High multicollinearity among the indicators in formative models is highly unusual since for formative models, the indicators represent a complete set of the separate dimensions which compose the factor. The dimensions are not expected to correlate highly. For instance, for the factor "Philanthropy", formative items might be dollars given to church, dollars given to environmental causes, dollars given to civil rights causes, etc. Different respondents will give in different patterns and correlation of items will not be high.

Regarding multicollinearity among the factors, since the PLS factors are orthogonal, by technical definition mathematical multicollinearity is not a problem in PLS. This is a major reason why PLS models may be selected over OLS regression models or structural equation modeling

Proper use of dummy variables

The dummy variable representing desired reference category must be omitted in the model. Coefficients for the remaining dummy variables in the set for a given categorical variable must be interpreted with respect to the reference category. When refining a model, dummy variables are treated as a set: the entire set is added to or deleted from the model.

Standardized variables

When interpreting output, keep in mind that all variables in the model have been centered and standardized, including dummy variables for categorical variables.

Frequently Asked Questions

How does PLS-SEM compare to SEM using analysis of covariance structures?

The primary difference between variance-based PLS and covariance-based SEM in SPSS AMOS, SAS, or Stata, is that PLS is component-based, using OLS regression in PLS-SEM or using principal components analysis in PLS-regression. In contrast, SEM is covariance-based, using common factor analysis, with the result that the latent variables in each are constructed quite differently as described earlier above. That is, the meanings of the latent variables will differ for the same model using analysis of covariance structures (ordinary SEM) compared to analysis of principal components in PLS-SEM. A corollary is that most of the model fit measures differ between the two.

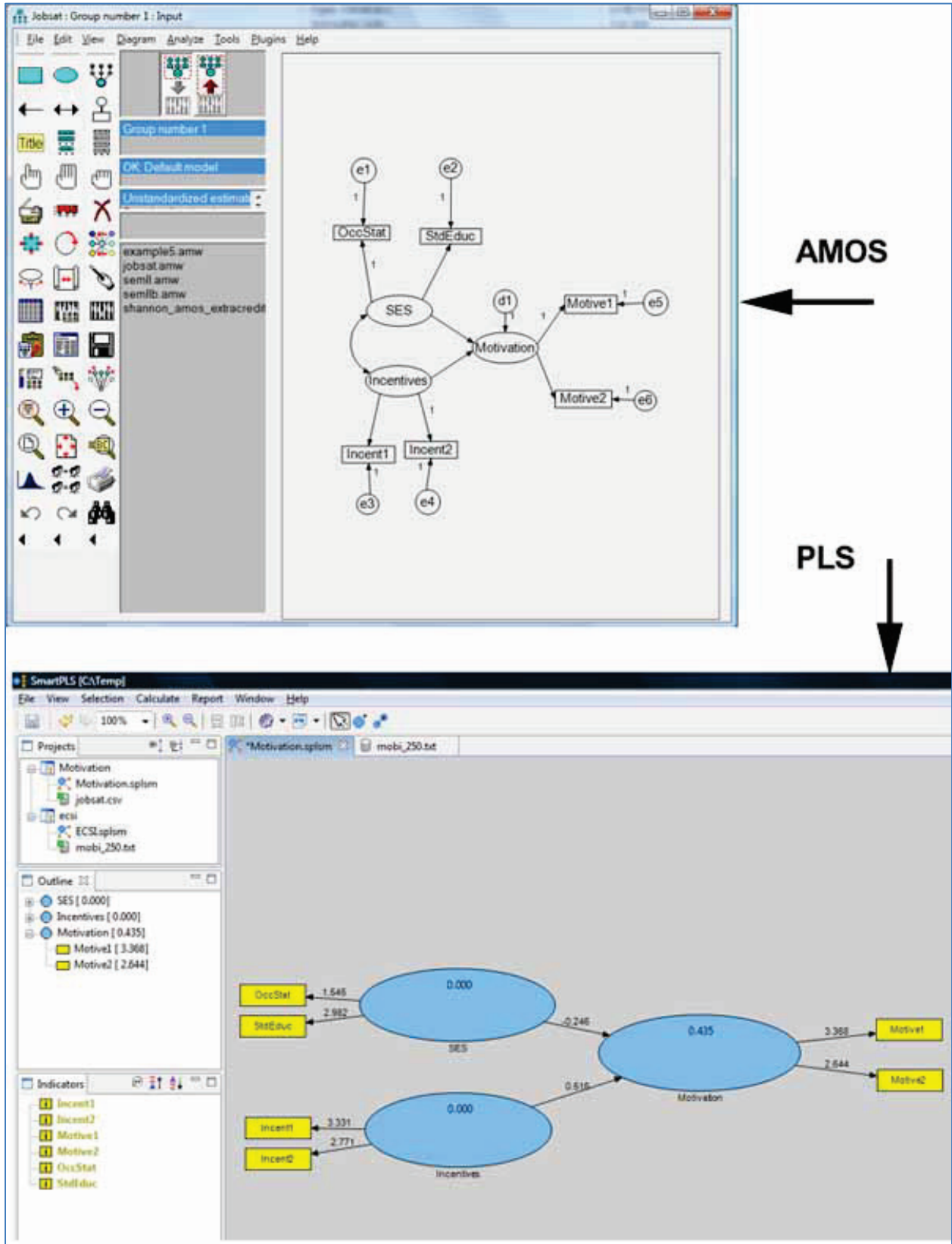
In PLS-regression, a variance-based approach, principal components analysis seeks optimal components which reproduce the total variance of the variables. Principle components analysis determines the factors which can account for the total (unique and common) variance in a set of variables. Manifest variables reflect the total variance and unique variance explained by the components, plus error variance not explained by the components. This approach to creating latent variables is appropriate for creating a typology of variables or reducing attribute space, or for exploratory purposes, or for non-causal prediction.

