Università degli Studi di Napoli
Federico II

Ph.D. Thesis

in Statistics

XXVII Ciclo

Nonlinear Approach to PLS Path Modelling

Methodology, Software and Application

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April 2017

to my family:

Rita, Salvatore and Andrea

Joana and little Manuel

"Inspiration exists, but it has to find you working."

Pablo Picasso

Abstract

This thesis proposes a flexible nonlinear alternative to the PLSPM algorithm which tackles two main issues identified and motivated throughout this study: (i) the presence of linearity assumptions; and (ii) the path direction's incoherence within the inner model estimation phase.
The proposed approach can be seen, when it comes to the inner model, as a data-driven estimation approach. In fact, the algorithm adapts to the form assumed by the inner relationships among composites by means of a piecewise estimation method. As detailed and motivated along this work, another added value is represented by the possibility of defining a non-symmetrical weighting system designed to accommodate a coherent path direction modelling among composites.
The customer satisfaction application to the energy supply market shows how using the proposed nonlinear approach to PLSPM allows the definition of a more precise business strategy.
The results obtained are very promising and the proposed Nonlinear PLSPM approach achieved two main goals: (i) the relation defined in the theoretical model are free from the linearity assumption; (ii) the results provided set the basis for a more suitable interpretation of the relation between composites, based on the natural patterns present in the data.

Keywords: PLS Path Modelling, Nonlinear PLSPM, Component-Based approach, ECSI, Customer Satisfaction, Energy Supply Market

Acknowledgements

This thesis represents the end result of my long journey towards the Ph.D. in which I could count with the support of many people and institutions.
First of all, I want to express my deep thankfulness to Prof. Carlo Lauro who has the merit (or the blame) for convincing me to take this path. His mentorship, leadership and ideas helped shaping the professional I am today.
A special gratitude message goes to Prof. Marina Marino who dedicated me many hours of her precious time with a positive attitude, constructive questions and knowledgeable counselling. I also thank Prof. Germana Scepi who agreed to be the second examiner of this thesis and supported my work with her advices and encouragement.
I would also like to show my gratitude to Pasquale Dolce who has been a constant presence during the whole journey helping me validating the methodology and the coherence of my ideas with his distinguishing calm.
At the institutional level, I would like to thank my employer EDP for sharing the relevant data for this work and in particular to Ferrari Careto for creating the necessary conditions to make it possible.
Still on a professional level I would like to thank Nick Eayrs for being an inspirational leader and a reference in my years at SAS.
On a very personal note, to all my dearest friends and family who, regardless of the distance, have supported me with their presence and cheerfulness. I will greet each one of them personally as soon as I close this thesis...!

A special word of thanks goes to my parents-in-law Manuel and Lina, to João, Ana and Pedro and to Mary.
There will never be enough words to express my gratefulness to my mother Rita and my father Salvatore, they have always been my inspiration and my lighthouse. A special note goes to my brother Andrea who always believed in me and supported me throughout this long journey.
This work is also dedicated to my dear nonna!
My last efforts to express my feelings goes to my dear Joana and my little Manuel simply for being who they are and for making my life a wonderful place... Thank you!

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Abbreviations

AVE	Average Variance Extracted
CATI	Computer-Assisted Telephone Interview
CCA	Canonical Correlations Analysis
ECSI	European Customer Satisfaction Index
EDP	Energias de Portugal
EDPC	EDP Comercial
GME	Generalised Maximum Entropy
GoF	Goodness of Fit
GSCA	Generalised Structured Component Analysis
GUI	Graphical User Interface
IPA	Importance-Performance Analysis
LISREL	LInear Structural RELations
LS	Least Squares
LV	Latent Variable
LVPLS	Latent Variables Partial Least Squares
MIMIC	Multiple Indicators for Multiple Causes
ML	Maximum Likelihood
MV	Manifest Variable
NILES	Nonlinear Iterative LEast Squares
NIPALS	Nonlinear Iterative PArtial Least Squares
OLS	Ordinary Least Squares
PCA	Principal Component Analysis
PLS	Partial Least Squares
PLSPM	Partial Least Squares Path Modelling
PLS-R	Partial Least Squares - Regression
RGCCA	Regularised Generalised Canonical Correlation Analysis
SEM-ML	Structural Equations Model - Maximum Likelihood
TOL	Tolerance
VIF	Variance Inflation Factor

Introduction

All models are wrong, but some models are useful.
George E.P. Box

Statistics researchers and business practitioners are constantly confronted with new challenges characterised by an ever-growing size and complexity.

Efron (2009) describes the current century as a period where the relation between data size and challenge complexity is characterised by large data sets and more sophisticated and targeted questions.

Hastie et al. (2009) explain that vast amounts of data are being generated in many fields, and the statistician's job is to make sense of it all: to extract important patterns and trends, and understand "what the data says". The authors believe that the growing complexity associated to the process of "learning from data" have led to a revolution in the statistical sciences. Since computation plays such a key role, much of the new development has been done by researchers in other fields such as computer science and engineering. This "cross-pollination" made new developments possible setting the foundations for a multidisciplinary research area: Computational Statistics, which is today a consolidated field aiming at analysing complex real phenomena using advanced computational techniques.

The complexity of real phenomena is related to both the larger data set available and the amount of unknown influential factors present in real world. These changes in paradigm require the design of analyses that have to be customised and flexible, focussed on unveiling the real structure underlying the available data.

A real phenomenon can be analysed by identifying its main dimensions and defining a set of influential factors related to them. Scientific modelling aims at making a particular feature of the world easier to understand, define, quantify and visualise. As referred above, this process requires selecting and identifying relevant aspects of a situation in the real world and then applying different types of models based on the main goal; these models include conceptual models to better understand, operational models to operationalise, mathematical models to quantify and graphical models to visualise the phenomenon under analysis.

However, when the analysed phenomenon presents sources of heterogeneity, comes from several sub-populations or is influenced by other disturbance factors, traditional methods often fail to recover the real structure underlying the data and more sophisticated procedures are required.

This situation is no different for models like Partial Least Squares Path Modelling (PLSPM); this model aims at estimating the relationships among blocks of observable variables, which in turn are expression of latent (unobservable) variables.

The PLSPM algorithm is characterised by a system of interdependent equations based on simple and multiple linear regressions. The algorithm estimates the dependence relationships among latent variables (inner or structural model) as well as the relationships between manifest variables and their own latent variable (outer or measurement model). All the relations present in both inner and outer models are estimated under the assumption of linearity.
Although attractively simple, the traditional linear model often fails in some situations: in real life, effects are often not linear (Hastie et al., 2009).
The objective of this thesis is to propose a flexible data-driven alternative to the PLSPM algorithm tackling two main issues: (i) break the linearity assumptions present in the standard PLSPM algorithm; and (ii) accommodate path direction within the inner model estimation phase through a non-symmetrical weighting estimation technique.

Thesis Outline Chapter 1 presents an historical overview of PLSPM from its origins up to the latest developments; followed by theoretical analysis on measurement and structural models. Section 1.2.3 presents a state of the art on PLSPM algorithm and its extensions. The following section shows an overview on model validation techniques and comments the main issues related to the current assessment metrics. The chapter ends with a thorough study on open issues and sets the ground for the following chapters introducing the challenges related with linearity assumption and path direction incoherence.
Chapter 2 starts with an introduction on the linear assumptions made

in PLSPM and motivates the need for new developments focussed at answering the aforementioned questions. The subsequent sections show an overview on nonlinear modelling techniques and a detailed critical analysis on the available nonlinear approaches to PLSPM. Section 2.4 introduces and draws up the proposed approach, developed as part of this thesis; the final part of this section compares Nonlinear PLSPM results against the standard PLSPM model.

The algorithm presented in chapter 2 is tested for convergence and stability in chapter 3. This chapter presents a wide Monte Carlo simulation analysis based on a comprehensive scenarios design phase. The results are then analysed and compared with the standard PLSPM algorithm.

Chapter 4 presents an application focussed on a Customer Satisfaction study developed at EDP Comercial, one of the leaders in the Portuguese liberalised energy supply market. This application introduces a novel results interpretation tool provided by the proposed nonlinear approach to PLSPM.

The EQS code for the Monte Carlo simulated data and the R code for the nonlinear approach to PLSPM are provided in the appendix.

Chapter 1

PLS Path Modelling

1.1 Historical Review

Partial Least Squares (PLS) methods made their first appearance in the 1960s when a research group at the Uppsala University, led by Herman Wold, developed the foundations of all modern PLS tools.

Herman Wold work was focussed on estimation methods for systems of simultaneous equations using least squares (LS) rather than Maximum-Likelihood (ML) (Mateos-Aparacio, 2011). His developments led him to a different estimation technique using iterative procedures, from which he created a new method called the Fixed-Point algorithm. This method uses an iterative ordinary least squares (OLS) algorithm to estimate the coefficients in a system of simultaneous equations (Wold, 1965).

Based on a comment received in 1964, during a conference on the Fixed-Point at the University of North Carolina, Wold steered the algorithm in order to calculate Principal Components (PCA) using an iterative process (Fornell, 1982). Later developments led Wold to apply the algorithm for calculating Canonical Correlations (CCA) (Hotelling, 1936). Fornell and Larcker (1987, p 408) define these approaches as belonging to a “second generation of multivariate analysis”.

The Fixed-Point algorithm, some years later, led him to his final domain of interest: multivariate analysis and projection methods (Principal Components Analysis and its extension, PLS projection to latent structures) (Johnson and Kotz, 1998).

Herman Wold formalised the idea of partial least squares in his work on principal component analysis (Wold, 1966a,b) where the NILES algorithm, short for “Nonlinear Iterative LEast Squares”, was introduced. The latter paper presented a collage of examples solved by means of iterative procedures based on steps of least squares regressions.

Wold (1973) and Noonan and Wold (1977) works strengthen the foundations of PLS methods and renamed the category of methods from NILES to NIPALS (“Nonlinear Iterative PArtial Least Squares”). Given the fact that these first publications emphasised the iterative least squares approach to PCA, most authors refer to NIPALS as the PLS algorithm for PCA.

These first NIPALS procedures were never tagged as a single methodology. On the contrary, they were seen as a collection of different algorithms for solving a diversity of methods such as PCA, CCA, regressions, and systems of econometric equations. The common goal of these procedures was to linearise problems that were originally nonlinear in their parameters.

The 1970s started with some turbulence for all NIPALS related procedures. In fact, a Wold's former Ph.D. student, Karl Jöreskog, designed a novel approach to path modelling with latent variables based on ML estimation (i.e., models connecting two blocks of variables). Although Wold's and Jöreskog's proposals present an approach to path modelling with latent variables, there are several differences between the two approaches (see Astrachan et al. (2014); Dolce (2015); Dolce and Lauro (2015); Rigdon (2012, 2016); Vilares et al. (2010)).

Jöreskog's major accomplishments came from a multidisciplinary research that merged econometric simultaneous equations models, psychometric latent variable models, sociology causal analysis, and biometric path analysis in a computer algorithm using the ML approach for parameters estimation (Jöreskog, 1970).

The combination of latent variables modelling and path models opened a whole new range of opportunities for researchers in the latent variables modelling area. Wold realised that some of the NIPALS procedures could be adapted for this new type of models.

In 1973, Wold re-branded again his methods from NIPALS procedures to NIPALS modelling with the intent of presenting NIPALS as a modelling framework (Wold, 1973). He positioned NIPALS modelling as "a design for the linearisation of models that are not linear in the parameters. The design is an *ad hoc* combination of (i) model specification in terms of causal and/or predictive relations, and (ii) parameters estimation". That being said, NIPALS modelling was thus clearly reflecting a more mature but still incomplete modelling framework.

Still on the completeness of the NIPALS modelling framework, Joseph Kruskal once asked Wold "whether an explicit definition can be given for the class of nonlinear models that constitute the scope of NIPALS modelling" (Wold, 1973). Wold answered that "NIPALS modelling is highly flexible, allowing the combined used of several devices, including parameter grouping and relaxation; auxiliary transformation of the model; and modelling the predictors in terms of indirectly observed manifest variables and other hypothetical constructs", identifying "NIPALS modelling as an open ended array of models with unlimited complexity in the combined use of several devices".

In mid-1970s, Wold and his team at the University of Göteborg refined and published several versions of a common methodology to estimate path models by using an iterative algorithm of least squares regressions. It is worth mentioning: (i) an extension of the algorithm that allows handling three blocks (as opposed to the previous two blocks algorithm); and (ii) the extension of handling more than one between-block relation (Wold, 1974, 1975a,b).

During the same period Wold encased his modelling framework based on the PLS approach under the "Soft Modelling" insignia (Wold, 1975b). The NIPALS approach is applied to the "soft" type of model used in social sciences in the last years, specifically path models affecting latent variables which serve as proxies for blocks of indirectly observed variables. "Soft modelling" implies the idea of modelling in "complex situations where data and prior information are relatively scarce and without specifying assumptions about the stochastic-distributional properties of variables and residuals" (Wold, 1975b).

Johnson and Kotz (1998) describes Herman Wold as "a very practical man, and wanted estimation and modelling methods to work with a minimum of assumptions, for incomplete data, with many variables and collinear variables, etc.; and he developed PLS accordingly". This practicality is confirmed in "Path Models with Latent Variables: The NIPALS Approach" (Wold, 1975a), where Wold states that sometimes "the model builder has little or no more prior information at disposal for the model construction than its intended operative use. The NIPALS models are designed with particular view to applications in such low-information situations".

After several adjustments made during the 1970s, Wold and his team arrive to a more defined framework and the acronym NIPALS is shortened to PLS. The end of the 1970s decade sees the official presentation of the so-called Basic Design for PLS path modelling.

The Basic Design represents the basic method for PLS Path Analysis with Latent Variables and it has been firstly published in "Causal-Predictive Analysis of Problems with High Complexity and Low Information: Recent Developments of Soft Modelling" and then in Wold (1980). This method represents the main reference on top of which all extensions and modifications are based on. More theoretical details can be found in Wold (1982a,b,c) and a practical application to the chemometric area is provided in Gerlach et al. (1979). Geometric interpretations are provided by Fred Bookstein (Bookstein, 1980, 1982).

Also in 1979, Karl Jöreskog and Herman Wold organised a meeting that brought together the LISREL[1] (or SEM-ML community) and PLS com-

[1] LISREL (LInear Structural RELations) is the "informal" name that the community gave to the ML approach to Structural Equations Modelling published by Jöreskog in Jöreskog (1970). The term LISREL was the name given to the implemented software (Jöreskog and Sorbom, 1993). However, it had such a rapid development that the

munity generating interesting contents then published in the form of the classic two-volume book: "Systems under indirect observation: Causality, structure, prediction".

In 1989, Jan-Bernd Lohmöller published the book "Latent Variable Path Modeling with Partial Least Squares" (Lohmöller, 1989) where he presented the basic PLS Path Modelling (PLSPM) algorithm and his extended version. For many years LVPLS 1.8 (developed by Lohmöller, 1984) was the unique available software on PLS Path Modelling. What is perhaps the first pseudo-code description of the basic algorithm is also provided in Lohmöller (1989) (p. 29).

As mentioned in the previous paragraph, Lohmöller extended the basic PLS algorithm in various directions. More details can be found in section 1.2.

Strangely enough, during the 1990s, the theoretical developments on PLS Path Modelling slowed down dramatically. One of the most interesting work was presented on the computational side with the development of PLS-Graph by Wynne Chin (Chin, 1998b).

The beginning of the XXI century saw a renewed interest in PLSPM and major contributions were made. The main reference in this period was the paper "PLS path modeling" by Tenenhaus, Esposito Vinzi, Chatelin, and Lauro (2005). Other relevant authors in this field are Ringle, Henseler and Dijkstra.

In 2005 a new software was made available by Ringle et al. (2005b) and their work has been an on-going process with a series of versions (the current one being SmartPLS 3).

methodology and the software have been associated to each other (Trinchera, 2008).

On the theoretical side, Hanafi (2007) and Tenenhaus and Hanafi (2010) presented two fundamental works that aimed at better understanding the PLSPM algorithm. They developed extensions to the multi-block approach initiated by Lohmöller and Hanafi has resolved some of the issues around the convergence of the PLSPM algorithm. An interesting work on the convergence issue has been provided by Krämer (2007). Its findings will be presented with more detail in section 1.3.

Other alternative approaches to PLSPM have been proposed. Namely, the Generalised Maximum Entropy (GME) presented by Al-Nasser (2003) and the Generalised Structured Component Analysis (GSCA) by Hwang and Takane (2004).

Two interesting reviews on PLS path modelling empirical applications can be found in Marcoulides et al. (2009) and Ringle et al. (2012).

More recently, Tenenhaus and Tenenhaus (2011) proposed the Regularised Generalised Canonical Correlation Analysis (RGCCA), a new modification to the PLSPM algorithm in such a way that convergence is guaranteed; additionally, PLS Regression[2] is presented as one of its special cases. This approach represents a generalisation of regularised canonical correlation analysis to three or more sets of variables. It constitutes a general framework for many multi-block data analysis methods and combines the power of multi-block data analysis methods, such as the maximisation of well identified criteria, and the flexibility of PLS path modelling. The big achievement is the fact that this paper, extending Hanafi (2007) work on convergence, presents a new monotonically

[2]PLS Regression (PLS-R) (Tenenhaus, 1998; Wold et al., 1983) represents a slightly modified PLSPM algorithm with the objective of obtaining a regularised component based regression tool Tenenhaus (1998); Wold et al. (1983).

convergent algorithm very similar to the PLS algorithm proposed by Herman Wold. This new proposal achieves convergence introducing a modified Mode A in which the outer weights are normalised to unitary variance at each step of the algorithm. Contrary to classical Mode A, this new estimation mode has the major advantage to maximise a known criterion.

During the last year, a set of papers discussed the differences between the SEM-ML approach and the PLS approach to Structural Equation Modelling. The review papers by Rigdon (2012) and Ronkko and Evermann (2013) started two interesting and active discussion streams.

The first critical review published by Rigdon in 2002 (Rigdon, 2012) states that PLS path modelling "has strengths as a tool for prediction which have not been fully appreciated" and "can move forward by freeing itself entirely of its heritage as 'something like but not quite factor analysis', by fleshing out inferential tools appropriate for a purely composite method and by developing approaches for assessing measurement validity that properly recognise the distinction between theoretical concepts and empirical proxy".

The paper published by Sarstedt, Ringle, Henseler, and Hair (2014) criticises the comments made by Rigdon in the aforementioned review, giving "their version of the truth" focussing mainly on prediction, explanation and model assessment. The authors clarify that there should not be a dichotomy between predictive and explanatory modelling and that PLS path modelling (referred as PLS-SEM in their paper) should not be forced to "choose a side".

Dijkstra (2014) also commented the review made by Rigdon going through the PLS genesis and focussing on two main topics: (i) suitability of PLS path modelling as a tool for estimating structural relationships; and (ii) whether the factor scores produced by PLS path modelling can be determined unambiguously or they should be obtained by using composites instead. Other critics to Rigdon's strong statements are presented in Bentler and Huang (2014).

This sequence of comments ends, at least for now, with a "closing" and clarifying paper presented by Rigdon (2014). The author tries to answer all the comments and flaws highlighted in the previous reviews. Rigdon subdivides the challenges in nine main arguments described in his work. In addition to the previous paper, Rigdon (2016) published a thorough analysis on the practical use of PLS path modelling identifying: (i) flaws related to invalid arguments in favour of using PLSPM; and (ii) invalid arguments opposing its use within the context of a unifying framework to be used as an analytical method in European management research.

Other authors focussed on developing a unified framework are Sarstedt et al. (2016). The authors validated their conceptual considerations based on a simulation study, highlighting the biases that occur when using (i) composite-based partial least squares path modelling to estimate common factor models, and (ii) common factor-based covariance-based structural equation modelling to estimate composite models. Their results show that the use of PLSPM is preferable, particularly when it is unknown whether the data's nature is common factor-based or composite-based.

Ronkko and Evermann (2013) presented a review on the application and applicability side of PLS path modelling. This paper strongly criticises

PLS path modelling suitability for different applications and presents the authors' doubts regarding its effectiveness in building and testing theory in organisational research. This review generated a detailed answer from Henseler et al. (2014) who pointed out that "the shortcomings of PLS are not due to problems with the technique, but instead to three problems with Ronkko and Evermann (2013) study: (i) the adherence to the common factor model; (ii) a very limited simulation design; and (iii) over-stretched generalisations of their findings".