As a variance-based approach. PLS-SEM using OLS regression seeks to maximize the explained variance in the endogenous latent variables and subsequently of the indicators for them. Covariance-based SEM (hereafter called CB-SEM for convenience of contrast), seeks to minimize the difference between the observed and model-implied covariance matrices. The common factor analysis used in CB-SEM seeks optimal factors which reproduce the covariation among the variables. Common factor analysis determines the least number of factors which can account for the common variance in a set of variables. Manifest variables reflect the common variance explained by the factors, plus unique and error variance not explained by the factors. This approach to creating latent variables is appropriate for confirming that the hypothesized dimensionality of a set of variables such as a set of items in a scale, is consistent with the observed data. It is also appropriate for confirming that hypothesized causal relations and their associated implied covariance matrix, are consistent with the observed data.

Other statistical and practical differences between PLS-SEM and CB-SEM:

- CB-SEM is used much more widely than PLS-SEM, especially in sociology and the primary social sciences. PLS-SEM has been more widespread in specialized fields, such as market research, where prediction is a central research goal.
- PLS-SEM lacks global model goodness-of-fit (GOF) measures, which are a central feature of CB-SEM. This advantage of CB-SEM is one major reason it is preferred for confirmatory research. The global scalar function used as the basis of most GOF measures in CB-SEM involve minimizing the residuals reflecting the difference between the observed and the model-implied covariance matrices. PLS-SEM lacks any such global GOF criterion and the goodness-of-fit measures used in CB-SEM do not appear in PLS-SEM output.
- Parameter estimates tend to be more accurate in CB-SEM than in PLS-SEM (see Reinartz, Haenlein, & Henseler, 2009). PLS-SEM is associated with a bias which tends to underestimate structural path parameters and overestimate measurement path parameters (see Hair et al., 2014: 47-48). PLS-SEM bias becomes negligible when sample size is large and the number of indicators per latent variable is large (Lohmöller, 1989). Simulation studies suggest PLS-SEM bias is low in most situations (Reinartz et al., 2009; Ringle et al., 2009).