The result of such a rich amount of ideas and views allows us to get a deeper view on PLS path modelling capability and suitability in different situations and application areas.

More recently, a group of researchers shifted their focus on PLSPM prediction capabilities. Shmueli et al. (2016) stated that, so far, PLSPM literature has not made a full use of these predictive proprieties, using instead an explanatory approach focussed on statistical significance and power (Becker et al., 2013). Shmueli and Koppius (2010, 2011) reinforced the previous statements saying that quantitative research in management has been dominated by causal-explanatory statistical modelling at the expense of predictive modelling. More details on this topic are presented in section 1.2.5.

Our position with regards to the aforementioned papers is that PLS path modelling is often discussed and used as if it was a kind of factor analysis but, as mathematically shown by Rigdon, it is a purely composite-based method. Also, the fact that PLS path modelling represents a better model for prediction does not imply that the same cannot be used for explanatory analysis. The PLS path modelling community needs to em-

brace the method's character as a composite-based method; this requires shedding the factor-based jargon, perspectives, evaluation tools and measurement framework of factor-based SEM and developing alternatives. Another important set of opportunities is related to the predictive assessment of PLSPM. The latest steps toward prediction-driven PLSPM applications and the formalisation of a predictive assessment framework are widening the possibilities associated to the use of PLSPM.
The next sections present the original algorithm by Herman Wold, its extensions and open issues.

1.2 PLS Path Modelling

As discussed in the previous sections, PLS path modelling can be described as a composite-based estimation method which aims at analysing the complexity existent in a specific system by estimating the causal relations between latent variables (LVs) defined as components or composites and measured by a set of manifest variables (MVs).
Formalising the previous concepts, PLS path modelling focusses on studying the relationships among J blocks $\boldsymbol{X_1, \ldots, X_j, \ldots, X_J}$ of MVs, which represent J latent variables $\boldsymbol{\xi_1, \ldots, \xi_j, \ldots, \xi_J}$, defined as composites.
PLSPM adhere to a specific graphical convention (see Figure 1.1) based on the drawing principles defined in the path analysis (Wright, 1921, 1934). More in detail, ellipses or circles represent the latent variables, and rectangles or squares refer to manifest variables, whereas unidirectional arrows are used to relate MVs with LVs and also causations among LVs.

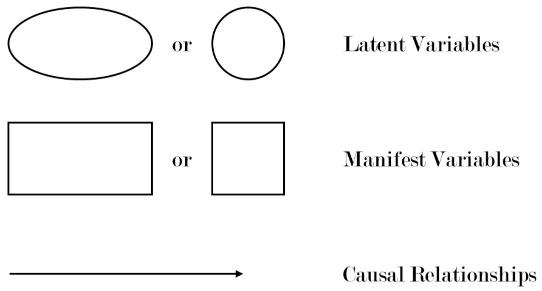


Figure 1.1: PLSPM Graphical Notation

A PLS path model (see Figure 1.2) is made up of two elements: (i) the measurement model (or outer model) which describes the relationships between the MVs and their respective LVs; and (ii) the structural model (or inner model) which describes the relationships between the LVs. Both models are described in the next sections.

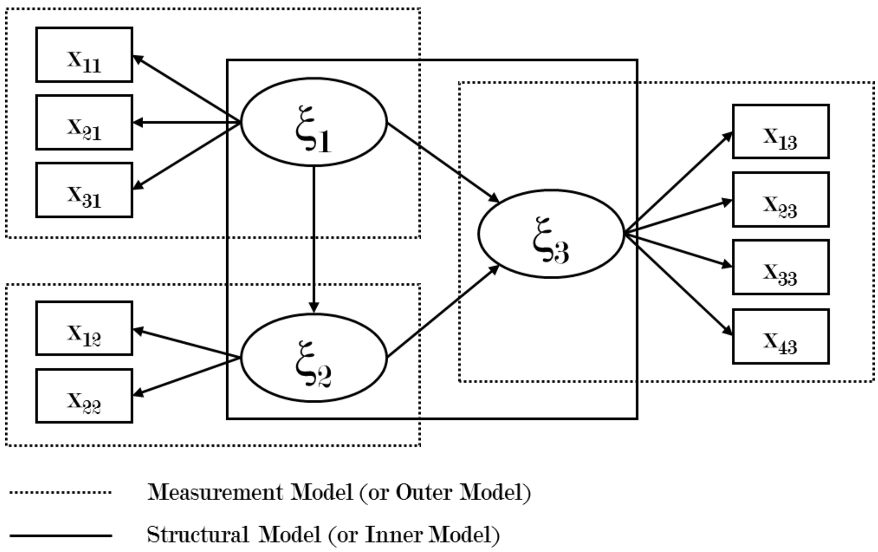


Figure 1.2: PLSPM Graphical Representation

1.2.1 The Measurement Model

A LV ξ_j is an unobservable variable (also named composite or construct) indirectly described by a block of observable variables $\boldsymbol{X_j}$ which are called MVs or indicators. There are several ways to relate the MVs to their LVs:

– The reflective way (or outwards directed way);

– The formative way (or inwards directed way);

– The MIMIC way (a combination of both reflective and formative).

Reflective Way

In the reflective way each MV reflects the corresponding LV (see Figure 1.3). A block is defined as reflective if the LV is assumed to be a common factor that reflects itself in its respective MVs.

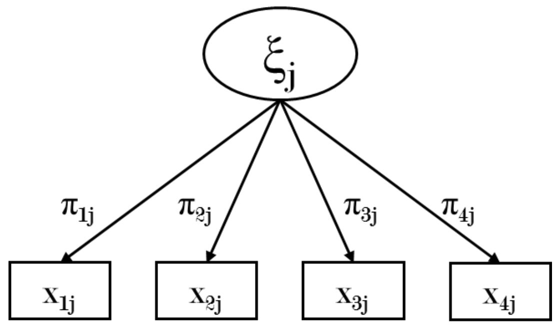


Figure 1.3: Measurement Model: the Reflective Way

In this model each MV is related with its LV by a simple linear regression.

$$x_{pj} = \pi_{p0} + \pi_{pj}\xi_j + \epsilon_p \tag{1.1}$$

where ξ_j has mean m and standard deviation equal to 1.

The model defined in equation 1.1 has to follow only one hypothesis named *predictor specification* and defined by H. Wold in his seminal papers:

$$E\left(x_{pj}|\xi_j\right) = \pi_{p0} + \pi_{pj}\xi_j \tag{1.2}$$

This hypothesis implies that the residual ϵ_p has a zero mean and is uncorrelated with the LV ξ_j.

In the reflective model each block of MVs $\boldsymbol{X_j}$, has to be unidimensional in the sense of factor analysis. The ultimate goal is that all the MVs belonging to one block have to present a strong correlation.

When working with real data and using a reflective model, it is very important to check the unidimensionality for each block of MVs.

There are three main techniques used to check the unidimensionality:

– *Principal Component Analysis*: a block can be considered unidimensional if the first eigenvalue of the correlation matrix, built based on all the MVs related to the block, is greater than 1 and the second one smaller than 1, or at least far enough from the first one. After checking the eigenvalues, it is important to verify that all the MVs are positively correlated with the first factor (in the sense of PCA). A MV becomes inadequate to measure the LV when its correlation with the first factor is negative.

– *Cronbach's* α: this statistic can be used to check unidimensionality in a block of P_j manifest variables $\boldsymbol{X_j}$, when they are all positively correlated. Cronbach proposed the following procedure for standardised variables:

The variance of $\sum_{p=1}^{P_j} x_{pj}$ is developed as follows:

$$Var\left(\sum_{p=1}^{P_j} x_{pj}\right) = P_j + \sum_{p \neq p'} corr\left(x_{pj}, x_{p'j}\right) \tag{1.3}$$

The larger $\sum_{p \neq p'} corr\left(x_{pj}, x_{p'j}\right)$ the more the block $\boldsymbol{X_j}$ is unidimensional.

Based on equation 1.3 is possible to calculate the following ratio:

$$\alpha^{'} = \frac{\sum_{p \neq p'} corr\left(x_{pj}, x_{p'j}\right)}{P_j + \sum_{p \neq p'} corr\left(x_{pj}, x_{p'j}\right)} \tag{1.4}$$

When all correlations $corr\left(x_{pj}, x_{p'j}\right)$ are equal to 1, $\alpha^{'}$ reaches its maximum value, i.e., $(P_j - 1)P_j$.

The maximum value is then used to obtain the Cronbach's α dividing $\alpha^{'}$ by its maximum value:

$$\alpha = \frac{\sum_{p \neq p'} corr\left(x_{pj}, x_{p'j}\right)}{P_j + \sum_{p \neq p'} corr\left(x_{pj}, x_{p'j}\right)} \times \frac{P_j}{P_j - 1} \tag{1.5}$$

When working with the original manifest variables (non-standardised), Cronbach's α is calculated as follows:

$$\alpha = \frac{\sum_{p \neq p'} corr\left(x_{pj}, x_{p'j}\right)}{Var\left(\sum_{p=1}^{P_j} x_{pj}\right)} \times \frac{P_j}{P_j - 1} \tag{1.6}$$

The following table (Cortina, 1993) can help assessing α's values:

Cronbach's α	**Internal Consistency**
$\alpha \geq 0.9$	Excellent
$0.9 > \alpha \geq 0.8$	Good
$0.8 > \alpha \geq 0.7$	Acceptable
$0.7 > \alpha \geq 0.6$	Questionable
$0.6 > \alpha \geq 0.5$	Poor
$0.5 > \alpha$	Unacceptable

Table 1.1: Cronbach's α Assessment

In accordance with (Cortina, 1993) a block can be considered unidimensional when α is larger than 0.7.

– *Dillon-Goldstein's* ρ: by construction, the correlation signs between manifest variables x_{pj} and the latent variable ξ_j have to be positive, that is, in the equation 1.1 all loadings π_{pj} are positive. A block can be defined unidimensional when all loadings are large.

The first step is represented by defining the variance of $\sum_{p=1}^{P_j} x_{pj}$. For this specific case the variance is calculated from equation 1.1 assuming that the residual terms ϵ_p are independent:

$$\begin{aligned} Var\left(\sum_{p=1}^{P_j} x_{pj}\right) &= Var\left(\sum_{p=1}^{P_j} (\pi_{p0} + \pi_{pj}\xi_j + \epsilon_p)\right) \\ &= \left(\sum_{p=1}^{P_j} \pi_{pj}\right)^2 Var\left(\xi_j\right) + \sum_{p=1}^{P_j} Var\left(\epsilon_p\right) \end{aligned} \tag{1.7}$$

The larger $\left(\sum_{p=1}^{P_j} \pi_{pj}\right)^2$ the more the block $\boldsymbol{X_j}$ is unidimensional. The Dillon-Goldstein's ρ is defined as:

$$\rho = \frac{\left(\sum_{p=1}^{P_j} \pi_{pj}\right)^2 Var\left(\xi_j\right)}{\left(\sum_{p=1}^{P_j} \pi_{pj}\right)^2 Var\left(\xi_j\right) + \sum_{p=1}^{P_j} Var\left(\epsilon_p\right)} \tag{1.8}$$

In an initial stage, the values of ξ_j are not available and an approximation is needed. Based on the assumption that all MVs x_{pj} and the LV ξ_j are standardised, it is possible to obtain a LV approximation using the first factor t_1 from a PCA on all MVs related with the block.

The loading π_{pj} can be estimated by $corr\left(x_{pj}, t_1\right)$ and, based on equation 1.1, the a $Var\left(\epsilon_p\right)$ is estimated by $1 - corr^2\left(x_{pj}, t_1\right)$.

The estimated Dillon-Goldstein's ρ can be calculated as:

$$\hat{\rho} = \frac{\left[\sum_{p=1}^{P_j} corr\left(x_{pj}, t_1\right)\right]^2}{\left[\sum_{p=1}^{P_j} corr\left(x_{pj}, t_1\right)\right]^2 + \sum_{p=1}^{P_j} \left[1 - corr^2\left(x_{pj}, t_1\right)\right]} \tag{1.9}$$

A block can be considered unidimensional when $\hat{\rho}$ is larger than 0.7.

This statistics is considered to be a better option to check unidimensionality for a block of manifest variables (Chin, 1998a).

Formative Way

In a formative model the latent variable ξ_j is obtained through a linear combination of the related manifest variables (see Figure 1.4) and a residual term:

$$\xi_j = \sum_{p=1}^{P_j} \omega_{pj} x_{pj} + \delta_j \tag{1.10}$$

Using this measurement model scheme, unidimensionality of the block is not required (i.e., a block of manifest variables is allowed to be multidimensional).

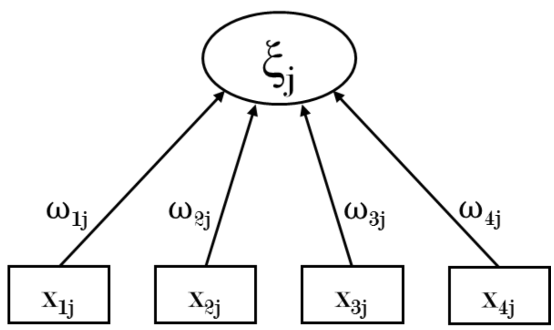


Figure 1.4: Measurement Model: the Formative Way

The hypothesis related to the predictor specification for the equation 1.10 is:

$$E\left(\xi_j | x_1, \ldots, x_{P_j}\right) = \sum_{p=1}^{P_j} \omega_{pj} x_{pj} \quad (1.11)$$

This hypothesis implies that the residuals δ_j has mean 0 and is not correlated with the manifest variables x_{pj}.
In this scheme the LV is generated from a linear combination of its MVs and there is no sign constraints on the weights ω_{pj}, but unexpected signs show problems in data that might be related to multicollinearity. If the model's results present unexpected signs the user can remove the MV from input data or, as shown in Tenenhaus, Esposito Vinzi, Chatelin, and Lauro (2005), sign constraints can be easily added to the PLS algorithm.

MIMIC (*Multiple Indicators for Multiple Causes*)

In a MIMIC scheme the latent variables are seen as a mix of formative and reflective relationships. The measurement model for a specific block $\boldsymbol{X_j}$ is defined as follows.
Let P^R represent the set of MVs following the reflective scheme,
when the arrows are outward directed (reflective scheme) the simple regression on x_{pj} can be written as:

$$x_{pj} = \pi_{p0} + \pi_{pj}\xi_j + \epsilon_p \quad \text{for} \quad p \in P^R \quad (1.12)$$

when the MVs are inward directed (formative scheme), the latent variable ξ_j can be determined as:

$$\xi_j = \sum_{p \notin P^R} \omega_{pj} x_{pj} + \delta_j \quad (1.13)$$

The predictor specification hypothesis for equations 1.12 and 1.13 are the same mentioned in the previous sections.

Thoughts on Measurement Model's Schemes

The previous paragraphs presented three measurement model schemes related, in some way, to the assumed directions of the connections between manifest and latent variables.

The "reflective" measurement scheme is used to describe an outer model where manifest variables act as dependent upon an unmeasured variable. Reverting the direction of the outer relation, the unobserved variable is modelled as dependent from the manifest variables; this scheme is known as "formative". A mixture of inward and outward directed connection belonging to the same block corresponds to the MIMIC scheme.

It is important to separate the conceptual analysis of these measurement schemes from the technique used to calculate the latent variables proxies (or composites).

The PLS path modelling presents several options to calculate the latent variables proxies; the most known techniques are "Mode A" and "Mode B" (explained in detail throughout this chapter). For years Mode A and Mode B have been associated to reflective and formative schemes, respectively. As Rigdon (2016) strongly affirms, "this is an illusion". In fact, both modes create composites and the only difference standing between the two is the way how weights are obtained (using Mode A instead of Mode B means using correlation weights instead of OLS regression coefficients).

Differently from OLS regression coefficients, correlation weights ignore collinearity among predictors. This difference represents an advantage for the users that prefer correlation weights because this technique does not experience unexpected weights signs driven by collinearity.

As confirmed by Becker et al. (2013) for PLS path modelling, Dana and Dawes (2004) demonstrated that, while correlation weights yield a somewhat lower in-sample R^2 than OLS regression weights, they yield a higher out-of-sample R^2 when sample size and true predictability are moderate, potentially covering a much larger range of practice than the special conditions required for OLS regression weights to stand out.

There can be good reasons to choose Mode A or Mode B within a PLS path modelling; this choice has nothing to do with the conceptual scheme idealised for the measurement model (choice between "formative" and "reflective").

The real choices a researcher faces whilst implementing a PLS path model are between common factor proxies and composite proxies, and between regression weighted composites and correlation weighted composites.

In summary, this work shares Rigdon's position on this matter: "the the terms formative and reflective only obscure the statistical reality" (Rigdon, 2016).

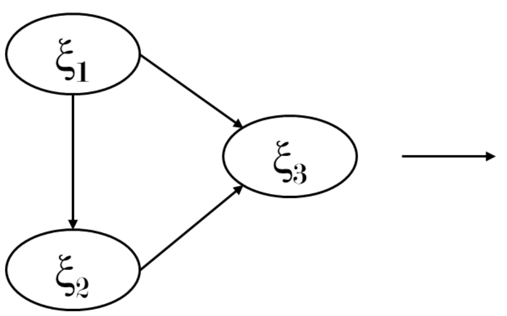
The MIMIC conceptual scheme is difficult to implement within a PLSPM context (Fornell and Bookstein, 1982), but the problem may be faced by splitting the MIMIC variable into two blocks of manifest variables (an endogenous and an exogenous one) with a known relationship between original and new path coefficients.

1.2.2 The Structural Model

The causal model shown in figure 1.2 presents three latent variables connected by a causal relationship. These relationships build the structural model (or inner model) and can be formalised as follows:

$$\xi_j = \beta_{j0} + \sum_{j \neq j'} \beta_{jj'} \xi_{j'} + \nu_j \tag{1.14}$$

The predictor specification hypothesis also applies for equation 1.14.
A latent variable which never appears as dependent in equation 1.14 is known as exogenous variable. The other LVs are defined as endogenous variables.
The causality model must be a causal chain. That means that there is no loop in the model. This kind of model is called recursive, from the Latin *Recursio*, which means I can return (Tenenhaus et al., 2005).
Every structural model can be described through a square matrix containing binary values (see Figure 1.5). Its dimension is equal to the number of latent variables J. Lohmöller defines this matrix as inner design matrix (Lohmöller, 1989).



0	0	0
1	0	0
1	1	0

Figure 1.5: Inner Design Matrix

Let l and k be respectively rows and columns indexes of the aforementioned matrix, cell (l, k) has value of 1 when latent variable ξ_k causes ξ_l; 0 otherwise.

The structural model estimation process is shown in the next sections.

1.2.3 Algorithm: State of the Art

PLS path modelling has been firstly developed by Wold (1975b). Lohmöller (1989) presented new theoretical and computational developments (LV-PLS software). A first software with graphical interface (PLS-Graph) has been developed by Chin (1998a,b). PLS-Graph is based on Lohmöller's proposed algorithm presenting some new and improved validation techniques.

The current work is based on the algorithm proposed by Lohmöller (1989) which is described in the next paragraphs.

As discussed in the previous sections, PLS path modelling aims to estimate relationships among J $(j = 1, \ldots, J)$ blocks of variables, which are expression of unobservable constructs. The algorithm is composed by a system of interdependent equations based on simple and multiple linear regressions. The algorithm estimates the causal effects among LVs as well as the relationships between MVs and their own LVs.

Starting Weights Definition

The first step of the PLSPM algorithm regards the definition of a set of arbitrary weights w_{pj} to be used as starting point. The weights are then normalised in order to produce LVs with unitary variance.
There are several ways to define the starting weights. One of the most common choices is $w_{pj} = sign\left[corr\left(x_{pj}, \xi_j\right)\right]$; this is applied in practice by setting $w_{pj} = sign\left[corr\left(x_{pj}, \xi_j\right)\right]$ when $p = 1$ and 0 otherwise.
As of today, the starting weights choice does not seem to interfere with the final results but it does have an impact on how quickly the algorithm reaches convergence.