- When the assumptions of CB-SEM are violated (inadequate sample size, non-normal data, lack of parsimony), standard errors in CB-SEM are inflated and PLS-SEM tends to exhibit lower variability of estimates (Reinartz et al., 2009).
- CB-SEM uses maximum likelihood estimation whereas standard PLS-SEM uses ordinary least squares. The former requires larger sample sizes. For smaller samples, PLS-SEM is sometimes preferred.
- Compared to CB-SEM, PLS-SEM makes fewer distributional assumptions about the data, as discussed [above](#).
- PLS-SEM will have greater statistical power and hence fewer Type II errors at any sample size.
- Whereas CB-SEM may be prone to problems with models being underidentified, especially with small samples, PLS-SEM is not constrained by identification considerations associated with small samples. PLS-SEM is much more likely to converge for small samples than CB-SEM. CB-SEM cannot handle data at all when sample size is less than the number of variables whereas PLS-SEM can handle even this. Henseler, Dijkstra, Sarstedt, et al. (2014: 199) observe, based on their simulation studies, that “nonconvergence and Heywood cases occur quite frequently with common factor models (Krijnen, Dijkstra, & Gill, 1998) and that PLS in general only rarely has convergence problems (Henseler, 2010).”
- Single-indicator variables may cause identification and convergence problems in CB-SEM, but are not a problem in PLS-SEM, whose practitioners are more likely to use single-indicator variables.
- PLS-SEM converges quickly and is less likely to fail to converge on a solution compared to CB-SEM. A corollary is that compared to CB-SEM, PLS-SEM may be able to handle much larger and more complex models.
- As illustrated in the figure below, PLS-SEM models indicators without error whereas CB-SEM models error terms explicitly. Likewise, PLS-SEM models endogenous latent factors without disturbance terms. As a result, CB-SEM is more useful for modeling different error assumptions.



While the choice between CB-SEM and PLS-SEM depends on the researcher's purpose and data, as a rule of thumb, PLS-SEM is used for exploratory purposes and analysis of covariance structures (ordinary SEM) is used for confirmatory purposes (e.g., see Hair et al., 2014: 2). CB-SEM and PLS-SEM each yield different information and in some research contexts, both may be used on a complementary basis.

What are higher order/hierarchical component models in PLS-SEM?

Models dealt with in this volume are “first-order models” because all latent variables are based on observed (measured, manifest) indicator variables. A “higher-order model” is one in which at least one of the latent variables has as its indicators not the usual measured variables but rather at other latent variables in the causal model. Also called “hierarchical component models” (HCM), in principle higher order models might have several levels. In practice, almost all involve just second-order factors.

Three major reasons for using HCM are given by Hair et al. (2014: 229-230):

1. To reduce the number of structural relationships under analysis in PLS, for parsimony reasons.
2. To deal with collinearity among first-order latent constructs by using them to create more general second-order constructs.
3. When formatively-modeled indicators for a first-order construct are collinear, if justified by a theoretical rationale, the indicators may be separated into sets, each set being the indicators for a different formative first-order construct, then these first-order constructs may formatively measure a second-order construct.

Recall that in HCM, the centroid weighting scheme may not be used, as discussed [above](#).

Let there be multiple first order components (FOCs) each measured reflectively or formatively by multiple measured indicators. Let the second order component (SOC) be the higher order latent variable. As discussed by Ringle et al. (2012) and others, there are four types of higher order models in PLS:

1. *Reflective-Reflective*: The SOC is measured reflectively by the FOCs (arrows go from the SOC to the FOCs) and, in a “repeated indicators approach” (the

most common but not the only approach), also reflectively by all of the indicator variables for all of its FOCs (arrows go from the SOC to all of the repeated indicators). The same indicators are modeled reflectively with respect to each FOC (arrows go from the FOC to their own indicator variables). This is perhaps the most common type.

2. *Reflective-Formative*: The indicators for the FOCs are modeled reflectively as is the entire set of repeated indicators for the SOC (as in reflective-reflective models), but the SOC is modeled formatively with respect to the FOCs (arrows go from the FOCs to the SOC).
3. *Formative-Reflective*: The indicators for the FOCs are modeled formatively as is the entire set of repeated indicators for the SOC, but the SOC is modeled reflectively with respect to the FOCs (arrows go from the SOC to the FOCs).
4. *Formative-Formative*: The indicators for the FOCs are modeled formatively as is the entire set of repeated indicators for the SOC, and the SOC is modeled formatively with respect to the FOCs (arrows go from the FOCs to the SOC).

In the repeated indicator approach for reflective-reflective and formative-formative models, the FOCs will explain nearly all of the variance in the SOC (R^2 will approach 1.0). The corollary is that paths from other latent variables prior in causal order to the SOC will approach 0. In such a situation, a two-stage approach is recommended: (1) first the repeated indicator approach is used to get factor scores for the FOCs, then (2) the FOC factor scores are used as indicators for the SOC. In both stages, other latent variables are included in the model also.

For further discussion and a worked example of HCM with respect to SmartPLS, see Hair et al. (2014: 229-234). For another example, see Wetzels, Odekerken-Schroder, & van Oppen (2009).