Measurement Model: Latent Variables Calculation

Once defined the initial weights the algorithm moves to the outer estimate y_j of the standardised (with mean = 0 and standard deviation = 1) latent variables $(\xi_j - m_j)$. The composites are calculated as linear combination of their centered MVs:

$$y_j \propto \pm \left[\sum_{p=1}^{P_j} w_{pj}\left(x_{pj} - \bar{x}_{pj}\right)\right] \tag{1.15}$$

where the $\propto$ symbol means that the variables on the left is proportional to the operator on the right; the $\pm$ sign represents the sign ambiguity. This problem is solved by selecting the sign that makes the variable y_j positively correlated with the majority of manifest variables x_{pj}.
The j-th estimated latent variable (or composite) is obtained as follows:

$$y_j = \sum_{p=1}^{P_j} \tilde{w}_{pj} \left(x_{pj} - \bar{x}_{pj} \right) \tag{1.16}$$

The coefficients w_{pj} and $\tilde{w}_{pj}$ are called outer weights.

The mean value m_j is estimated as:

$$\hat{m}_j = \sum_{p=1}^{P_j} \tilde{w}_{pj} \bar{x}_{pj} \tag{1.17}$$

and the latent variable ξ_j is estimated by:

$$\hat{\xi}_j = \sum_{p=1}^{P_j} \tilde{w}_{pj} x_{pj} = y_j + \hat{m}_j \tag{1.18}$$

Structural Model: Inner Weights Estimation

The structural model aims to give an estimate of the LVs based on the causal relations present in the inner model. The inner weights $e_{jj'}$ can be estimated through several techniques.

Centroid Scheme The centroid scheme represents the original technique proposed by H. Wold and is also one of the most used techniques to estimates inner weights. Following this technique $e_{jj'}$ can be obtained as:

$$e_{jj'} = sign\left[corr\left(y_j, y_{j'} \right) \right] \tag{1.19}$$

In this case $e_{jj'}$ are expressed as the correlation sign between y_j and the latent variable $y_{j'}$ connected to y_j (see Equation 1.19). Two LVs are connected if they are linked in the structural model (i.e., an arrow goes from one variable to the other describing their causality relation).

The centroid scheme presents some inconvenience when correlations between LVs are very close to 0. In fact, when this situation happens, correlations fluctuate between positive and negative values creating apparent instability. Tenenhaus, Esposito Vinzi, Chatelin, and Lauro (2005) state that this choice does not seem to be a problem in practical applications.

Factorial Scheme The Factorial Scheme is one of the two techniques proposed by Lohmöller where inner weights $e_{jj'}$ are calculated as follows:

$$e_{jj'} = r_{jj'} = corr\left(y_j, y_{j'}\right) \tag{1.20}$$

By choosing this technique, the inner weights correspond to the correlation between latent variables. According to Lohmöller (1989), this technique should solve the drawbacks presented by the Centroid Scheme. Even though this new scheme do not significantly influence the results, it is very important for theoretical reasons. In fact, as shown in Tenenhaus, Esposito Vinzi, Chatelin, and Lauro (2005), it allows to relate PLS path modelling to usual multiple table analysis methods.

Path Weighting (or Structural) Scheme The Path Weighting Scheme is the second technique proposed by Lohmöller. The LVs connected to ξ_j are divided into two groups: the predecessors of ξ_j which are LVs explaining ξ_j, and the followers which are LVs explained by ξ_j. For a predecessor $\xi_{j'}$ of the LV ξ_j, the inner weight $e_{jj'}$ is equal to the

regression coefficient of $y_{j'}$ in the multiple regression of y_j on all the $y_{j'}$'s related to the predecessors of ξ_j. If $\xi_{j'}$ is a successor of ξ_j then the inner weight $e_{jj'}$ is equal to the correlation between $y_{j'}$ and y_j.
Summarising, when using the Path Weighting scheme, inner weights $e_{jj'}$ are calculated as:

$$\begin{aligned} e_{jj'} &= \text{regression coefficient of } y_j \text{ on all } y_{j'} \text{ if } \xi_{j'} \text{ explains } \xi_j \\ &= r_{jj'} \text{ if } \xi_j \text{ explains } \xi_{j'} \end{aligned} \tag{1.21}$$

The Path Weighting Scheme represents the only scheme where the direction of structural relations is taken into account (Dolce, 2015). As referred for the Factorial Scheme, this technique also allows to relate PLS path modelling to usual multiple table analysis methods.

Structural Model: Latent Variables Calculation

In the inner LVs calculation stage, the standardised $(\xi_j - m_j)$ latent variables inner estimation z_j is given by:

$$z_j \propto \sum_{j' \,:\, \xi_{j'} \text{ } adjacent \text{ } to \text{ } \xi_j} e_{jj'} \circ y_{j'} \tag{1.22}$$

where $\circ$ denotes the Hadamard product.

Measurement Model: Outer Weights Estimation

There are several ways to estimate the outer weights w_{jh}. Originally, H. Wold's algorithm included two estimation techniques: Mode A, Mode B

(Wold, 1975b). Later on, Lohmöller proposed a third technique: Mode C (Lohmöller, 1989). More recently, two more techniques have been proposed: Mode PLS (Esposito Vinzi, 2008, 2009; Esposito Vinzi and Russolillo, 2013) and New Mode A (Tenenhaus and Tenenhaus, 2011).

Mode A Each outer weight w_{pj} is the regression coefficient in the simple linear regression of the p-th MV x_{pj}, belonging to the j-th block $\boldsymbol{X_j}$, on the composite z_j of the j-th LV. As a matter of fact, as z_j is standardised, the generic outer weight w_{pj} is represented by the regression coefficient associated to z_j in the simple linear regression of x_{pj} on z_j. In more detail:

$$w_{pj} = cov\left(x_{pj}, z_j\right) \tag{1.23}$$

where, as referred above, the estimated latent variable z_j is standardised.

Mode B In mode B, the outer vector w_j of weights w_{pj} is composed by the regression coefficient vector in the multiple regression of z_j on the centered manifest variables $(x_{pj} - \bar{x}_{pj})$ related to the same latent variable ξ_j:

$$w_j = \left(\boldsymbol{X}_j^t \boldsymbol{X}_j\right)^{-1} \boldsymbol{X}_j^t z_j \tag{1.24}$$

where $\boldsymbol{X_j}$ is a matrix having on the columns the centered manifest variables $(x_{pj} - \bar{x}_{pj})$ related with the same latent variable ξ_j.

Mode C Lohmöller added a new mode C for the calculation of the outer weights (Lohmöller, 1989). In mode C, the weights are all equal in absolute value and reflect the signs of the correlations between the MVs and their LVs:

$$w_{pj} = sign\left(corr\left(x_{pj}, z_j\right)\right) \tag{1.25}$$

These weights are then normalised so that the resulting LV has unitary variance. Mode C actually refers to a formative way of linking MVs to their LVs and represents a specific case of mode B whose comprehension is very intuitive to practitioners.

Mode PLS In order to solve the problems related with multi-collinearity a new way to compute outer weights, in the case of a formative block, has been recently proposed by Esposito Vinzi (2008, 2009); Esposito Vinzi and Russolillo (2013). This approach involves using PLS Regression (PLS-R) (Tenenhaus, 1998; Wold et al., 1983) in order to compute significant outer weights. In particular, Esposito Vinzi (2009) proposes to calculate at each iteration the outer weights as coefficients in a PLS Regression of the LV inner composite on the MVs linked to the same LV. PLS-R method has been extensively described in literature (Tenenhaus, 1998; Wold et al., 1983). PLS-R is a linear regression technique that allows relating a set of predictor variables to one or several response variables. PLS-R shrinks the predictor matrix by sequentially extracting orthogonal components which, at the same time, summarise the explanatory variables and allow modelling and predicting the response variables. Finally, it provides a classical regression equation, in which the response is estimated as a linear combination of the predictor variables.

New Mode A Traditional Mode A applied to all the blocks does not seem to optimise any criterion; as Krämer (2007) showed, Wold's Mode A technique does not lead to a stationary equation related to the optimisation of a twice differentiable function. However, Tenenhaus and Tenenhaus (2011) recently extended the results of Hanafi (Hanafi, 2007) to a slightly adjusted Mode A in which a normalisation constraint is placed on outer weights rather than on LV composites. In particular, they showed that Wold's procedure, applied to a PLS path model where the new Mode A is used in all the blocks, monotonically converges to the following criterion:

$$\underset{||\boldsymbol{w}_j||^2=||\boldsymbol{w}_{j'}||^2=1}{\arg\max} \sum_{j \neq j'} c_{jj'}\, g\left(cov\left(\boldsymbol{X}_j \boldsymbol{w}_j, \boldsymbol{X}_{j'} \boldsymbol{w}_{j'}\right)\right) \tag{1.26}$$

where g is defined as:

$$g(x) = \begin{cases} x^2 & \text{if factorial} \\ |x| & \text{if centroid} \end{cases} \tag{1.27}$$

In the new mode A, the outer vector w_j of weights w_{pj} is

$$w_j = \frac{\boldsymbol{X}_j^t z_j}{||\boldsymbol{X}_j^t z_j||} \tag{1.28}$$

We may note that the outer composite $y_j = \boldsymbol{X_j a_j}$ is the first PLS component in the PLS regression (Tenenhaus, 1998; Wold et al., 1983) of the inner composite z_j on block $\boldsymbol{X_j}$. In the original mode A of the PLS approach, the outer weights are computed in the same way as formula 1.23 but normalised so that the outer component $y_j = \boldsymbol{X_j a_j}$ is standardised. This new mode A shrinks the intra-block covariance matrix to the identity. This shrinkage is probably too strong, but is useful for very high-dimensional data because it avoids the inversion of the intra-block covariance matrix.

Iterative Process and Convergence

After the first cycle the algorithm iterates the following steps:

1. Measurement Model: Latent Variables Calculation
2. Structural Model: Inner Weights Estimation
3. Structural Model: Latent Variables Calculation
4. Measurement Model: Outer Weights Estimation
5. Outer Weights Convergence Check

The aforementioned algorithm is described in figure 1.6 and its pseudocode is shown in Algorithm 1.

After reaching the algorithm convergence, the outer weights w_{jh} are used to obtain the final estimation of ξ_j calculated as $\hat{\xi}_j = \sum w_{jh} x_{jh}$.

In the last step of PLSPM algorithm, path coefficients are estimated through an OLS multiple regression among the estimated latent variables composites, according to path diagram structure. Denoting ξ_j $(j = 1, \ldots, J)$ as the generic endogenous LV and $\boldsymbol{\Xi}_{\rightarrow j}$ as the matrix

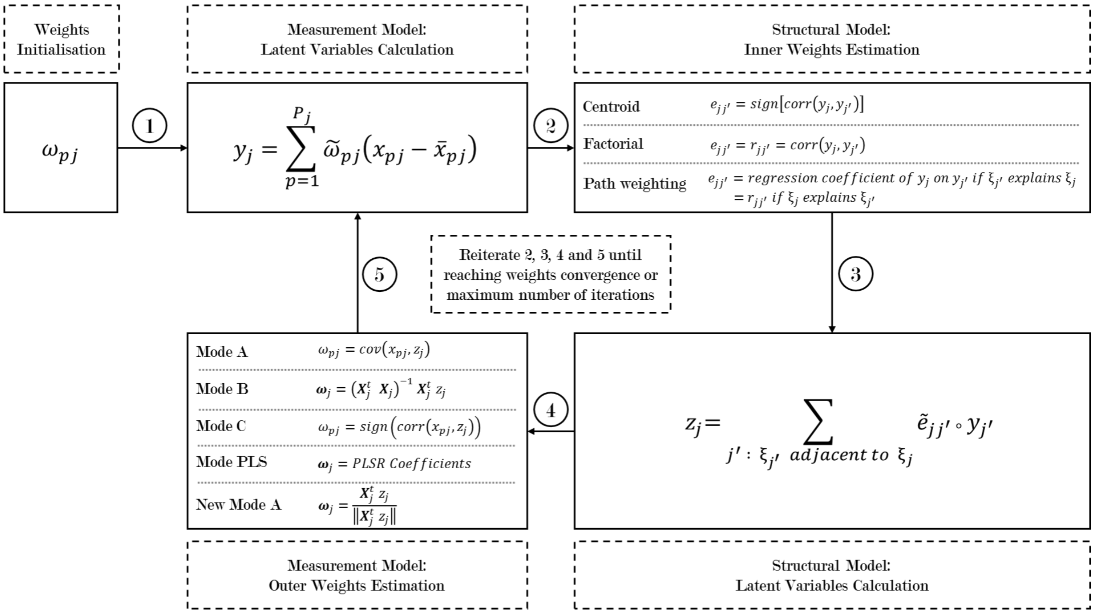


Figure 1.6: PLSPM Iterative Estimation Process

of the corresponding latent predictors, the path coefficient vector $\boldsymbol{\beta_j}$ for each ξ_j is obtained as:

$$\boldsymbol{\beta_j} = \left(\boldsymbol{\Xi}'_{\rightarrow j}\boldsymbol{\Xi}_{\rightarrow j}\right)^{-1}\boldsymbol{\Xi}'_{\rightarrow j}\hat{\xi}_j \tag{1.29}$$

Algorithm Convergence As previously mentioned, PLS path modelling is mostly used to analyse complex relationships among latent variables.

Many fields of research have embraced the specific advantages of PLSPM, behavioural sciences for instance (Bass et al., 2003) as well as many disciplines of business research such as marketing (Anderson et al., 1994; Fornell and Larcker, 1987; Matzler et al., 2004) and many others. The PLSPM advantages highlighted in these papers are confirmed in practice by its wide adoption in many organisations.

Algorithm 1: PLS Path Modelling (Lohmöller's Algorithm)

Input : $\boldsymbol{X} = [\boldsymbol{X_1}, \ldots, \boldsymbol{X_j}, \ldots, \boldsymbol{X_J}]$

Output: $w_{pj}, \hat{\xi}_j, \boldsymbol{\beta_j}$

1 Arbitrary Weights Initialisation: $w_{pj} = w_{pj}^{(0)}$

2 **while** *Convergence of* w_{pj} *is not reached (or max number of iterations)* **do**

3 **Latent Variables Composites Calculation** (Measurement Model):
$y_j \propto \pm \left[\sum w_{pj} \left(x_{pj} - \bar{x}_{pj}\right)\right]$

4 **Inner Weights Estimation** (Structural Model):
$e_{jj'} = f\left(y_j, y_{j'}\right)$ according to the chosen scheme

5 **Latent Variables Composites Calculation** (Structural Model):
$z_j \propto \sum_{j' \,:\, \xi_{j'} \text{ adjacent to } \xi_j} \left(e_{jj'} \circ y_{j'}\right)$

6 **Outer Weights Estimation** (Measurement Model):
$w_{pj} = f\left(\boldsymbol{X}, \boldsymbol{Z}\right)$ according to the chosen estimation technique

7 **Final Latent Variables Composites Calculation**:
$\hat{\xi}_j = \sum w_{pj} x_{pj}$

8 **Path Coefficients Calculation**:
$\boldsymbol{\beta_j} = \left(\boldsymbol{\Xi}'_{\boldsymbol{\to j}} \boldsymbol{\Xi}_{\boldsymbol{\to j}}\right)^{-1} \boldsymbol{\Xi}'_{\boldsymbol{\to j}} \hat{\xi}_j$

Henseler (2010) in his paper states that the popularity of PLSPM among scientists and practitioners results from four genuine advantages:

- Can be used when distributions are highly skewed (Bagozzi and Yi, 1994), because "there are no distributional requirements" (Fornell and Bookstein, 1982);

- Can be used to estimate relationships between latent variables with several indicators when sample size is small (Chin and Newsted, 1999);

– Availability of modern and easy-to-use software with graphical user-interface, like SmartPLS (Ringle et al., 2005b) and PLS-Graph (Chin, 1998b), have contributed to increase the attractiveness of PLSPM;

– PLSPM is preferred over covariance-based structural equation modelling when improper or non-convergent results are likely, as for instance in more complex models, when the number of latent and manifest variables is high in relation to the number of observations and the number of indicators per latent variable is low.

Notwithstanding the fact that the algorithm saw its first formalisation decades ago, the scientific and professional community mainly focussed on its practical implementations and standard algorithm expansions. When it comes to a thorough analysis of convergence the literature is scarce.

Tenenhaus et al. (2005) state that convergence is "always verified in practice but mathematically proven only for the two-block case"; Hanafi (2007) reinforces the previous statement adding that the "convergence ... is always verified in practice". Henseler (2010) presented in his work six cases where convergence is not reached under a set of specific circumstances; the author also states that "PLS does not always converge" and "the further search for a proof of convergence, at least for the general PLS path modelling algorithm, can thus be abandoned".

Analysing the different developments made during the last decades, it is possible to say that when first developed by Wold one of the advantages of its procedure was the monotonic propriety. More recently Hanafi (2007) demonstrated, for the case of Mode B, that Wold's procedure is monotonically convergent for more than two blocks of manifest variables; the author also demonstrated that Wold's PLSPM reaches a stable solution faster than Lohmöller's procedure.

Henseler (2010) presented a exhaustive summary of the PLSPM convergence across several configurations shown in table 1.2.

	Inner scheme	**One or two LVs**		**More than two LVs**	
		Mode A	**Mode B**	**Mode A**	**Mode B**
Wold	Centroid	Converges	Converges	Unproven	Converges
	Factorial	Converges	Converges	Unproven	Converges
	Path	Converges	Converges	Unproven	Unproven
Lohmöller	Centroid	Converges	Converges	Unproven	Unproven
	Factorial	Converges	Converges	Not Always	Unproven
	Path	Converges	Converges	Not Always	Unproven

Table 1.2: Convergence Scenarios for the PLSPM Algorithm (Henseler, 2010)

In his paper, Henseler (2010) showed that using Lohmöller algorithm, factorial or path weighting schemes and Mode A, the convergence is not proven.

Analysing in detail the summary presented in table 1.2, it is possible to conclude that the efforts related to the convergence of PLSPM can be focussed on cases where this situation is still to be proven. For these cases there are two possible future developments: (i) empirical proof through simulation techniques; and (ii) mathematical proof of the procedure's convergence.

Future studies are needed in order to better understand PLSPM and assess its limitations related to how the structure of the used inner model or the manifest variables affect convergence.

1.2.4 Model Validation

PLSPM produces several analytical results for both measurement (relations between manifest and latent variables) and structural models (causal relations between latent composites).

These indicators allow a comparison between empirical results and the theoretical models built on top of the input data. In other words, we can determine how well the theory fits the data.

The quality of a PLS path model should be assessed in different ways based on the analysis' main goals. For instance, when the main objective is to use PLSPM for predictive purposes, researchers often rely on measures indicating the model's predictive capabilities to judge the overall model quality. Those indicators are different from the ones used for model assessment when the objective is to validate a causal theory.

The next sections present several assessment indicators and show details on how and when they should be used.

The aforementioned evaluation measures build a set of non-parametric evaluation criteria and use procedures such as bootstrapping and blindfolding. These two techniques require a separate assessment for the measurement model and the structural model.

Measurement Model

This section presents the model assessment measures related with the measurement model. Their main objective is to enable researchers to

evaluate the reliability and validity of the composite measurement.
When evaluating the measurement model, it is mandatory to distinguish between reflectively and formatively measured composites because they are based on different underlying concepts.
Reflective measurement models are evaluated on their internal consistency, reliability and validity. These measures include composite reliability (addressed to assess internal consistency), convergent validity, and discriminant validity.
When working with formative measures, the first step is to ensure content validity even before collecting data and estimating the PLSPM model. Once the model reaches its convergence, the formative measures are assessed for their convergent validity, significance and relevance. Additionally to these measures, it is important to check for the presence of collinearity among the indicators.

Outward Directed Model As described in the previous paragraphs, the assessment of reflective measurement models includes composite reliability to evaluate the internal consistency, individual indicator reliability, and Average Variance Extracted (AVE) to evaluate the convergent validity. In addition to the previous techniques, the Fornell-Larcker criterion (Fornell and Larcker, 1981) and cross loadings are also used to assess the discriminant validity.

Internal consistency and individual indicator reliability have already been described in section 1.2.1.

Convergent Validity The main goal of convergent validity is to assess the extent to which a measure correlates positively with alternative measures of the same construct. Therefore, the MVs that are indicators of a specific construct should converge or share a high proportion of variance (Hair et al., 2014).

To establish convergent validity, researchers mainly consider the outer loadings associated to the indicators and the Average Variance Extracted (AVE).

High outer loadings on a construct indicate that the associated indicators have much in common, which is captured by the construct. This characteristic is also commonly called indicator reliability. At a minimum, all indicators outer loadings should be statistically significant.

A common measure to establish convergent validity on the construct level is the AVE (Fornell and Larcker, 1981) that expresses the degree of variance of the block explained by $\hat{\xi}_j$:

$$AVE_j = \frac{\sum_{p=1}^{P_j} \hat{\lambda}_{pj}^2}{\sum_{p=1}^{P_j} var(x_{pj})} \tag{1.30}$$

This criterion is defined as the overall average of the squared loadings associated to the indicators belonging to the j-th construct.

When the $AVE_j \geq 0.5$ is possible to state that, on average, the j-th construct explains more than half of the variance of its indicators. Conversely, an $AVE_j < 0.5$ indicates that, on average, more error remains in the items than the variance explained by the j-th construct.

Therefore, the AVE can be interpreted as the communality of a construct. In a well defined measurement model, each MV is well represented by its own LV. So, for each block j, the Communality Index is computed as:

$$Com_j = \frac{1}{P_j}\sum_{p=1}^{P_j} cor^2(x_{pj}, \hat{\xi}_j) = \frac{1}{P_j}\sum_{p=1}^{P_j} \hat{\lambda}_{pj}^2 \tag{1.31}$$

that is the average of the communalities between each MV belonging to the j-th block and $\hat{\xi}_j$.

The communality index measures the capability of the LV to explain the variance of its MVs. When the manifest variables are standardised, AVE and Communality coincide for less than the constant $1/P_j$.

Goodness of the whole measurement model could be measured by using the Average Communality index, that is the weighted average of all J blocks specific Communality indices, with weights equal to the number of MVs in each block:

$$\overline{Com} = \frac{1}{P}\sum_{j=1}^{J} P_j Com_j \tag{1.32}$$

where P_j is total number of MVs in the j-th block and P is the total number of MVs present in the model (considering all blocks J).

Discriminant validity The discriminant validity lies on the principle that a construct is truly distinct from other constructs by empirical standards. In other words, a construct is unique and captures phenomena not represented by other constructs in the model. Alternative measures of discriminant validity have been proposed. One of the proposed methods for assessing discriminant validity is based on the examination of the indicators' cross loadings. Specifically, an indicator's outer loading on the associated construct should be greater than all of its loadings on other constructs (i.e., the cross loadings):

$$H_0 : cor(\xi_j, \xi_{j'}) = 1 \text{ against the } H_1 : cor(\xi_j, \xi_{j'}) < 1 \tag{1.33}$$

The presence of cross loadings exceeding the indicators' outer loadings represents a discriminant validity problem. This criterion is generally considered rather liberal in terms of establishing discriminant validity (Hair et al., 2011). This means that it is very likely to indicate that two or more constructs exhibit discriminant validity.

Another approach for assessing discriminant validity has been proposed by Fornell and Larcker (1981). This approach compares the square root of the AVE values with the LVs correlations.

Specifically, the square root of each composite's AVE should be greater than its highest correlation with any other construct. The logic of this method is based on the idea that a construct shares more variance with its associated indicators than with any other construct:

$$(\sqrt{AVE_j} \text{ and } \sqrt{AVE_{j'}}) > cor(\hat{\xi_j}, \hat{\xi_{j'}}) \tag{1.34}$$

This means that each latent variable explains better the MVs belonging to its block than other LVs in the model.

Inward Directed Model A review on PLSPM studies in the strategic management and marketing disciplines presented by Hair et al. (2012b) showed that many researchers incorrectly use validity measures built for outward directed models (shown in the previous paragraphs) to assess the quality of inward directed models.

In the original PLSPM conception, researchers focussed on establishing content validity before empirically evaluating formatively measured constructs. One of the main concerns for the inward directed models is to ensure that the conceptually formative indicators capture as many facets as possible of the LV. In creating composites, content validity issues are addressed by the content specification in which the researcher clearly specifies the domain's content the indicators are intended to measure. Researchers must include a comprehensive set of indicators that fully covers the formative blocks' domain. Failing to gather all facets of the construct may lead to the exclusion of important parts of the construct itself.

The evaluation of inward directed measurement models mandates the establishment of convergent validity measures, the assessment of indicators' collinearity, and an analysis of the indicators' relative and absolute contributions, including their significance.

Convergent Validity The main goal of convergent validity is to assess whether each measure correlates positively with other measures of the same construct. In other words, it is important to test whether the measured construct is highly correlated with an outward directed measure of the same construct. This analysis is also known as redundancy analysis (Chin, 1998c). The term redundancy analysis stems from the information in the model being redundant in the sense that it is included in the inward directed construct ξ_1 and again in the outward directed one ξ_2 (see Figure 1.7).

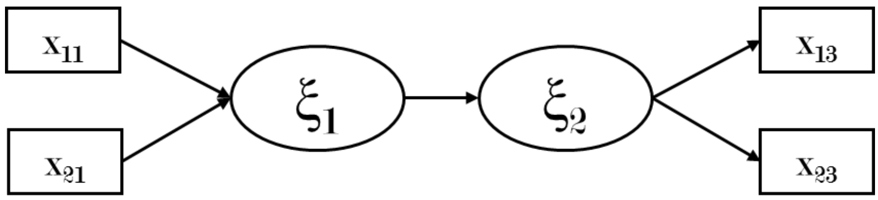


Figure 1.7: Redundancy Analysis for Convergent Validity

The strength of the path coefficient linking the two blocks (ξ_1 and ξ_2) indicates the validity of the designated set of inward directed indicators in tapping the LV of interest.

If the analysis exhibits a lack of convergent validity (i.e., the R^2 value of $\xi_2 < 0.6$), then the inward directed indicators belonging to the block ξ_1 do not contribute at a sufficient level to its intended content. In this situations, the block needs to be theoretically and conceptually refined by removing, exchanging and/or adding indicators.

In order to assess collinearity among indicators the researchers can use several statistics. The most used are: Tolerance (TOL) and Variance Inflation Factor (VIF). The Tolerance represents the amount of variance of one indicator not explained by the other indicators in the same block. It can be obtained by following a two steps approach:

1. The first indicator x_1 is regressed on all the remaining indicators in the same block and it is calculated its proportion of variance associated with the other indicators $R^2_{x_1}$;

2. Tolerance for the indicator (TOL_{x_1}) is computed:

$$TOL_{x_1} = 1 - R^2_{x_1} \tag{1.35}$$

The Variance Inflation Factor (VIF), is defined as the reciprocal of the tolerance:

$$VIF = \frac{1}{TOL_{x_1}} \tag{1.36}$$

A tolerance value of 0.20 or lower and a VIF value of 5 and higher respectively indicate a potential collinearity problem (Hair et al., 2011).

Significance and Relevance of the Formative Indicators Significance and relevance represent important criteria to evaluate the contribution of a formative indicator. The values of the outer weights can be compared with each other and can therefore be used to determine each indicator's relative contribution to the block, or its relative importance. We must test if the outer weights in inward directed measurement models are significantly different from zero by means of the bootstrapping procedure. It is important to note that the values of the indicators' weights are influenced by other relationships in the model (see Section 1.2.3).
Non-significant indicators' weights should not be automatically interpreted as indicative of poor measurement model quality. Conversely, researchers should consider an inward directed indicator's absolute contribution to its block. The absolute contribution is given by the indicator's outer loading, which is always provided along with the indicator weights. Differently from the outer weights, the outer loadings come from simple linear regressions of each indicator on its corresponding LV. When an in-

dicator's outer weight is non-significant but its outer loading is high (i.e., above 0.5), the indicator should be interpreted as absolutely important but not as relatively important. In this situation, the indicator would generally be kept in the model. When an indicator has a non-significant weight and the outer loading is below 0.5, the researcher should decide whether to keep or delete the indicator by examining its theoretical relevance and the potential content overlap with other indicators of the same construct.

Structural Model

The structural model estimates are not examined until the reliability and validity of the constructs have been established. If the assessment of reflective and formative measurement models provides evidence of sufficient quality in the measurement model then the structural model estimates are evaluated.

The assessment of the structural model is focussed on the model's predictive power. Once the measurement model has been analysed, the first evaluation criteria for the inner model are the coefficients of determination (R^2 values) as well as the level and significance of the path coefficients.

The assessment of the PLSPM outcomes can be extended to more advanced analyses such as examining the mediating and/or moderating effects, considering any unobserved heterogeneity, multi-group testing, and common method variance (Cataldo, 2016).

The structural model assessment can be done once the construct measures are reliable. This assessment is done by focussing on two main

parts: (i) the model's predictive capabilities; and (ii) the relationships between the constructs.
The key criteria for assessing the structural model in PLSPM are the significance of the path coefficients, the level of the R^2 values, the f^2 effect size, the predictive relevance Q^2 and the q^2 effect size.

Path Coefficients In a structural model the paths represent the hypothesised relationships among the LVs. In order to asses the significance of a coefficient the researchers need to rely on the path coefficients standard error obtained by means of bootstrapping.
The bootstrap standard error allows a computation of an empirical t-value:

$$t = \frac{\bar{\beta}^*}{\sigma_{\beta^*}} \tag{1.37}$$

where $\bar{\beta}^* = \frac{\sum_{i=1}^{n} \beta_i^*}{n}$, $\sigma_{\beta^*} = \sqrt{\frac{\sum_{i=1}^{n} \left(\bar{\beta}_i^* - \bar{\beta}^*\right)^2}{n-1}}$ and β_i^* represents the parameter's bootstrap estimation β in the i-th simulation.
When the empirical t-value is larger than the critical value, the coefficient is significant at a certain error probability (i.e., significance level); commonly used critical values for two-tailed tests are 1.65 (significance level = 10%), 1.96 (significance level = 5%), and 2.57 (significance level = 1%). In addition to calculating the t and p values, the bootstrapping confidence interval for a pre-specified probability of error can also be determined.

Coefficient of Determination The coefficient of determination (more commonly known as R^2) is a measure of the model fit and is calculated as the squared correlation between a specific endogenous composite's actual and predicted values. It represents the amount of variance in the endogenous constructs explained by all of the exogenous constructs linked to it. The R^2 value ranges from 0 to 1 with higher levels indicating higher levels of model fit; the acceptable R^2 value depends on the model complexity and the research discipline (Hair et al., 2012b).

Effect Size The effect size (f^2) represents an additional measure in evaluating the R^2 value of all endogenous constructs. The change in R^2 is explored to see whether a specific exogenous LV has a substantive impact on the R^2:

$$f^2 = \frac{R^2_{included} - R^2_{excluded}}{1 - R^2_{included}} \tag{1.38}$$

where $R^2_{included}$ and $R^2_{excluded}$ are the R^2 value of the endogenous LV when a selected exogenous LV is respectively included in or excluded from the model. Guidelines for assessing f^2 are proposed by Cohen (1988):

– if $f^2 \approx 0.02 \rightarrow$ small impact

– if $f^2 \approx 0.15 \rightarrow$ medium impact

– if $f^2 \approx 0.35 \rightarrow$ large impact

Predictive Relevance The last indicator is known as predictive relevance (Q^2) and it has been developed by Stone (1974) and Geisser (1975).

The PLSPM adaptation of this approach follows a blindfolding procedure. Given a block of n cases and P manifest variables, the procedure extracts a portion of the considered block during the parameters estimation steps and then attempts to estimate the omitted part by using the estimated parameters. In order to estimate the model, omitted values are typically replaced with the variable mean (even though other imputation techniques may be used (Chin, 1998a)). Based on the model's outcomes, the estimates obtained for the omitted value are compared to the observed values, using the squared difference (E). At the same time, the difference between the variable mean (or otherwise imputed value) and the observed values are also compared using the squared difference (O). This procedure is repeated until every data point has been omitted and estimated. The predictive measure Q^2 is then calculated as:

$$Q^2 = 1 - \frac{\sum_m E_m}{\sum_m O_m} \tag{1.39}$$

where m is the number of times the procedure is repeated in order to ensure that every data point has been omitted.

Q^2 measures how well observed values are reconstructed by the model and its parameters estimates (Chin, 2010). When PLSPM exhibits predictive relevance, it accurately predicts the data points of indicators in outward directed measurement models of endogenous constructs and endogenous single-item constructs (this procedure does not apply for inward directed endogenous constructs). $Q^2 > 0$ implies that the model has predictive relevance whereas $Q^2 \leq 0$ represents the lack of predictive relevance.

In the structural model, Q^2 values greater than zero for a certain outward directed endogenous LV indicate the path model's predictive relevance for a particular composite. In contrast, values of 0 and below indicate the lack of predictive relevance.

Similar to the f^2 effect size approach for assessing R^2 values, the relative impact of predictive relevance can be compared by means of the q^2 effect size, formally defined as follows:

$$q^2 = \frac{Q^2_{included} - Q^2_{excluded}}{1 - Q^2_{included}} \tag{1.40}$$

where $Q^2_{included}$ and $Q^2_{excluded}$ are the Q^2 values of the endogenous LV when a selected exogenous LV is respectively included or excluded from the model. Similarly to the aforementioned effect size statistic, as a relative measure of predictive relevance, values of 0.02, 0.15 and 0.35 indicate that an exogenous construct has a respectively small, medium or large predictive relevance for a certain endogenous construct (Hair et al., 2012b).

Different forms of Q^2 can be obtained through different procedures for predicting observations from the model. In the cross-validated communality Q^2, the prediction of observations is obtained by the computed composite and the estimated loadings. The cross-validated redundancy Q^2 is also based on the estimated loadings but the composites are predicted from the structural model using the estimated path coefficients. The redundancy-based Q^2 is applicable only to observations of MVs of the endogenous blocks, while the communality-based Q^2 can be applied to all MVs (Chin, 2010).

Tenenhaus, Esposito Vinzi, Chatelin, and Lauro (2005) and Tenenhaus, Amato, and Esposito Vinzi (2004) proposed a PLSPM Goodness-of-Fit (GoF) as an operational solution to validate the PLSPM model globally. The GoF can be proposed as the geometric mean of the average communality and the average of R^2:

$$GoF = \sqrt{\overline{Com} \times \overline{R^2}} \tag{1.41}$$

where $\overline{R^2} = \frac{\sum_{j=1}^{J} R_j^2}{J}$.

The GoF has been positioned as a compromise between the quality of the outer model and the quality of the inner model, so that the normalised index is obtained by bringing each part to its maximum value. In particular, for the outer estimation (represented by the first part of the formula with the average communality) for each block the maximum is the first eigenvalue; while for the inner estimation, the maximum is given by the square of first canonical correlation. To verify the GoF significance it is possible to build a confidence interval with the Bootstrap technique, as done for the R^2.

Henseler and Sarstedt (2013) criticise the usefulness of the GoF both conceptually and empirically. Their research shows that the GoF does not represent a goodness-of-fit criterion for PLSPM (referred as PLS-SEM in the original paper). Using simulated data, they illustrated that the GoF is not suitable for model validation. Since the GoF is also not applicable to inward directed measurement models and does not penalise over-parametrisation efforts, researchers are advised not to use this measure.

1.2.5 Thoughts on PLSPM Predictive Power

As previously mentioned, many authors criticise the lack of a global validation measure in PLSPM (Dijkstra and Henseler, 2015; Henseler and Sarstedt, 2013; Sharma et al., 2015). In addition to this gap, there is another topic that is driving a large production of scientific research: the assessment of predictive power in PLSPM.

Analysing historical scientific works related to PLSPM and its adoptions in business research, it is possible to see that its use resemble a descriptive approach where explanation and exploration are key. This usage is slightly contradictory to the PLSPM nature, which can be summarised as a non-parametric estimation procedure that is "slated" to be predictive (Hair et al., 2011). Also, Evermann and Tate (2014) note that "Herman Wold, who originally developed PLSPM, clearly and explicitly positioned it as a method for prediction (Dijkstra, 1983, 2010; Wold, 1982c)".

Shmueli et al. (2016) stated that, so far, PLSPM literature has not made a full use of these predictive proprieties, using instead an explanatory approach focussed on statistical significance and power (Becker et al., 2013).

Shmueli and Koppius (2010, 2011) reinforced the previous statements saying that quantitative research in management has been dominated by causal-explanatory statistical modelling at the expense of predictive modelling.

In the last five years the PLSPM community has shown an increasing interest in exploiting the predictive nature of PLSPM and recognising the insufficiency of considering only its theoretical validity as a statistical model fit; it is fundamental to assess its predictive performance

(Armstrong, 2012; Woodside, 2013).

Additionally, as stated by Gregor (2006), explanation and prediction are the two main purposes of theories and statistical methods.

In every statistical application, explanation is primarily concerned with testing the faithful representation of causal mechanisms by the statistical model and making valid inferences to population parameters. In contrast, prediction is synthesised as the ability to predict values for individual cases based on a statistical model whose parameters have been estimated from a suitable training sample (Evermann and Tate, 2016).

Shmueli and Koppius (2010, 2011) believe that emphasising predictive approaches on existing and new data sources can generate fresh insights for business practitioners and driving new theoretical hypothesis to be studied from a business and management research perspective.

When the focus is pointed at building a predictive model, the objective is to retrieve a predictive function (classification or regression, Hastie et al. (2009)) that can be applied to new observations. With that in mind, one of the most important elements to consider is making sure that the predictive function is generalisable.

Sharma et al. (2015) identify several types of generalisations:

– **Statistical Generalisation**: where the model estimated from the sample generalises to the population from which the sample was drawn;

– **Scientific Generalisation**: where the model estimated from the sample generalises to other populations (e.g., to other contexts);

– **Predictive Generalisation**: where the model estimated from the sample provides sufficiently accurate predictions for new records from that population (out-of-sample prediction).

Focussing on predictive generalisation, Shmueli et al. (2016) proposed a framework based on three dimension where the prediction measures in PLSPM can be defined: (i) Construct-Level versus Item-Level; (ii) In-Sample versus Out-of-Sample; and (iii) Average Case versus Case-wise. Changing slightly the design proposed by the authors, this framework is summarised in figure 1.8.

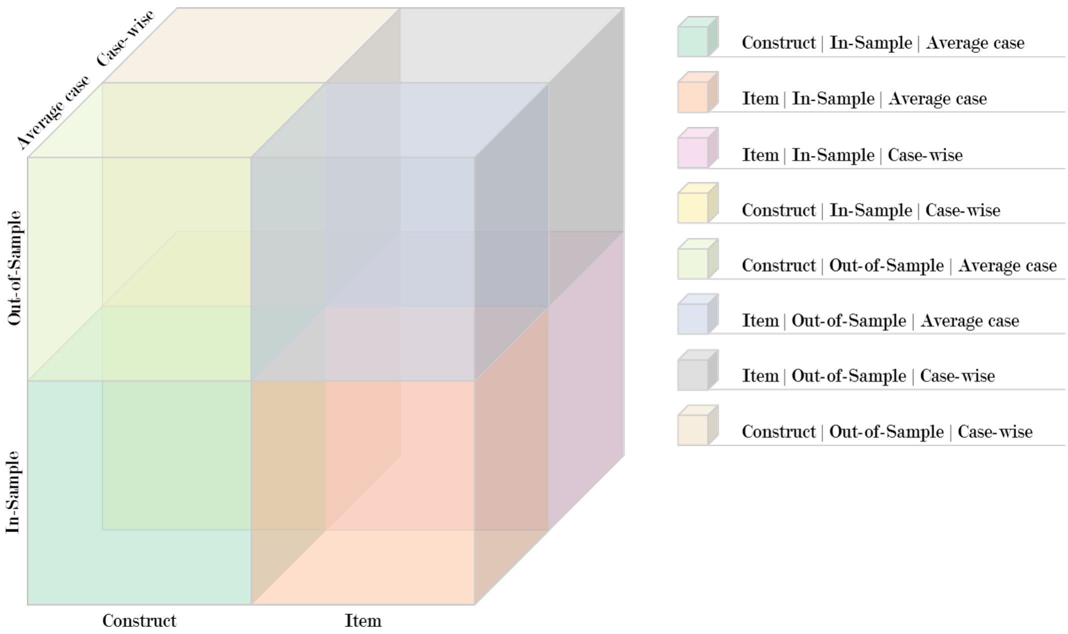


Figure 1.8: A Prediction Framework for PLSPM Assessment Measures

From the eight available types of predictions presented in figure 1.8, only two allow for evaluating predictive performance in the sense of the aforementioned predictive generalisation: (Item-Level, Out-of-Sample, Case-wise) and (Item-Level, Out-of-Sample, Average Case).