How does norming work?

To understand how norming a set of values to range from 0 to 100, consider the simple case of values for a set which varies from 3 to 7. After norming, 3 should become 0, 7 should become 100, and 5 (the middle value) should become 50. This can be accomplished with the following formula:

$$\text{Normed value} = 100 * [(\text{original value} - \text{minimum}) / (\text{maximum} - \text{minimum})]$$

- Thus the normed value for 5 = $100 * [(5-3)/(7-3)] = 100 * [2/4] = 50$
- Likewise for the value for 7 = $100 * [(7-3)/(7-3)] = 100 * [4/4] = 100$
- And for the value of 3 = $100 * [(3-3)/(7-3)] = 100 * [0/4] = 0$

For purposes of norming the unstandardized latent variable scores for importance-performance matrix analysis (IPMA, discussed [above](#)), the same formula may be applied, as it may to any series.

What other software packages support PLS-regression?

PLS-GUI, from the PLS Institute, is software which extends SmartPLS functionality. SA input, it reads in SmartPLS models (.spslm files) and data in comma-delimited (.csv) or SPSS (.sav) files. Primary features are 2- and 3-group MGA (multigroup analysis) and use of jackknifing estimates (leave-one-out) of standard errors in addition to bootstrapping (random resampling with replacement). PLS-GUI also performs linear path analysis and interfaces with (calls) R Commander, a statistical package which adds non-linear, logistic, generalized linear, generalized additive, mixed-effects, and other modeling procedures, with dozens of high definition graphics options. The PLS-GUI url is <http://www.pls-institute.org/>.

GENSTAT is a full-featured statistics package which also implements PLS regression. Url: <http://www.vsni.co.uk/software/genstat> .

The Unscrambler. This software from Camo, Inc. implements PLS regression and PLS-DA, a PLS-based version of discriminant analysis. Url: <http://www.camo.com/rt/Products/Unscrambler/unscrambler.html> .

MorphoJ supports two-block partial least squares modeling. Url: http://www.flywings.org.uk/MorphoJ_page.htm .

tpsPLS is free software also supporting two-block partial least squares modeling, geared toward analysis of shapes as well as variables. Url: <http://tpspls.software.informer.com/> .

XLSTAT-PLS is an add-on module for Excel spreadsheets, supporting PLS regression as well as principal component regression (PCR). Url: <http://www.xlstat.com/en/products-solutions/pls.html> .

Implementations of PLS regression also exist for S-Plus, Matlab, and R, among others.

How is PLS installed for SPSS?

This section is quoted from SPSS 22 installation notes.

The Partial Least Squares Regression procedure is a Python extension command and requires IBM® SPSS® Statistics - Essentials for Python, which is installed by default with your IBM SPSS Statistics product. It also requires the NumPy and SciPy Python libraries, which are freely available.

Note: For users working in distributed analysis mode (requires IBM SPSS Statistics Server), NumPy and SciPy must be installed on the server. Contact your system administrator for assistance.

Windows and Mac Users

For Windows and Mac, NumPy and SciPy must be installed to a separate version of Python 2.7 from the version that is installed with IBM SPSS Statistics. If you do not have a separate version of Python 2.7, you can download it from <http://www.python.org>. Then, install NumPy and SciPy for Python version 2.7. The installers are available from <http://www.scipy.org/Download>.

To enable use of NumPy and SciPy, you must set your Python location to the version of Python 2.7 where you installed NumPy and SciPy. The Python location is set from the File Locations tab in the Options dialog (Edit > Options).

Windows and Unix Server

NumPy and SciPy must be installed, on the server, to a separate version of Python 2.7 from the version that is installed with IBM SPSS Statistics. If there is not a separate version of Python 2.7 on the server, then it can be downloaded from <http://www.python.org>. NumPy and SciPy for Python 2.7 are available from <http://www.scipy.org/Download>. To enable use of NumPy and SciPy, the Python location for the server must be set to the version of Python 2.7 where NumPy and SciPy are installed. The Python location is set from the IBM SPSS Statistics Administration Console.

Linux Users

We suggest that you download the source and build NumPy and SciPy yourself. The source is available from <http://www.scipy.org/Download>. You can install NumPy and SciPy to the version of Python 2.7 that is installed with IBM SPSS Statistics. It is in the Python directory under the location where IBM SPSS Statistics is installed.