Shmueli et al. (2016) also present a deep analysis on the existing approaches highlighting their main limitations and some of the available opportunities. The authors reinforced that R^2 in PLSPM allows to assess the in-sample predictability (or fit) of endogenous average case composite scores and it is not concerned with each of the other seven prediction options presented in figure 1.8. In order to assess the predictive power, Becker et al. (2013) defined and used an "out-of-sample R^2" which is based on case-wise, out-of-sample predictions of the endogenous composites scores. Shmueli et al. (2016) also commented on the Q^2 and on the Operative Prediction Approach proposed by Evermann and Tate (2014): the first only concerns with an aggregate sense of predictability of a dataset, rather than gauging the predictability of particular cases and it is also considered, together with the q^2, as ad-hoc metrics that do not provide highly interpretable results in terms of error magnitude; the second (Operative Prediction Approach) is classified as a case-wise, out-of-sample technique that produces operative predictions at item-level. Shmueli et al. (2016) find that this approach still presents several challenges to overcome before being considered as a truly useful and informative predictive evaluation for PLSPM.

Shmueli et al. (2016) presented a new procedure for evaluating predictive performance for PLSPM model with the aim of diagnosing whether the PLSPM model is overfitting the training data. The approach proposed by the authors generates item-level case-wise and average case predictions for both out-of-sample and in-sample cases. The out-of-sample allows assessing predictive performance on new data and its comparison with the in-sample results allows to assess the aforementioned issue related to the overfitting of the training data.

The last years highlighted some insufficiency related to the assessment measures present in the PLSPM literature. These limitations open a whole new set of opportunities related to the predictive assessment of PLSPM. These steps towards prediction-driven PLSPM applications and the formalisation of a predictive assessment framework are widening the possibilities associated to the use of PLSPM and reducing the gap between PLSPM and the predictive analysis world.

1.3 Open Issues

This section summarises the open issues discussed through this chapter and some other research challenges worth mentioning.

– **Algorithm Optimisation Criteria**: as discussed in the previous sections, PLSPM does not have an overall scalar function to optimise. This is mainly due to the different available options in the inner and outer estimation steps, but also to the fact that PLSPM can be present in several configuration (number of latent variables, inner relationships, etc.) (Esposito Vinzi and Russolillo, 2013). Hanafi (2007) proved that the PLSPM iterative procedure is monotonically convergent to a specific criteria. Traditional Mode A applied to all the blocks does not seem to optimise any criterion, as Krämer (2007) showed that Wold's Mode A technique does not lead to a stationary equation related to the optimisation of a twice differentiable function. However, Tenenhaus and Tenenhaus (2011) recently extended the results of Hanafi (Hanafi, 2007) to a slightly adjusted Mode A in which a normalisation constraint is placed on outer weights rather than on LV composites. In particular, they showed that Wold's procedure, applied to a PLS path model where the new Mode A is used for all the blocks, monotonically converges to the criterion shown in equation 1.26.

– **Sample Size**: one of the main reasons justifying the use of PLSPM found in literature is the minimal demands in terms of sample size (Chin, 1998a). This topic has been widely debated in recent research (Hair et al., 2012a; Henseler et al., 2014; Marcoulides and Saunders, 2006; Ronkko and Evermann, 2013; Rönkkö et al., 2016) and has been empirically studied in several simulation studies (e.g., Hulland et al. (2010); Vilares and Coelho (2013)). Within the PLSPM community, there seems to be a common belief that sample size does not affect PLSPM estimation in practice applications (Henseler et al., 2014). Many authors follow the "ten times" rule of thumb according to which the sample size should be equal to the larger of the following: (i) ten times the largest number of formative indicators used to measure one construct; or (ii) ten times the largest number of inner model paths directed at a particular construct in the inner model (Barclay et al., 1995). However, this rule of thumb does not take into account several important factors (i.e., the magnitude of the relationships, the reliability, the number of indicators, distributional characteristics of the data, etc.) and its use could affect the model's statistical power. Some authors (Henseler et al., 2009; Marcoulides and Saunders, 2006) stated that this rule cannot be applied indiscriminately.

- **Model Quality Assessment**: another important challenge is to fine-tune the model assessment measures. These measures, as presented in the previous section, can be focussed on the inner model, outer model or on the PLSPM as a whole. When the goal is to use PLSPM for descriptive or explanatory analysis, the priority should be focussed on finding a measure for global fit. Henseler and Sarstedt (2013) criticise the usefulness of the GoF both conceptually and empirically. Their research shows that the GoF does not represent a goodness-of-fit criterion for PLSPM. Using simulated data, they have illustrated that the GoF is not suitable for model validation. Since the GoF is also not applicable to inward directed measurement models and does not penalise over-parametrisation efforts, researchers are advised not to use this measure and to propose alternative ones.

- **Prediction Assessment Techniques**: when the objective is to use PLSPM as a predictive model, there is a need for defining a new framework to assess its predictive power. Dolce (2015) stated that frequently composite-based methods are preferred to factor-based methods since their objective is to develop a predictive model. In the last five years, many researchers focussed their efforts to present new procedures and frameworks for evaluating predictive performance (Becker et al., 2013; Evermann and Tate, 2014; Shmueli et al., 2016). These researches set the foundations for future works. New techniques should allow model generalisation to new data (out-of-sample testing) and avoid situations where the PLSPM model is overfitting the training data.

– **Multicollinearity**: another issue to take into account concerns the situation in which input data presents multicollinearity. This issue affects solely Mode B (Diamantopoulos and Winklhofer, 2001); in fact, being based on multiple regression, the stability of the MVs outer weights is affected by the strength of the manifest variables inter-correlations and by the sample size (Dolce, 2015). In case of perfect collinearity between two formative MVs (i.e., one MV can be expressed as a linear combination of another MV belonging to the same block), PLSPM cannot estimate the model's parameters since the covariance matrix is singular and cannot be inverted (action required in a multiple regression model when using Mode B).

– **Path Direction Incoherence**: the previous sections presented three main options to calculate the inner weights: Centroid scheme, Factorial scheme and Path weighting scheme. One of the main advantages appointed to the path weighting scheme is the fact that this technique takes into account both strength and direction of the paths present in the inner model. Dolce (2015) shows that the path direction is only taken into account in the way the inner weights are computed, but each LV is still defined as a function of all the connected LVs. These steps of the algorithm lead to some inconsistencies when it comes to the relationships' directions specified in the path diagram. This same situation is verified for all the inner weighting schemes. The same author adds that the PLSPM estimation process amplifies interdependence among blocks and, as a consequence, it fails to distinguish between dependent and explanatory latent variables.

- **Unobserved Heterogeneity**: an important topic related to the input data structure is the unobserved heterogeneity. Usually, in order to understand heterogeneity the researchers use various marketing research techniques (i.e., interviews, focus groups, surveys, etc.) to identify *a priori* segments upon which subsequent research and analysis is based (Hahn et al., 2002). Henseler et al. (2009) verified that, based on their review of PLSPM applications in international marketing, there is a mixed picture regarding the examination of heterogeneity. Although a significant number of studies take observed heterogeneity into account by means of multi-group comparisons, none of the studies analysed by the authors account for unobserved heterogeneity. In literature there are several PLSPM-based techniques that approach the detection of unobserved heterogeneity (Esposito Vinzi et al., 2008; Hahn et al., 2002; Ringle et al., 2010a,b; Trinchera, 2008). This situation shows the need for an exhaustive analysis (theoretical and empirical) of all available techniques aiming at building a reference framework to use when there is a need to detect and handle situations of unobserved heterogeneity.

- **Linear and Nonlinear Moderation Variables**: another topic that is awakening interest within the PLSPM community is the introduction of linear and nonlinear moderation (Hair et al., 2017). As presented in this chapter, PLSPM algorithm is an iterative process based on simple and multiple OLS regressions aiming at obtaining a unique system of weights for the computation of scores calculated as linear combinations of the corresponding items. These scores are then used to estimate relationships between composites. Although attractively simple, traditional linear models often fail in these situations: in real life, effects are often not linear (Hastie et al., 2009).

Many authors decided to tackle the linearity assumption by using moderating effects within the PLSPM algorithm (Chin et al., 2003; Henseler and Chin, 2010; Henseler et al., 2008, 2012; Krämer, 2005), others used nonlinear functions to fit the inner relationships (Jakobowicz, 2007a,b; Jakobowicz and Saporta, 2007) and other presented approaches that subdivide the nonlinearity present in the data by using a set of linear submodels (Esposito Vinzi et al., 2008; Farooq et al., 2013; Hahn et al., 2002; Martínez-Ruiz and Aluja-Banet, 2013; Ringle et al., 2005a; Sánchez and Aluja-Banet, 2006; Trinchera, 2008).

The objective of this work is to propose a flexible alternative to the PLSPM algorithm which tackles two of the aforementioned issues by: (i) breaking the linearity assumptions present in the inner model estimation phase; and (ii) accommodating path direction within the inner model estimation phase.

Chapter 2

Nonlinear Approach to PLSPM

2.1 Introduction and Motivations

PLS path modelling is a statistical approach for modelling complex multivariate relationships among observed and latent variables. It allows to model a system of relationships that are separated in: relations between manifest and latent variables (measurement model) and relations between latent variables (structural model).

The algorithm is represented by an iterative process based on simple and multiple OLS regressions that aim at obtaining a unique system of weights for the computation of the composites as linear combinations of the corresponding manifest variables. These scores are then used to estimate relationships between composites.

Although attractively simple, the traditional linear model often fails in some situations: in real life, effects are often not linear (Hastie et al., 2009). The following paragraphs present a set of concrete examples on the underlying relations among composites.

Crainer and Dearlove (2004) verified that most customer-driven organisations' goal is to have satisfied and loyal customers. Many of these companies fail to find a positive link between customer satisfaction and loyalty. This situation often leads to poor return on investments caused in part by the intrinsic relation among customer satisfaction and loyalty which is often nonlinear. The linearity assumption about this specific relation can lead to wrong assessments and inappropriate marketing initiatives.

Paulssen and Sommerfeld (2006) affirm that, despite high rates of satisfied customers, organisations experience high rates of customer defection. In general, the relationship between satisfaction and loyalty has often been assumed to be linear and symmetrical. However, this linearity assumption has recently been questioned in studies from Mittal et al. (1998) and Matzler et al. (2004).

Matzler et al. (2004) presented an interesting work on the relation between customer satisfaction, investments and profitability. They found several empirical studies confirming a positive relationship between customer satisfaction and profitability (e.g., Anderson et al. (1994); Eklof et al. (1999)).

Matzler et al. (2004) also stated that, in order to build a loyal relationship with their customers, organisations must identify the critical factors that determine satisfaction and loyalty. An effective method to set priorities is given by the Importance–Performance Analysis (IPA).

Two implicit assumptions underlie the IPA: (i) attribute performance and attribute importance are two independent variables; and (ii) the relationship between quality attribute performance and overall performance is linear and symmetrical. Research in the customer satisfaction field, however, suggests that quality attributes fall into three categories: basic factors, performance factors, and excitement factors (Anderson and Mittal (2000); Johnston (1995); Matzler et al. (1996)). In the model of customer satisfaction presented by Kano et al. (1984), the relationship between performance and importance of basic and excitement factors is nonlinear and asymmetrical.
Other interesting works questioning the linearity assumption often defined between satisfaction and loyalty are: Kumar (2007), Tuu and Olsen (2010) and Zhang and Li (2009).
The current thesis is based on the assumption that the application of nonlinear transformations represents a better fit when estimating some of the relationships among the variables (manifest and/or latent) present in the model.
In PLSPM, the nonlinear model can be applied to relationships belonging to the measurement model and/or to the structural model. Several bibliographic references on the application of nonlinear techniques will be presented in section 2.3.1.
Two interesting papers were presented by Emancipator and Kroll (1993) and Kroll and Emancipator (1993) which proposed a quantitative measure of nonlinearity based on a comparison between a straight line and a curve function. In their work they fit curvilinear relationships between variables using extensions of linear regression models (they used stepwise

polynomial regression as curve-fitting function).

The next section presents several nonlinear estimation techniques based on the well-known linear regression model.

2.2 Nonlinear Modelling Techniques

Nonlinear models can be classified into two main categories:

1. The first category includes models that are nonlinear in the variables, but linear in terms of the unknown parameters. This category includes models which become linear in the parameters after a transformation. For example, the Cobb-Douglas (Cobb and Douglas, 1928) production function that relates output (Y) to labour (L) and capital (K) can be formalised as:

$$Y = \alpha L^{\beta} K^{\gamma} \tag{2.1}$$

   Applying a logarithmic transformation gives:

$$\ln Y = \delta + \beta \ln(L) + \gamma \ln(K) \tag{2.2}$$

   where $\delta = \ln(\alpha)$.

   This function is nonlinear in the variables Y, L, and K, but it is linear in the parameters δ, β and γ. Models of this kind can be estimated using the least squares technique.

2. The second category of nonlinear models contains models which are nonlinear in the parameters and which cannot be made linear in the parameters using a transformation. These models are usually estimated using an extension of the least squares technique known as nonlinear least squares.

The next sections briefly present these two modelling category using the regression as baseline model and showing its extensions to fit nonlinear relationships among variables.

2.2.1 Nonlinear in the Variables but Linear in Parameters

When a regression model is nonlinear in the variables but linear in the parameters, data transformations are often used to describe curvature and can sometimes be usefully employed to correct for the violation of the assumptions related to a multiple linear regression model (particularly the linearity[1] and equal variances[2] assumptions).

Let x be a matrix containing P input variables $x = (x_1, x_2, ..., x_P)$, and let the objective be the prediction of a real-valued output y. The linear regression model has the following form:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \ldots + \beta_p x_p + \ldots + \beta_P x_P + \epsilon \tag{2.3}$$

The linear model either assumes that the regression function $E\left(y|x\right)$ is linear, or that the linear model is a reasonable approximation. The β_p are

[1] The mean of the response , $E(y_i)$, at each value of the predictor, x_i, is a linear function of the x_i.

[2] The errors, ϵ_i, at each value of the predictor, x_i, have equal variances (denoted σ^i)

unknown parameters or coefficients, and the variables x_p in a linear regression are usually defined as quantitative inputs and no transformation is needed because the relation between target variable and predictors is linear (Draper et al., 2014). There are cases where the relation between target variable and predictors is not linear but linearisable. In these cases the variables x_p can be linearised as follows:

- Transformations of quantitative inputs, such as logarithmic, square-root or square;
- Numeric or "dummy" encoding of the levels of qualitative inputs. For instance, if G is a five-level factor input we might create x_p, $p = 1, \ldots, 5$, such that $x_p = I(G = p)$. Together this group of x_p represents the effect of G by a set of level-dependent constants, since in $\sum_{p=1}^{5} x_p \beta p$, one of the x_p's is equal to one, and the others are set to zero;
- Interactions between variables, for instance, $x_3 = x_1 \times x_2$;
- Basis expansions, such as $x_2 = x_1^2$, $x_3 = x_1^3$, leading to a polynomial representation.

Independently of which of the aforementioned forms of the x_p is used, the model is still linear in the parameters.

Variables Transformations The issues related with nonlinear relationships among variables might be solved by replacing the predictor x_p values with a transformation technique. This is usually the first approach tried when lack of linear trend in data is found. In fact, transforming the x_p values is appropriate when nonlinearity is the only problem and the independence, normality and equal variance conditions are met.

One of the most used data transformation techniques is the "logarithmic" transformation. The default logarithmic transformation merely involves taking the natural logarithm, denoted ln or $\log_e$ or simply log, of each data value. One could consider taking a different base for the logarithm, such as log base 10 or log base 2. However, the natural logarithm, which can be thought of as log base e (where e is the constant $2.718282\ldots$) represents the most common logarithmic scale used in scientific works. When using the natural logarithmic transformation, small values that are close together are spread further out and large values that are spread out are brought closer together.

Other predictors transformations are exponential ($\exp^{x_p}$), reciprocal ($1/x_p$), square root ($\sqrt{x_p}$), square (x_p^2), etc. and their use depends on the type of relationship existing between a predictor and its response variable.

Numeric or Dummy Encoding of Categorical Variables When a predictor is categorical, such as gender or academic level, it is common to decompose the predictor into separate variables, each one containing a part of the variable information. In order to use a categorical predictor in a model, the categories need to be re-encoded into smaller bits of information called "dummy" variables. Usually, each category get its own dummy (binary) variable. When the predictor has 5 levels, this encoding process creates 4 dummy variables. This approach goes by the name of "full-rank" encoding and the dummy variables do not always add up to 1 (Kuhn and Johnson, 2013).

Sometimes a similar transformation is applied to continuous variables. This process is also known as discretisation and is not generally recommended due to the loss of information. Royston et al. (2006) and Harrell (2008) discussed drawbacks to categorising continuous variables, including loss of power and sensitivity to the choice of cut-points. One of the strong points they made is related with the fact that it is a risky strategy to estimate cut-points for discretisation based on the response variable, y. In addition to that, even when the cut-points are set based on the predictor x, there is generally a loss of efficiency compared to its use as a continuous variable when fitting a regression model (Gelman and Park, 2009).

An example of dummy encoding is presented in table 2.1 where the original categorical variable "Hair" is encoded in three dummy variables.

Hair	**Brown**	**Red**	**Black**
Brown	1	0	0
Black	0	0	1
Brown	1	0	0
Brown	1	0	0
Red	0	1	0
Black	0	0	1
Brown	1	0	0
Red	0	1	0

Table 2.1: An example of Dummy Encoding

Variables Interactions Jaccard and Turrisi (2003) stated that there are many ways in which interaction effects have been conceptualised in the social sciences and there is controversy about the best way to think about this concept. They also define the moderated relationships as one of the most popular interaction effects. This configuration is illustrated in figure 2.1 by using a three variables system: a first variable (y) as dependent, a second (x) declared as independent variable and a third one (z) viewed as a moderator variable. An interaction effect is said to exist when the effect of the independent variable on the dependent variable differs depending on the value of a third variable (moderator variable).

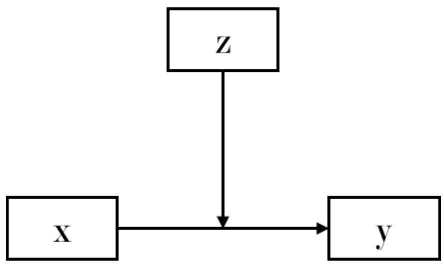


Figure 2.1: Moderated Causal Relationship

In other words, interaction effects represent the combined effects of variables on the dependent measure. When an interaction effect is present, the impact of one variable depends on the level of the moderator variable. As Pedhazur (1997) noted, the idea of multiple effects should be studied in research rather than the isolated effects of single variables. When interaction effects are present, it means that interpretation of the individual variables may be incomplete or misleading.

In a regression model in the form of equation 2.3 with only two predictors x_1 and x_2, the interaction effects can be built as follows:

$$y = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2 + \epsilon \tag{2.4}$$

where β_3 represents the coefficient measuring the impact of the interaction effect on the dependent variable y.

Interaction terms can be created between categorical (or binary) variables and quantitative predictors to allow for different slopes for levels of the categorical predictor. Interactions can also be created between quantitative predictors. This allows the relationship between the response and one predictor to vary with the values of another quantitative predictor. Interestingly, this provides a different way to introduce curvature into a multiple linear regression model.

Regression models that include interactions between quantitative predictors adhere to the hierarchy principle, which states that if the model includes an interaction term, $x_1 x_2$, and this is shown to be a statistically significant predictor of y, then the model should also include the "main effects", x_1 and x_2, whether or not the coefficients for these main effects are significant. Depending on the subject area, there may be circumstances where a main effect could be excluded, but this tends to be the exception.

Basic Expansions One of the most common ways to identify a nonlinear relationship among variables is during a visual check for the linearity assumption (i.e., scatter plot of the residuals versus the fitted values, scatter plot of the residuals versus each predictor, etc.).

A potential way to take into account this type of relationship is through the use of a polynomial regression model. Such a model for a single predictor, x, can be defined as:

$$y = \beta_0 + \beta_1 x + \beta_2 x^2 + \ldots + \beta_d x^d + \epsilon \tag{2.5}$$

where d is called the degree of the polynomial. For lower degrees, the relationship has a specific name (i.e., $d = 2$ is called quadratic, $d = 3$ is called cubic, $d = 4$ is called quartic, and so on). Although this model allows for a nonlinear relationship between y and x, polynomial regression is still considered linear regression since it is linear in the parameters (regression coefficients): $\beta_0, \beta_1, \beta_2, \ldots, \beta_d$.

In order to estimate equation 2.5, only two variables are needed (i.e., response variable y and the predictor variable x). The basic equation for the aforementioned polynomial regression model is relatively simple, but the model can grow depending on the specific case under analysis.

Some guidelines to take into account when estimating a polynomial regression model are:

– The fitted model is more reliable when it is built on a larger sample size;

– The results should not be used to extrapolate beyond the limits of the observed values present in the model;

– From a computational perspective, it is important to consider how large the size of the predictors will be when incorporating higher degree terms (this may cause numerical overflow for the statistical software used);

– It is important to be parsimonious when thinking about incorporating a higher degree term. This is a situation where it is fundamental to make a good trade off between "practical significance" versus "statistical significance";

– The models should adhere to the hierarchy principle, which states that if the model includes x^d, and this variable is shown to be a statistically significant predictor of y, then the model should also include each x^k for all $k < d$, whether or not the coefficients for these lower-order terms are significant.

2.2.2 Nonlinear in Parameters

All of the models presented in the previous sections are linear in the parameters (i.e., linear in the β's). For example, the polynomial regression model is often used to model curvature in the data by using higher-ordered values of the predictors. However, the final regression model was just a linear combination of higher-ordered predictors.
The least squares theory discussed in the previous sections is applicable when a model is linear or can assume a linear form via transformation techniques. For other non-normal error terms, different techniques need to be employed.
First, let

$$Q = \sum_{i=1}^{n} \left(y_i - f\left(\boldsymbol{X}_i, \beta\right)\right)^2. \tag{2.6}$$

In order to find

$$\hat{\beta} = \underset{\beta}{argmin}\ Q, \tag{2.7}$$

the first step is to calculate the partial derivatives of Q with respect to β_j. Then, each of the partial derivatives are set to 0 and the parameters β_k are replaced by $\hat{\beta}_k$. In this case, the functions to be solved are nonlinear in the parameter estimates β_k and, in order to be solved, iterative numerical methods are often employed.

Algorithms for nonlinear least squares estimation include:

– Newton-Raphson's method is a classical method based on a gradient approach. The drawbacks related to this technique are: (i) can be computationally challenging; and (ii) heavily dependent on good starting values;

– The Gauss-Newton algorithm represents a modification of Newton's method giving a good approximation of the solution reached by the latter method. The drawback is related to the fact that the convergence is not guaranteed;

– The Levenberg-Marquardt method which can take care of computational difficulties arising with the other methods. The drawback resides on the fact that it might require a tedious search for the optimal value of a tuning parameter.

A more detailed review on these methods can be found in Kutner et al. (2005).

In addition to the nonlinear least squares there are other modelling option such as "generalised additive models"[3] or neural networks[4]. These techniques work better with large amounts of variables and observations. More details can be found in Hastie et al. (2009).

From the large set of available nonlinear modelling techniques, it has been decided to use polynomial functions as the underlying technique for the proposed approach presented in the next sections. This decision is mostly related with the simplicity of polynomial functions and on its scalability to higher order functions.

2.3 Nonlinear Approaches in PLSPM: State-of-the-Art

2.3.1 Historical Review

This section aims to present the different nonlinear approaches developed for PLSPM and other interesting developments built for Covariance-Based SEM and PLS Regression.

[3] Generalised additive models can be seen more as automatic flexible statistical methods that may be used to identify and characterise nonlinear regression effects.

[4] Neural network can be thought of as a nonlinear generalisation of the linear model, both for regression and classification. By introducing the nonlinear transformations, it greatly enlarges the class of linear models.

In the PLSPM research field, several authors presented techniques to take into account nonlinear effects in the original PLSPM algorithm. Some of these approaches present a novel technique, others are adapted from developments made in covariance-based SEM and PLS Regression.

The presence of nonlinear transformations in the PLS path modelling algorithm are still marginal, however Wold (1982c) proposed the use of a variable transformation technique applied to the manifest variables. H. Wold suggested modelling nonlinear relationships in the structural model by using an additional step to the classical PLSPM algorithm. In particular, after the computation of each latent variable in the measurement model, Wold proposed computing interaction term proxies as an element-wise product of the outer estimates of the latent variables. Then the structural model is augmented in order to obtain inner estimates of endogenous latent variables by considering also the interaction term composites. The inner estimates of the latent variables are then used to update the outer weights as in the original PLSPM algorithm. One of the main critics made to this approach is that it does not take into account nonlinear links between the manifest and latent variables (Ingrassia and Trinchera, 2008).

Chin et al. (2003) presented an approach linkable to a "nonlinear" technique for PLSPM based on the so called product-indicator approach proposed by Kenny and Judd (1984) in which measures of latent constructs are cross-multiplied to form interaction terms that are used to estimate the underlying latent interaction construct within the LISREL algorithm. After the seminal paper from Kenny and Judd (1984), several covariance-based SEM specifications have been conducted (Jöreskog and Yang, 1996).

However, Ping Jr. (1996, p. 166) noted that covariance-based procedures "may produce specification tedium, errors, and estimation difficulties in larger structural equations models". Part of the difficulty involves the need to calculate and specify in the software the required set of nonlinear constraints, which increase exponentially with the number of indicators. In agreement, Bollen and Paxton (1998, p. 267), stated that "the best known procedures for models with interactions of latent variables are technically demanding. Not only does the potential user needs to be familiar with structural equation modelling (SEM), but the researcher must be familiar with programming nonlinear and linear constraints and must be comfortable with fairly large and complicated models". Again, these constraints tend to grow exponentially with the number of interaction terms.

Additionally Chin et al. (2003) showed that, based on their results, it is possible to achieve additional findings around known PLSPM biases, influences of different reliabilities, extensions for nonlinear indicators and use of formative indicators. In summary, the new PLSPM product-indicator approach, presented in their paper, seems to yield promising results for researchers interested in assessing interaction effects within the composite-based modelling area.

Ingrassia and Trinchera (2008) consider that Chin's approach presents two main weaknesses: (i) the number of indicators for the latent interaction terms directly increases the number of manifest variables in the model; and (ii) the latent interaction terms obtained by its indicators does not coincide with the product of the exogenous latent variable scores.

Another approach for handling nonlinear relations in PLSPM has been proposed by Krämer (2005). The author's underlying hypothesis is that the nonlinearity affects the outer model. In other words, nonlinear relations are supposed to exist among each manifest variable and the corresponding latent variable and these are modelled by means of a suitable data transformation called "kernel trick". In this approach each relation in the measurement model can be considered as a simple/multiple regression problem according to the chosen outer model scheme. This means that a kernel transformation is considered for each block of manifest variables and, after applying the transformation, the standard PLSPM algorithm is executed on the transformed data. Here the choice of a suitable kernel function can be considered as an additional parameter in the model. The kernel function should be identified for each block in the model but, for simplicity, Krämer (2005) suggested using only one family of kernels for all of the blocks present in the model. One of the drawbacks of this approach is related to the interpretability. In fact, the proposed algorithm does not provide any estimation of the outer weights. In order to overcome the issues related to the approach proposed by Chin et al. (2003) (i.e., exponential growth of the number of manifest variables), Henseler and Chin (2010); Henseler et al. (2008, 2012) proposed a two-stage procedure to model interaction effects. More in detail, the first stage presents a standard PLSPM analysis which aims to estimate the direct effect of each exogenous latent variable as well as the latent variable scores. In a second stage, the interaction effect is obtained as the product of endogenous latent variables scores. Then, the exogenous latent variable scores (estimated in the first-stage), and the interaction effect (obtained in the second-stage), are used as exogenous variables in a multiple linear regression to obtain path coefficients.

One of the principal criticism associated to the approach presented by Henseler et al. (2008) is related to the fact that the algorithm does not take into account nonlinear relationships among manifest and latent variables.

Recently Jakobowicz (2007a,b); Jakobowicz and Saporta (2007) proposed a modified version of the original PLSPM algorithm by adding an additional step. Based on an idea of Coolen et al. (1982), who combined optimal scaling techniques with B-splines, Jakobowicz applied a B-spline transformation to some of the latent variables in the model. In other words, the objective is to transform nonlinear variables into linear variables using monotonic B-spline transformations and alternating least squares (ALS). All exogenous construct of an endogenous unobservable variable are transformed such that the square multiple correlation coefficient of this endogenous construct is maximised. The ALS procedure is used to estimate the parameters of the monotonic B-spline function and the path coefficients for the inner model. However, this approach requires identifying a well-established target latent variable in the model. In particular, once the target latent variable is chosen, a B-spline transformation is applied to each exogenous latent variable impacting on the chosen target latent variable.

The approach developed by Jakobowicz (2007b) presents some difficulties related to its practical implementation, in fact, when working with complex models, the identification of a well-established target latent variable is not trivial.

Ingrassia and Trinchera (2008) concluded saying that the nonlinear transformations PLSPM approaches proposed by Krämer (2005) and Jakobowicz (2007b) did not improve the quality of the results when these are compared with the standard PLSPM algorithm.

In order to tackle the nonlinearity issue for the PLSPM, several researchers presented new approaches aiming at reaching a nonlinear approximation by using a set of linear submodels. Hahn et al. (2002) and Ringle et al. (2005a) presented two approaches for capturing unobserved customer heterogeneity in PLSPM using a modified finite-mixture distribution approach.

Another approach has been proposed by Sánchez and Aluja-Banet (2006) and consists of building a path model having a decision tree-like structure by means of the PATHMOX (Path Modelling Segmentation Tree) algorithm. This algorithm is specifically designed when prior information in form of external variables (such as socio-demographic variables) is available.

Trinchera (2008) and Esposito Vinzi et al. (2008) presented an approach called REBUS-PLS capable of estimating at the same time both the unit memberships to latent classes and the class specific parameters of the local models without making any kind of distributional assumption neither on the manifest variables nor on the latent variables. In other words this algorithm has been designed to "discover" latent classes inside a PLSPM global model by applying clustering principles.

Farooq et al. (2013) presented an interesting application of the REBUS-PLS algorithm applied to corporate social responsibility.

More recently Martínez-Ruiz and Aluja-Banet (2013) developed a two-step PLS path modelling MODE B procedure to estimate nonlinear and interaction effects among formative constructs. The procedure preserves the convergence properties of PLS MODE B with centroid scheme (Wold's algorithm) and offers a way to build proper indexes for linear, nonlinear and interaction terms, all of which are unobservable, and to estimate the relationships between them.

Other Nonlinear Approaches Many other nonlinear approaches have been proposed for covariance-based SEM and for PLS Regression. Some of these works were used as guideline for the proposals presented in the previous paragraphs.

Some of the most cited works in the covariance-based SEM field are: Kenny and Judd (1984), Bollen (1995),Jöreskog and Yang (1996), Wall and Amemiya (2003), Lee et al. (2004), Little et al. (2006), Paulssen and Sommerfeld (2006), Moosbrugger et al. (2006), Lee et al. (2007), Klein and Muthén (2007) and Mooijaart and Bentler (2010).

On te nonlinearity approach under the PLS Regression umbrella, it is worth mentioning Wilson et al. (1997), Baffi et al. (1999), Baffi et al. (2000), Rosipal and Trejo (2002) and Rosipal (2011).

Thoughs on Nonlinearity in PLSPM

As presented in the previous paragraphs, several approaches have been proposed to add nonlinear estimation as part of the PLSPM algorithm. Some researchers proposed to introduce the nonlinear estimation into the algorithm by changing the inner or outer model, by adding new composites built based on the product-interaction approach or by segmenting the observations prior to the algorithm.

Ingrassia and Trinchera (2008) see as a weakness the fact that some approaches do not account for nonlinear relationships among manifest and latent variables (i.e., considering only nonlinearity links in the structural model).

The approach proposed in this work, presented in the next sections, introduces a change in the structural model which is solving the nonlinearity by using a piecewise technique. The method does not apply nonlinear estimation for the measurement model even if the proposed technique is easily extensible to the outer model estimation phase.

2.4 Proposed Approach for Nonlinear PLSPM

As referred in the previous section, the proposed approach is based on a modification of the inner estimation process. As shown in the previous chapter (see section 1.2.3), the PLSPM algorithm presents three separate techniques to estimate inner weights estimation, several schemes have been showed (Centroid, Factorial and Path Weighting).

Independently from the estimation scheme selected, the relationship among two latent variables is always assumed to be linear even when empirical studies (see section 2.1) confirm the presence of nonlinearity.

Let us consider the relationship among two latent variables ξ_j and $\xi_{j'}$ and define y_j as the composite associated to the endogenous LV ξ_j and, $y_{j'}$ as the composite associated to the exogenous LV $\xi_{j'}$ directly connected to ξ_j.

Using the standard algorithm and following the factorial scheme, the inner weights $e_{jj'}$ are calculated as $e_{jj'} = r_{jj'} = corr\left(y_j, y_{j'}\right)$ and correspond to the correlations between sets of two composites. Since the composites are standardised, the correlation coefficient corresponds to the β_1 coefficient of the following regression model: $y_j = \beta_0 + \beta_1 y_{j'} + \epsilon$. The way how weights $e_{jj'}$ are calculated performs adequately when the relation between the two composites is linear as shown on the scatter plot in figure 2.2.

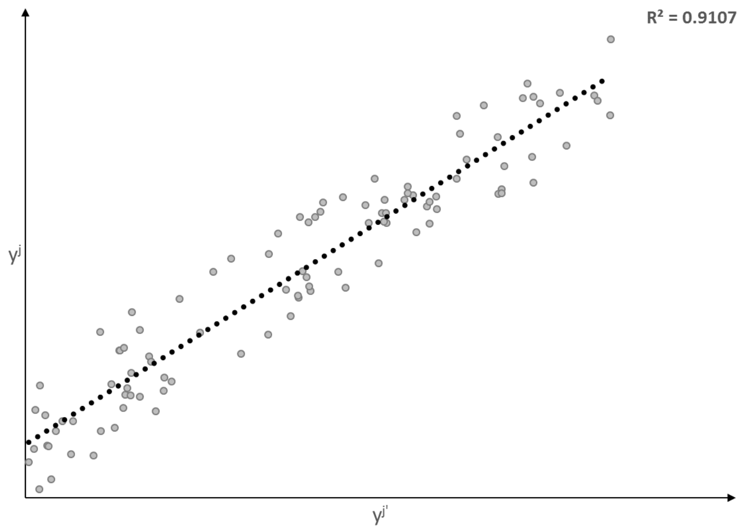


Figure 2.2: Structural relation between endogenous variable y_j and exogenous variable $y_{j'}$

The latter weight estimation technique shows some flaws when the relationship among the two variables is closer to a nonlinear relation. In those cases, the linear regression does not appear to be a good fit (see Figure 2.3) and better options are demanded by researchers.

Figure 2.3 presents a linear regression fit to clearly nonlinear data belonging to two composites and, in this case, the R^2 is equal to 0.3673.

2.4.1 Step-by-Step Introduction to Piecewise Inner Weights Estimation

This work presents a new technique aiming at improving the inner weights estimation phase in cases like the one presented in figure 2.3. From the vast set of nonlinear modelling techniques presented in section 2.2, it has been decided to estimate nonlinear relation using a custom approach based on polynomial functions.

Given the composites y_j calculated in the measurement model, the proposed inner weights estimation technique is composed of the following four steps:

1. **Fit Polynomial Functions**: the first step of the inner weights estimation process is focussed on understanding the nature of all the connections (paths) present in the structural model.

   In order to fit the data representing the relationship among each pair of composites, the proposed algorithm fits several polynomial functions: first (see Figure 2.3), second (see Figure 2.4) and third (see Figure 2.5) order.

   The three polynomial functions can be defined as follows:

   – First Order Polynomial

$$y_j = \beta_0 + \beta_1 y_{j'} + \epsilon \tag{2.8}$$

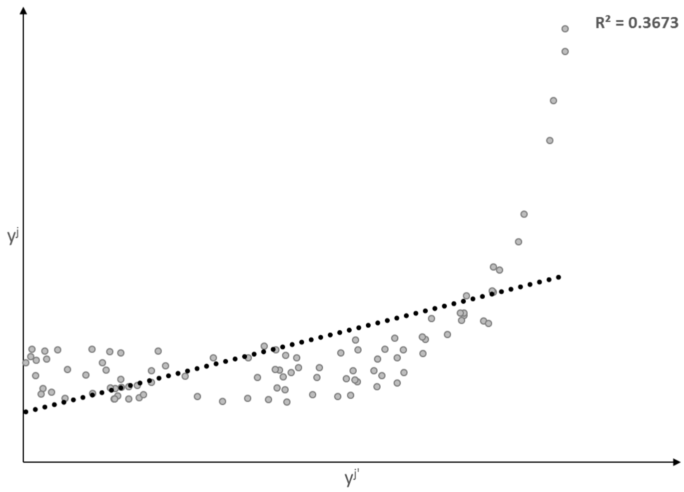


Figure 2.3: Linear Regression fit to nonlinear data

– Second Order Polynomial

$$y_j = \beta_0 + \beta_1 y_{j'} + \beta_2 y_{j'}^2 + \epsilon \qquad (2.9)$$

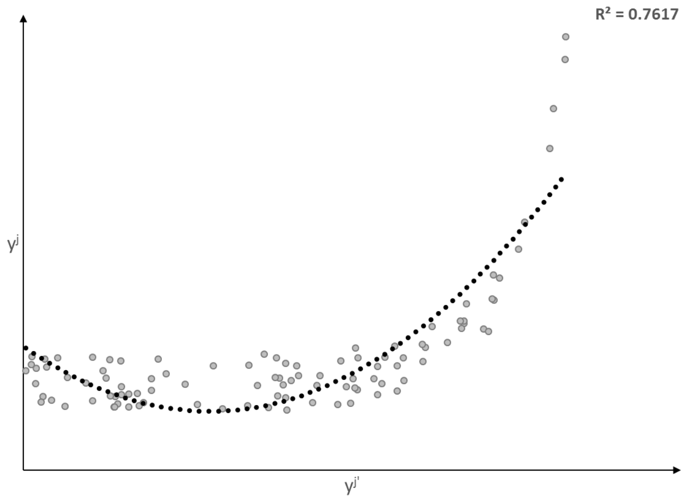


Figure 2.4: Second Order Polynomial Function fit to nonlinear data

– Third Order Polynomial

$$y_j = \beta_0 + \beta_1 y_{j'} + \beta_2 y_{j'}^2 + \beta_3 y_{j'}^3 + \epsilon \tag{2.10}$$

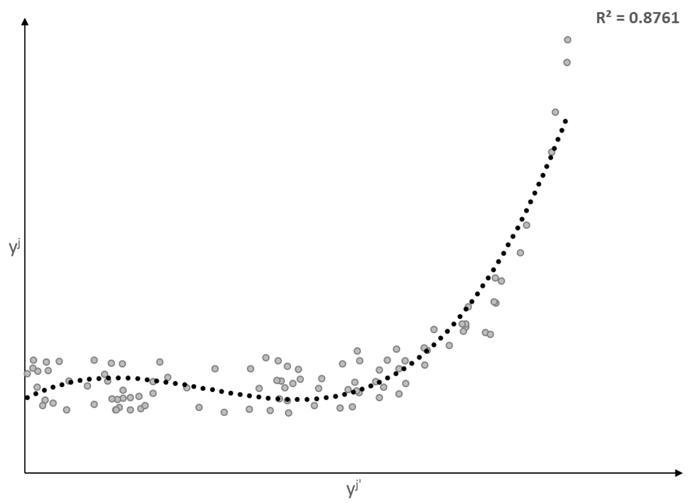


Figure 2.5: Third Order Polynomial Function fit to nonlinear data

Analysing the three different polynomial functions and their fit to the data, it is possible to understand that the third order polynomial presents a better fit to the actual data. In fact, when moving from a first degree function to a higher degree polynomial the fit shows an improvement even if the model is less parsimonious than the second degree function.

The second order polynomial (figure 2.4) presents an R^2 of 0.7617 and the third order polynomial (figure 2.5) presents an R^2 of 0.8761. The next phase will assess all fitting functions and select the polynomial that best represents the structural relation.

2. **Evaluate and Select Polynomial Functions**: The second stage of the proposed inner weights estimation process aims to assess the aforementioned functions and select the one presenting the best fit.

   The first decision to make is related to the criterion to be used for model selection. The proposed algorithm allows the use of three statistics: Bayesian Information Criterion (BIC) or Schwarz criterion, Akaike Information Criterion (AIC) and R-Squared.

   Assuming that the R-Squared is the statistic used for model selection, the choice falls on third order polynomial with an R^2 of 0.8761.

3. **Find Stationary Points**: once the best model (in the sense of the chosen statistic) is selected, the proposed algorithm moves to a function analysis focussed on determining stationary points.