If you choose to install NumPy and SciPy to a version of Python 2.7 other than the version that is installed with IBM SPSS Statistics, then you must set your Python location to point to that version. The Python location is set from the File Locations tab in the Options dialog (Edit > Options).

(Not from SPSS online Help): If you have the SPSS CD, you may be able to install PLS using the following steps:

1. Install SPSS (SPSS CD)
2. Install Python (SPSS CD)
3. Install SPSS-Python Integration Plug-in (from SPSS CD)
4. Install NumPy and SciPy (From SPSS CD under Python and Additional Modules; Note this option installs Python, NumPy, and SciPy in order if they are not already present)
5. Install PLS Extension available at:
<https://www.ibm.com/developerworks/mydeveloperworks/files/app/person/270002VCWN/file/33319ac0-6f93-4040-9094-f40e7da9e7a8?lang=en>.
You can log in as Guest/Guest.
6. After unzipping, copy `plscommand.xml` and `PLS.py` to the extensions subdirectory under the SPSS Statistics installation directory.

What other software packages support PLS-SEM apart from SmartPLS?

Neusrel, associated with a German team under Frank Buckler, is a PLS-SEM modeling package which supports exploratory analysis of categorical variables, nonlinear relationships, and interaction effects. Rather than using regression methods to estimate path parameters, it uses neural network analysis. Other features include an Excel interface, missing values data imputation using a nearest-neighbor algorithm, option for weighted cases, output of fit measures (R-Square, GOF, Cronbach's alpha, composite reliability, AVE) and effect sizes (path coefficients, factor scores, OEAD, an IE measure for interaction effects), support

for both reflective and formative models, segment models, non-recursive path models, bootstrapped significance, cross-validation, second-order models, time series, and data visualization through numerous types of plots. A trial version is available. Url: <http://www.neusrel.com/> .

WarpPLS. This package, first released in 2009, has been updated through 2013 as of this writing. It implements nonlinear (S-curve and U-curve) as well as linear paths and also outputs overall goodness-of-fit measures for PLS models. Other output includes p-values for path coefficients and also variance inflation factor (VIF) scores and multicollinearity estimates for latent variables. The development group is associated with Dr. Ned Kock of Texas A&M International University. and with Georgia State University. A free trial version is available. Url: <http://www.scriptwarp.com/warppls/> .

XLSTAT-PLSPM is path modeling software which operates as an Excel spreadsheet add-on. Scroll down on the company website to link to a series of tutorials. Url: <http://www.xlstat.com/en/products-solutions/plspm.html> .

PLS-Graph. An academic program developed by Wynne W. Chin. For information click here.. The url is <http://www.statisticssolutions.com/pls-graph-software/>. See Gefen & Straub (2005).

PLSPM. An R package for PLS, developed and maintained by Gaston Sanchez. Information at <http://cran.r-project.org/web/packages/plspm/index.html>.

LVPLS. LVPLS was the original software for PLS. The last version, 1.8, was issued back in 1987 for MS-DOS.

What are the SIMPLS and PCR methods in PROC PLS in SAS?

PROC PLS in SAS supports a METHODS= statement. With METHODS=PLS one gets standard PLS calculations. As this is the default method, the statement may be omitted. With METHODS=SIMPLS, one gets an alternative algorithm developed by de Jong (1993). SIMPLS is identical to PLS when there is a single response (dependent) variable but is computationally much more efficient when there are many. Results under PLS and SIMPLS are generally very similar.

PCR. With METHODS=PCR one is asking for principal components regression, which predicts response variables from factors underlying the predictor variables. Latent variables created with PCR may not predict Y-scores as well as latent variables created by PLS or SIMPLS.

Why is PLS sometimes described as a 'soft modeling' technique?

This is an allusion to assumptions of multiple linear regression compared to PLS. OLS regression makes "hard" assumptions, including lack of multicollinearity among the independent variables, which in turn often implies few independent variables with well-understood relationships to the dependent variable. "Soft modeling" refers to modeling when these assumptions cannot be met. PLS can handle multicollinearity, many independent variables, and because its focus is prediction, not explanation, lack of well-understood relationships of the independents to the dependent is not critical.

You said PLS could handle large numbers of independent variables, but can't OLS regression do this too?

In principle, yes. In practice, the larger the number of independent variables, the greater the likelihood of multicollinearity, which renders OLS regression results unreliable. Moreover, when the number of variables approaches or exceeds the number of cases, OLS regression will "overfit" the data and one will have a spurious perfect fit model which will fail to have predictive power for a new set of data.