   A stationary point can be defined as a point $y_{j'0}$ at which the derivative of a function $f(y_{j'})$ vanishes, $f'\left(y_{j'0}\right) = 0$.

   A stationary point may be a minimum, a maximum, or an inflection point.

   Each structural relation present in the models will have its set of stationary points and, based on those values, the $f(y_{j'})$ is segmented by dividing the domain of $y_{j'}$ into H contiguous intervals as shown in figure 2.6. From this point, the letter H will represent the number of segments created from the piecewise process introduced in the proposed algorithm.

   The model selected in the previous step is the third order polynomial (first and second order piecewise functions are only shown for information purposes).

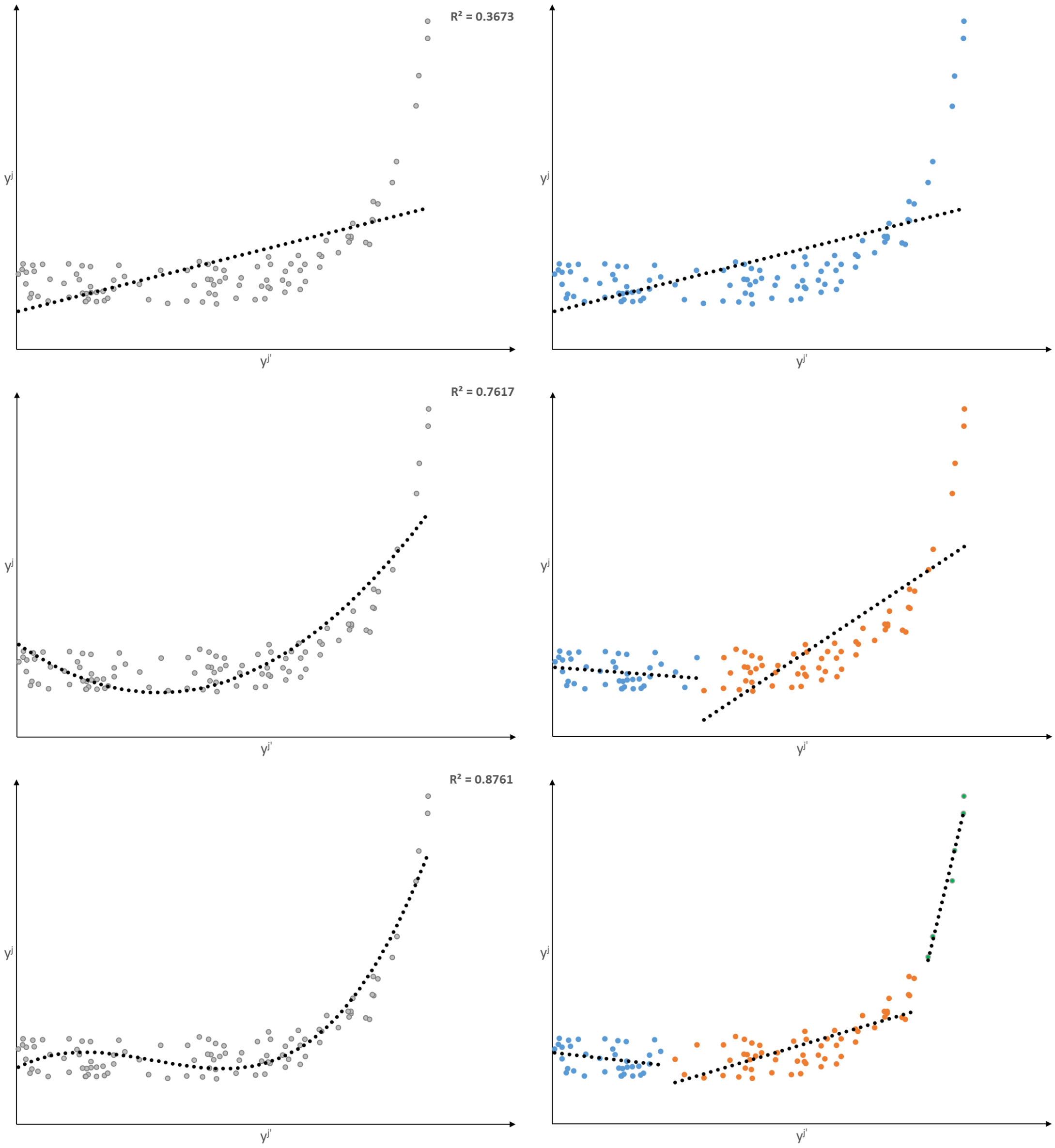


Figure 2.6: Piecewise Approach to nonlinear data based on First, Second and Third Order Polynomial Function

4. **Calculate Piecewise Correlations**: at this stage, for each connection present in the structural model, the algorithm has H sub-

sets of data originated by $H-1$ stationary points. When the chosen function is linear, there are no stationary points and H is equal to 1; for second order polynomial functions there is 1 stationary point and the algorithm identifies 2 subsets of data (i.e., $H = 2$); when the chosen function is a third degree polynomial, the 2 stationary points generate 3 subsets of data.

Given a $n \times 3$ matrix $Y_{jj'}$ containing the n observations of the two connected composites under analysis and the subset to which each observation belongs, defined as follows:

$$Y_{jj'} = \begin{bmatrix} y_{1j} & y_{1j'} & h_1 \\ y_{2j} & y_{2j'} & h_1 \\ \vdots & \vdots & \vdots \\ y_{ij} & y_{ij'} & h_h \\ \vdots & \vdots & \vdots \\ y_{nj} & y_{nj'} & h_H \end{bmatrix} \tag{2.11}$$

where H represent the number of subsets present in the relation between y_j and $y_{j'}$ (also corresponds to the order of the selected polynomial function). For a third degree polynomial function ($H = 3$), the matrix $Y_{jj'}$ will have a set of observations falling in the subset h_1, another group falling under h_2 and the remaining ones under h_3.

Once the previous matrix is built, it is possible to define a function $S^h\left(Y_{jj'}\right)$ defined as a generic piecewise function between y_j and $y_{j'}$ applied on each subset h. This function returns a $n \times 1$ vector and its i-th value represents the weight obtained using function S for the subset h to which the observation belongs. Figure 2.7 shows an example where the function $S^h\left(Y_{jj'}\right)$ corresponds to the piecewise correlation $corr^h\left(Y_{jj'}\right)$.

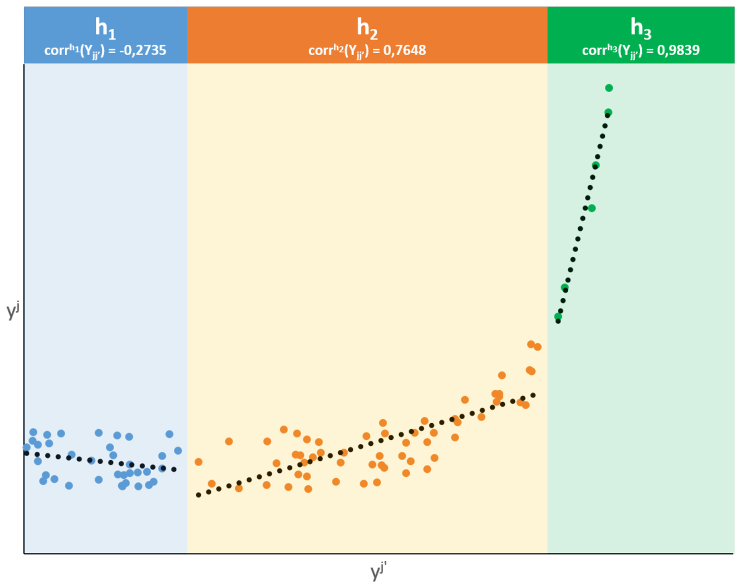


Figure 2.7: Piecewise Correlation built from a Third Order Polynomial Function

The next paragraphs present how these steps are embedded in the proposed algorithm. The main advantages of this technique when compared to the standard PLSPM inner weight estimation are:

- Allows to fit nonlinear estimation using a dynamic and scalable data-driven piecewise approach;

- Allows the definition of a non-symmetrical structural model estimation, where the step 1 (Fit Polynomial Functions) can be executed switching the dependent variable with the independent;

- Allows for the original inner weights estimation techniques to be applied through a data partitioning technique;
- When the relations among the composites is linear (i.e., the first order polynomial represents the best choice), the algorithm delivers the same results as the original PLSPM algorithm.

More details on the previous list of claims attributed to the proposed algorithm are presented in the next sections.
The next section will also present the full algorithm using the piecewise inner weights estimation process.

2.4.2 The PLSPM Algorithm using Piecewise Inner Weights Estimation

As discussed in the previous chapter, PLS path modelling aims to estimate the relationships among J $(j = 1, \ldots, J)$ blocks of manifest variables, which are expression of unobservable variables. The algorithm is characterised by a system of interdependent equations based on simple and multiple linear regressions. The algorithm estimates the dependence relationships among LVs as well as the relationships between MVs and their own LVs.
This section will present the proposed algorithm using piecewise inner weights estimation process, showing how this part is embedded in the standard algorithm.
With the aim of ease the readability of the proposed algorithm some of the steps presented in the previous chapter will be repeated.

Starting Weights Definition

The first step of the PLSPM algorithm regards the definition of a set of arbitrary weights w_{pj} to be used as starting point. These weights are then normalised in order to produce LVs with unitary variance. Common choices for starting weights are presented in subsection 1.2.3.

Measurement Model: Latent Variables Calculation

Once defined the initial weights the algorithm moves to the outer estimate y_j of the standardised (with mean = 0 and standard deviation = 1) latent variables $(\xi_j - m_j)$. The composites are estimated as linear combination of their centered MVs:

$$y_j \propto \pm \left[\sum_{p=1}^{P_j} w_{pj} \left(x_{pj} - \bar{x}_{pj} \right) \right] \tag{2.12}$$

where the $\propto$ symbol means that the variables on the left is proportional to the operator on the right; the $\pm$ operator represents the sign ambiguity. This problem is solved by selecting the sign that makes the variable y_j positively correlated with the majority of manifest variables x_{pj}.

The j-th estimated latent variable is obtained as follows:

$$y_j = \sum_{p=1}^{P_j} \tilde{w}_{pj} \left(x_{pj} - \bar{x}_{pj} \right) \tag{2.13}$$

The coefficients w_{pj} and $\tilde{w}_{pj}$ are called outer weights.

The mean value m_j is estimated as:

$$\hat{m}_j = \sum_{p=1}^{P_j} \tilde{w}_{pj} \bar{x}_{pj} \tag{2.14}$$

and the latent variable ξ_j is estimated by:

$$\hat{\xi}_j = \sum_{p=1}^{P_j} \tilde{w}_{pj} x_{pj} = y_j + \hat{m}_j \tag{2.15}$$

Structural Model: Piecewise Inner Weights Estimation

The structural model aims to give an estimate of the LVs based on the causal relations present in the inner model. Those relationship may present nonlinear patterns. In order to correctly estimate nonlinearity, the inner weights can be estimated by using the piecewise inner weight estimation process presented in the previous sections. This process can be applied transversally to most of the existing techniques referred in the standard algorithm.

Based on these assumptions, the piecewise inner weights $e^h_{jj'}$ can be estimated in different ways presented in the next paragraphs.

The piecewise inner weights $e^h_{jj'}$ can be defined as a vector of dimensions $n \times 1$. The i-th value of $e^h_{jj'}$ corresponds to the weight estimated for the subset (defined in the third column of the matrix $Y_{jj'}$) to which the i-th observation belongs.

Piecewise Centroid Scheme The piecewise centroid scheme represents an adaptation of the original technique proposed by H. Wold. The $n \times 1$ vector $e^h_{jj'}$ can be defined as having the i-th value corresponding to the sign of the correlation calculated in the subset h where the

i-th observation belongs. This can be obtained as:

$$e_{jj'}^{h} = sign\left[corr^{h}\left(Y_{jj'}\right)\right] \tag{2.16}$$

where $Y_{jj'}$ represents the matrix shown in 2.11 and the function $corr^h$ represents the piecewise correlation function among the two latent variables j and j'. As referred in the previous section, the piecewise function returns a $n \times 1$ vector where the generic value i belonging to the h-th subset, represents the correlation calculated within the subset h. In this case $e_{jj'}^{h}$ are the signs of this piecewise correlations (see Figure 2.7) between y_j and the latent variable $y_{j'}$ connected to y_j (see Equation 2.16).

Piecewise Factorial Scheme The Piecewise Factorial Scheme represents the proposed approach to one of the two techniques proposed by Lohmöller where inner weights $e_{jj'}^{h}$ are calculated as follows:

$$e_{jj'}^{h} = corr^{h}\left(Y_{jj'}\right) \tag{2.17}$$

where $Y_{jj'}$ represents the matrix shown in 2.11 and the function $corr^h$ represents the piecewise correlation function among the two latent variables j and j'. As referred in the previous sections, the piecewise function returns a $n \times 1$ vector where the generic value i belonging to the h-th subset, represents the correlation calculated within the subset h.

Some Observation It has been decided that the Path Weighting scheme proposed by Lohmöller would not be adapted to be included as a potential scheme for the proposed nonlinear approach.

The biggest argument in favour of Path Weighting scheme is the fact that this takes into account the path direction.

The proposed nonlinear approach presents the possibility of switching the inner weights estimation from symmetrical to non-symmetrical.

If a symmetrical approach is chosen, then the weighting system obtained to calculate the composite z_j is calculated using a symmetrical square matrix of dimensions $J \times J$. In this case, all weights present in the upper diagonal matrix are exactly the same as the ones present in the lower diagonal matrix.

In case the researcher wants to use the non-symmetrical approach, the weights present in the upper diagonal matrix are different from the ones in the lower diagonal matrix. In this situation, when estimating the weights, if $j > j^{'}$ (lower diagonal matrix), then the weight is calculated using y_j as dependent and $y_{j^{'}}$ as independent. When $j < j^{'}$ (upper diagonal matrix), then the weight is calculated using $y_{j^{'}}$ as dependent and y_j as independent.

Given to its flexibility, the proposed approach can be applied to other existing techniques and allow the development of novel customised weights estimation techniques.

Structural Model: Latent Variables Calculation

In the inner LVs calculation stage, the standardised $(\xi_j - m_j)$ latent variables inner estimation z_j is given by:

$$z_j \propto \sum_{j^{'} \, : \, \xi_{j^{'}} \; adjacent \; to \; \xi_j} e^h_{jj^{'}} \circ y_{j^{'}} \tag{2.18}$$

where $\circ$ denotes the Hadamard product.
Starting from this stage, the algorithm is exactly the same as the standard algorithm presented in section 1.2. The remaining step is the outer weights estimation related to the measurement model.

Iterative Process and Convergence

After the first cycle the algorithm iterates the following steps:

1. Measurement Model: Latent Variables Calculation
2. Structural Model: Piecewise Inner Weights Estimation
3. Structural Model: Latent Variables Calculation
4. Measurement Model: Outer Weights Estimation
5. Outer Weights Convergence Check

The aforementioned algorithm is described in figure 2.8 and its pseudocode is shown in Algorithm 2.
After reaching the algorithm convergence, the outer weights w_{pj} are used to obtain the final estimation of ξ_j calculated as $\hat{\xi}_j = \sum w_{pj} x_{pj}$.
In the last step of the proposed nonlinear approach to PLSPM, path polynomial functions are estimated. The final output is a function for each relationship existing in the path diagram structure. The generic function $\mathbf{\Gamma}_{jj'}$ representing the relation between y_j (i.e., the composite for the endogenous LV ξ_j) and $y_{j'}$ (i.e., the composite for the exogenous LV $\xi_{j'}$ directly connected to ξ_j), is obtained as:

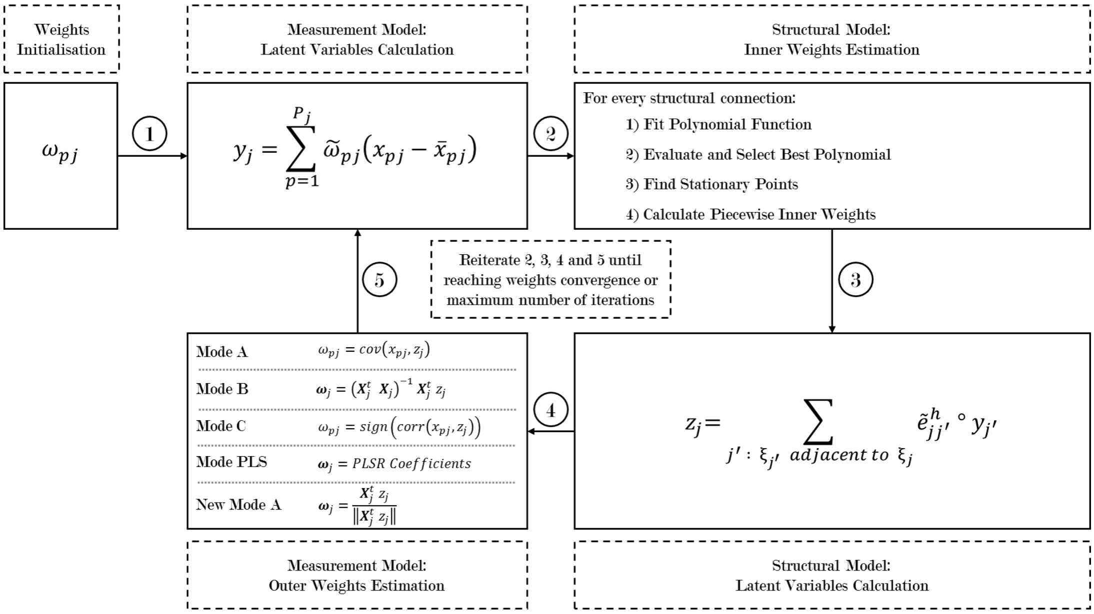


Figure 2.8: PLSPM Iterative Estimation Process using Piecewise Inner Weights Estimation

$$\boldsymbol{\Gamma_{jj'}} = \beta_0 + \beta_1 y_{j'} + \beta_2 y_{j'}^2 + \ldots + \beta_d y_{j'}^H \tag{2.19}$$

where the degree H is defined following the same proprieties used in the second step of the proposed algorithm (Evaluate and Select Polynomial Functions). These polynomial functions $\boldsymbol{\Gamma_{jj'}}$ are not easy to interpret. For this reason the algorithm produces a set of scatter plots (one for each inner relation) with the $\boldsymbol{\Gamma_{jj'}}$ function. An example can be seen in figure 2.9.

The algorithm convergence is analysed in the next chapter using several simulation scenarios.

Algorithm 2: Nonlinear PLSPM

Input : $\boldsymbol{X} = [\boldsymbol{X_1}, \ldots, \boldsymbol{X_j}, \ldots, \boldsymbol{X_J}]$
Output: $w_{pj}, \hat{\xi}_j, \boldsymbol{\Gamma_{jj'}}$

Arbitrary Weights Initialisation: $w_{pj} = w_{pj}^{(0)}$

while *Convergence of* w_{pj} *is not reached (or max number of iterations)* **do**

- **Latent Variables Proxies Calculation** (Measurement Model):
  $y_j \propto \pm \left[\sum_p w_{pj}\left(x_{pj} - \bar{x}_{pj}\right)\right]$
- **Piecewise Inner Weights Estimation** (Structural Model):
  for *Every structural connection between* y_j *and* $y_{j'}$ **do**
  - Fit Polynomial Functions
  - Evaluate and Select Polynomial Functions
  - Find Stationary Points
  - Calculate Piecewise Correlations as $e_{jj'}^{h} = f^{h}\left(y_j, y_{j'}\right)$
- **Latent Variables Proxies Calculation** (Structural Model):
  $z_j \propto \sum_{j' \,:\, \xi_{j'} \text{ adjacent to } \xi_j}\left(e_{jj'} \circ y_{j'}\right)$
- **Outer Weights Estimation** (Measurement Model):
  $w_{pj} = f\left(\boldsymbol{X}, \boldsymbol{Z}\right)$ according to the chosen estimation technique

Final Latent Variables Proxies Calculation:
$\hat{\xi}_j = \sum w_{pj} x_{pj}$

Path Polynomial Functions Estimation:
$\boldsymbol{\Gamma_{jj'}} = \beta_0 + \beta_1 y_{j'} + \beta_2 y_{j'}^2 + \ldots + \beta_d y_{j'}^H$ according to the chosen degree

2.4.3 A Practical Example on Simulated Data

The main objective of this section is to test the proposed algorithm presented in the previous sections, using data generated from a Monte Carlo simulation conducted in EQS 6.1 for Windows.