Is PLS always a linear technique?

While PLS is a linear technique, nonlinear PLS (NLPLS) has been advanced by Malthouse, Rasmussen, and others. This nonlinear approach combines PLS with feedforward neural network analysis (or in a variant with radial basis function neural network analysis). See Malthouse et al. (1997).

How is PLS related to principal components regression (PCR) and maximum redundancy analysis (MRA)?

All three are similar in sharing the strategy of indirect modeling, using factors derived from the X variables to predict factor scores of the Y variables, which are

then used to construct predictions of the raw Y variables. Where the PLS algorithm maximizes the strength of the relation of the X and Y factor scores, PCR maximizes the degree to which the X factor scores explain the variance in the X variables; and MRA maximizes the degree to which the Y factor scores explain the variance in the Y variables. Whereas the PLS algorithm chooses X-scores of the latent independents to be paired as strongly as possible with Y-scores of the latent response variable(s), PCR selects X-scores to explain the maximum proportion of the factor variation. Often this means that PCR latent variables are less related to dependent variables of interest to the researcher than are PLS latent variables. On the other hand, PCR latent variables do not draw on both independent and response variables in the factor extraction process, with the result that PCR latent variables are easier to interpret.

PLS generally yields the most accurate predictions and therefore has been much more widely used than PCR. PLS may also be more parsimonious than PCR. In a chemistry setting, Wentzell & Vega (2003: 257) conducted simulations to compare PLS and PCR, finding "In all cases, except when artificial constraints were placed on the number of latent variables retained, no significant differences were reported in the prediction errors reported by PCR and PLS. PLS almost always required fewer latent variables than PCR, but this did not appear to influence predictive ability."

Attempts have been made to improve the predictive power of PCR. Traditional PCR methods use the first k components (first by having the highest eigenvalues) to predict the response variable, Y. Hwang & Nettleton (2003: 71) note, "Restricting attention to principal components with the largest eigenvalues helps to control variance inflation but can introduce high bias by discarding components with small eigenvalues that may be most associated with Y. Jolliffe (1982) provided several real-life examples where the principal components corresponding to small eigenvalues had high correlation with Y . Hadi and Ling (1998) provided an example where only the principal component associated with the smallest eigenvalue was correlated with Y ." Recall variance inflation (measured in regression by the variance inflation factor, VIF) indicates multicollinearity: while a multicollinear model may explain a high proportion of variance in Y, but redundancy among the X variables leads to inflated standard error and inflated parameter estimates. Minimizing variance inflation may not minimize mean square error (MSE). To deal with the tradeoff between variance inflation and

MSE, some researchers employ an "inferential approach", which uses only components whose regression coefficients significantly differ from zero (Mason & Gunst, 1985). More recently, Hwang & Nettleton (2003) have proposed a PCR selection strategy which selects components which minimize mean square error (MSE) demonstrating through simulations studies that their estimator performed superior to traditional PCR, inferential PCR, or even traditional PLS (which ranked second in the simulation, among many variants tested). However, it appears that Hwang-Nettleton estimators are not employed by current software. .

What are the NIPALS and SVD algorithms?

There is more than one way to compute PLS coefficients. NIPALS is the nonlinear iterative partial least squares method and is the most common, developed by Wold (1975). SVD is the singular value decomposition method, which is computationally more exact but also less efficient than NIPALS. Results are very similar by either algorithm. EIG is an algorithm basing extraction on the eigenvalues. RLGW uses an iterative algorithm which handles models with many predictor variables. In SAS, in the PROC PLS statement, the ALGORITHM= option may be set to NIPALS | SVD | EIG | RLGW. NIPALS is the default.

How does PLS relate to two-stage least squares (2SLS)?

Thomas (2005) has argued that 2SLS, as implemented by Bollen's (1996) instrumental variables model, is similar to PLS in being free from distributional requirements, is even more robust in the face of model misspecifications, and is superior to it in generating consistent parameter estimates in latent variable equations. See the separate Statistical Associates "Blue Book" volume on two-stage least squares.

How does PLS relate to neural network analysis (NNA)?

Hsu, Chen, & Hsieh (2006: 369) compared PLS, SEM, and NNA in simulation studies, finding NNA results to be similar to PLS.

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