The data generation process is consistent with the procedure described

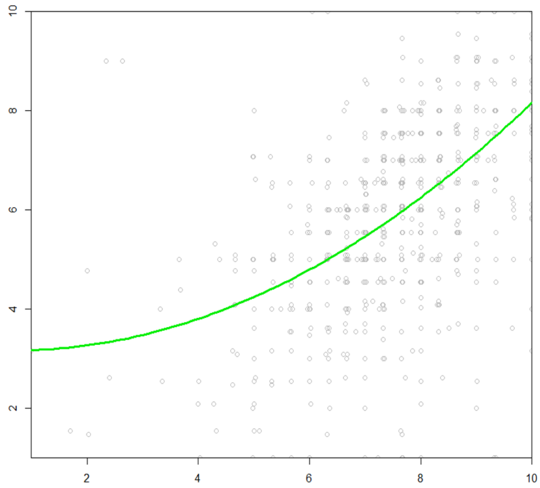


Figure 2.9: Nonlinear function $\mathbf{\Gamma}_{jj'}$ output example

in Paxton et al. (2001) for a Monte Carlo SEM study.

The generated data has been used for the analysis presented in this chapter and in a more detailed simulation study focussed on the algorithm convergence presented in chapter 3.

For this specific case, the desired target SEM model has been pre-specified and configured with a set of given parameters and then the data has been simulated following the previous assumptions and configuration.

The designed measurement model has 16 manifest variables x_p ($p = 1, \ldots, 16$) equally distributed across four reflective measurement blocks.

The structural model has been configured as follows:

$$
\begin{aligned}
\eta_2 &= 0.3\xi_1 + \zeta_2 \\
\eta_3 &= 0.3\xi_1 + 0.3\eta_2 + \zeta_3 \\
\eta_4 &= 0.5\xi_1 + 0.5\eta_2 + 0.5\eta_3 + \zeta_4
\end{aligned}
\tag{2.20}
$$

The variances of ξ_1 and the three endogenous latent variables (i.e., η_2, η_3, η_4) have been fixed to 1 and the errors' variances associated to the reflective measurement model equations have been set to 0.01.
The path diagram for the aforementioned model is presented in figure 2.10.

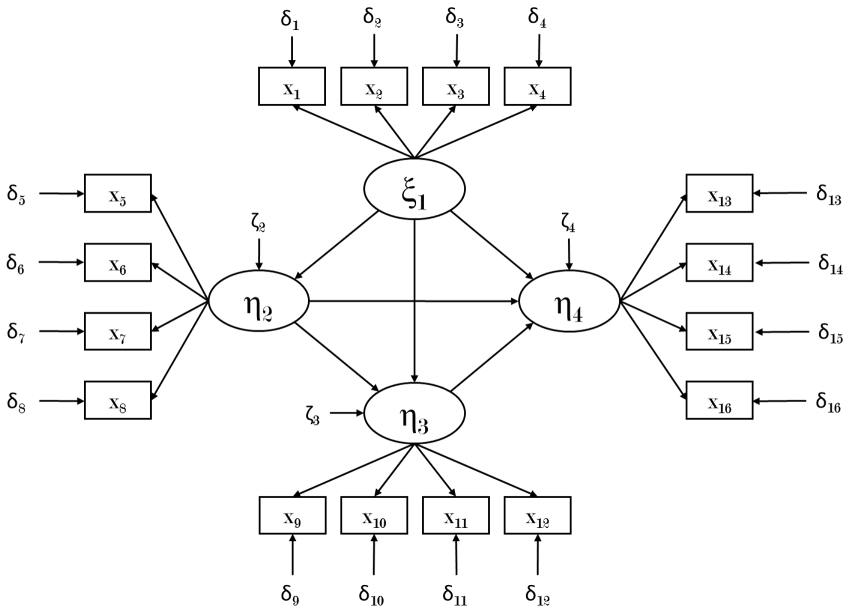


Figure 2.10: Simulated Structural Equation Model

The next sections present a comparison analysis between the proposed approach and the standard PLSPM algorithm, based on the Monte Carlo simulation described above.

Comparison Study

The comparative analysis has been developed on four simulated datasets generated using the aforementioned configuration. The only difference existing between the 4 datasets is the sample size; for this analysis the sample sizes used are 50, 100, 200 and 500.

The results for the standard PLSPM have been obtained using the *plspm* package developed by Sánchez (2013) with Mode A for outer weights estimation and Factorial Scheme for inner weights estimation. The nonlinear PLSPM algorithm has been executed with Mode A for outer weights estimation and Piecewise Factorial Scheme for inner weights estimation. All of the indicators and results are subdivided in three sections: Model Performance, Measurement Model Assessment and Structural Model Assessment.

Model Performance The first results to be analysed are the iterations to reach convergence. Even if the standard PLSPM presents a faster convergence in three out of four executions, the differences do not seem to be large enough to evidence a potential issue in the proposed algorithm (see Figure 2.11).

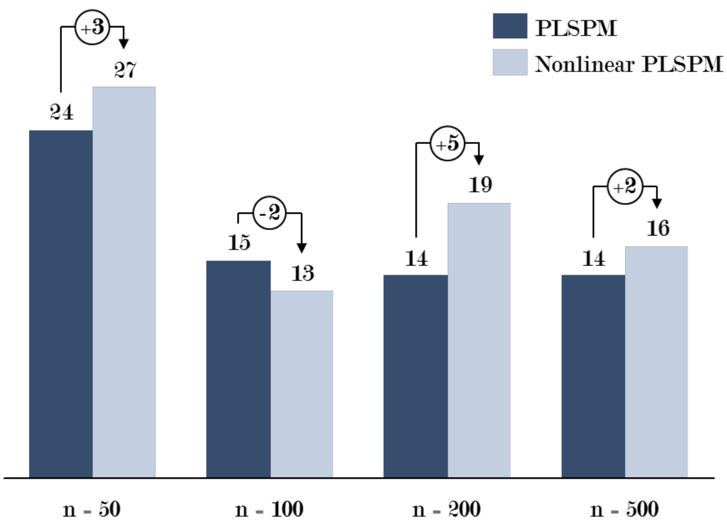


Figure 2.11: Model Performance: Iterations to Convergence

Measurement Model Assessment The main difference between the proposed approach and the standard algorithm is the way how the inner weights are estimated. Even though the new approach should mainly impact the structural model, the latent variable scores calculated internally impact in an indirect way the measurement model. This section presents the results obtained for communality and redundancy.

Figure 2.12 shows the communality results for both standard and Nonlinear PLSPM. The statistics are quite similar when $n = 50$ and $n = 500$. The sample size presents bigger differences when $n = 200$.

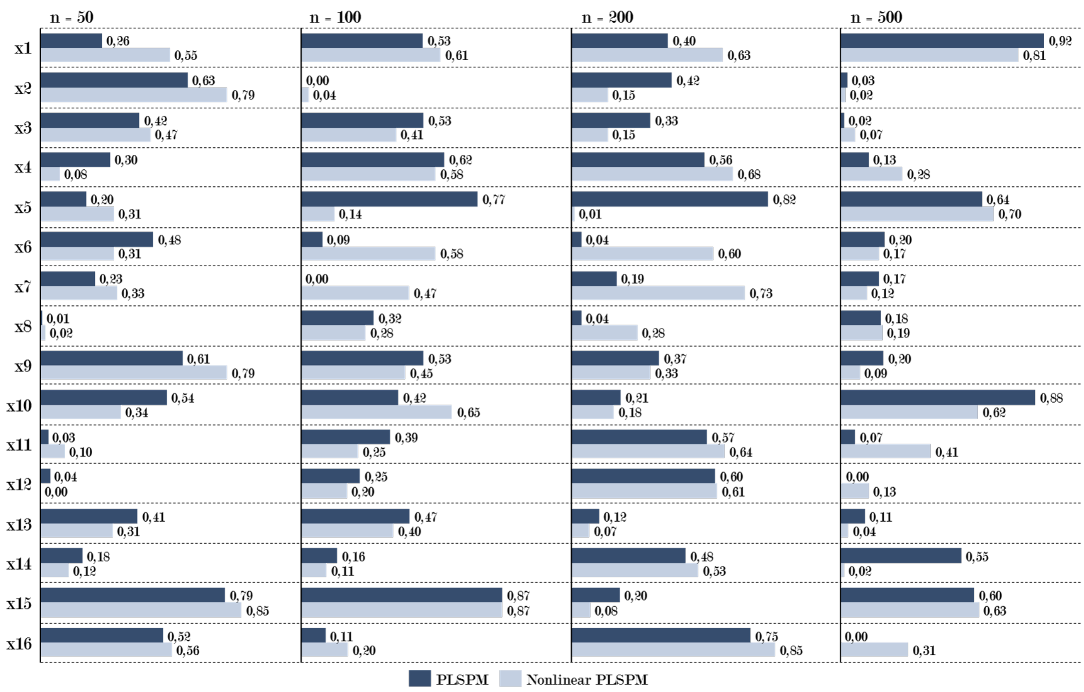


Figure 2.12: Measurement Model Comparison: Communality

Another way to assess the main differences between the two algorithms in the measurement model is by analysing the redundancy in figure 2.13. This graphical output, for sample sizes of at least 200 observations, shows that the Nonlinear PLSPM presents higher redundancy values when compared with the standard algorithm, even if not for all indicators.

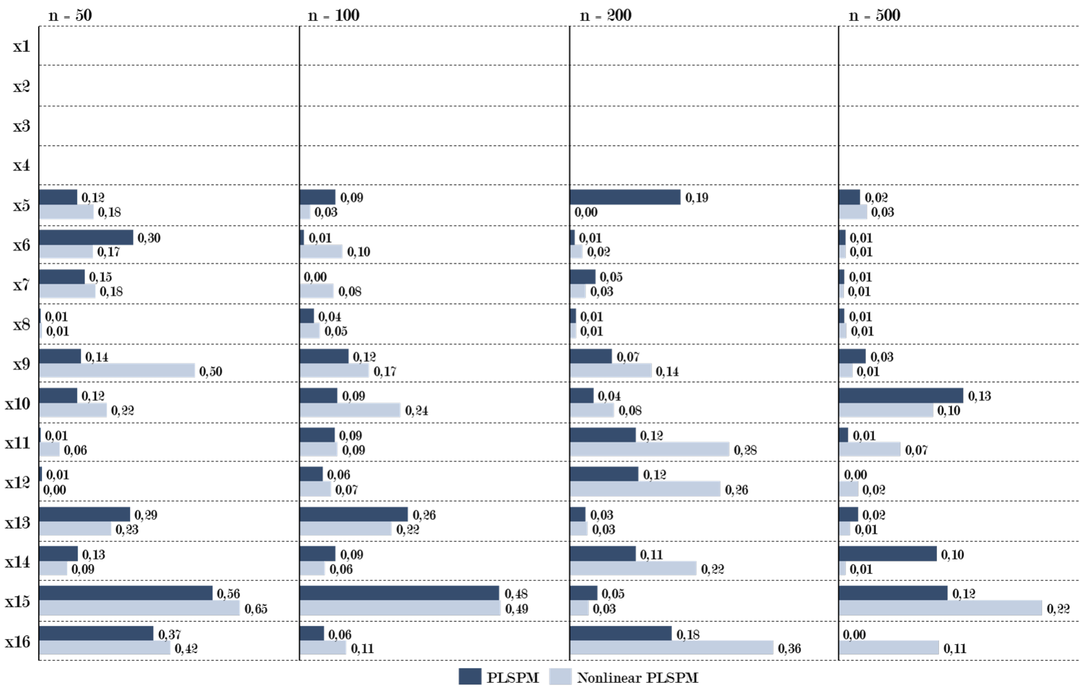


Figure 2.13: Measurement Model Comparison: Redundancy

Structural Model Assessment This section presents a comparison between the statistics related to the structural model. The assessment is based on a set of inner model statistics (such as R^2, Average Communality and Average Redundancy[5]).

Analysing the results in figure 2.14 it is possible to state that the proposed approach, for the selected samples, presents slightly higher results in terms of R^2, average communality and average redundancy. Whilst

[5] Average Variance Extracted (AVE) is not presented because when the variables are standardised AVE corresponds to the Communality multiplied by a constant parameter.

communality and redundancy results are quite similar, the R^2 presented by the proposed approach for endogenous latent variables η_2, η_3 and η_4 are most of the times consistently higher than the standard PLSPM algorithm.

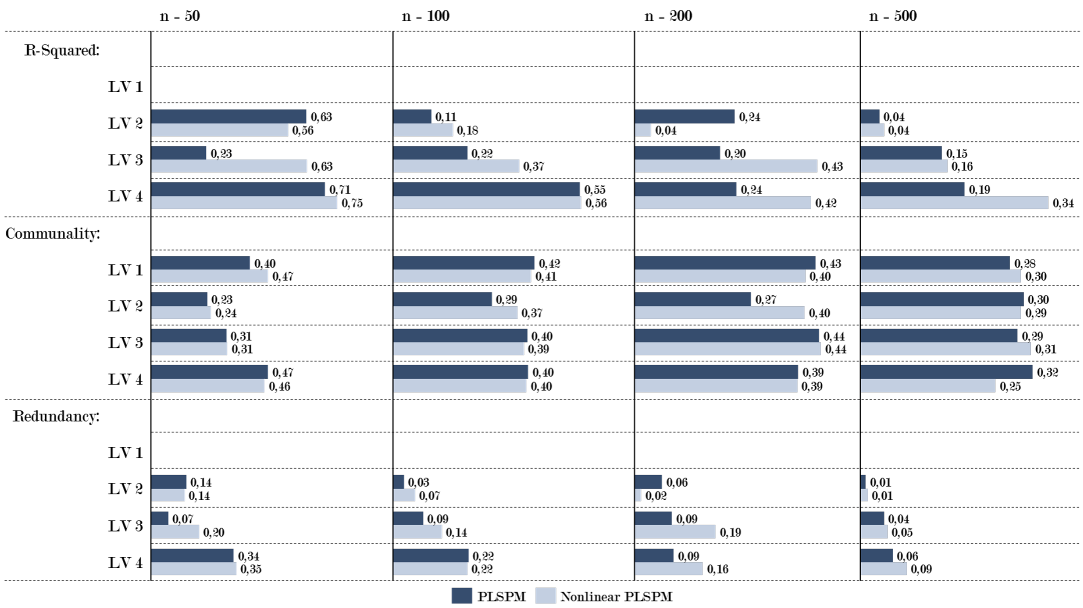


Figure 2.14: Structural Model Comparison: Latent Variables Statistics

2.5 Conclusions

As previously mentioned, PLS path modelling algorithm is an iterative process based on simple and OLS regressions. Although attractively simple, the traditional linear model often fails in these situations: in real life, effects are often not linear (Hastie et al., 2009).

The proposed nonlinear approach to the standard PLSPM can be seen, when it comes to the inner model, as a data-driven estimation approach.

In fact, the algorithm adapts to the form assumed by the inner relationships among latent variables defining a piecewise estimation method. Its flexibility allows using different inner weights estimation methods taking advantage of the piecewise algorithm's architecture. As detailed in the previous sections, another added value related to the proposed nonlinear algorithm is the possibility of defining a non-symmetrical weighting system in the structural model estimation.
The results obtained on the comparison study are promising and require a deeper analysis for other scenarios and model configurations.
The next chapter presents a Monte Carlo simulation to assess the algorithm stability and convergence.

Chapter 3

A Simulation Study on Nonlinear PLSPM

3.1 Introduction

This chapter presents a Monte Carlo simulation study focussed on assessing the algorithm's convergence and the stability of its estimates obtained by using the algorithm proposed in the previous chapter.

Monte Carlo computer simulations are used to model a variety of real-world statistical and psychometric processes. The value of a simulation is closely tied to the fidelity with which it represents the real-world environment that it attempts to model. All Monte Carlo procedures require the generation of random numbers. Random number generators typically available are limited to generating random numbers with uniform or normal distributions. However, to adequately replicate the real-world environment, random numbers with distinctly non-normal distributions

are often required (Vale and Maurelli, 1983).
In this work the data has been generated using EQS 6.1 (Bentler and Wu, 1995) and imported in R for the model estimation phase. More details on the scenarios and the theoretical model hypothesised are presented in the next sections.

3.2 Simulation and Scenarios Design

In order to build a systematic simulation process, this work approaches several questions related to model configuration, sample size and repetitions.
The following paragraphs present in detail the SEM model used to generate the simulated data in EQS and the several configuration considered for each scenario.

Simulated SEM Theoretical Model The designed measurement model has 16 manifest variables (x_1 to x_{16}) equally distributed among four reflective measurement blocks.
The structural model has been configured as follows:

$$\begin{aligned}
\eta_2 &= \beta_{21}\xi_1 + \zeta_2 \\
\eta_3 &= \beta_{31}\xi_1 + \beta_{32}\eta_2 + \zeta_3 \\
\eta_4 &= \beta_{41}\xi_1 + \beta_{42}\eta_2 + \beta_{43}\eta_3 + \zeta_4
\end{aligned} \tag{3.1}$$

The variances of ξ_1 and the three endogenous latent variables (i.e., η_2, η_3, η_4) have been fixed to 1 and the errors' variances associated to the reflective measurement model equations have been fixed to 0.01.

The path diagram for the aforementioned model is presented in figure 3.1.

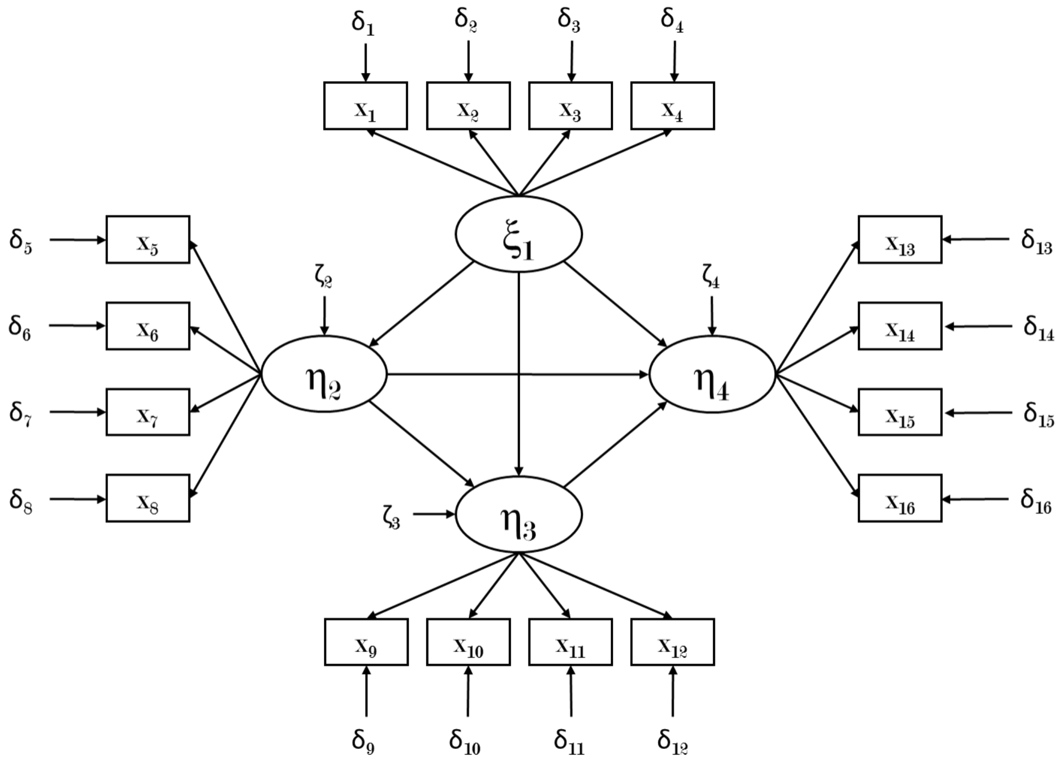


Figure 3.1: Simulated Structural Equation Model

In addition to the aforementioned model and configuration, the simulation scenarios differ on theoretical loadings (π_{ij}), path coefficients ($\beta_{jj'}$) and sample size.

Loadings Configurations Starting from the loadings, the simulation scenarios may follow two principal configurations: one where each block is heterogeneous, i.e., for each block j, the loadings are defined as $\pi_{1j} = 0.3$, $\pi_{2j} = 0.5$, $\pi_{3j} = 0.7$ and $\pi_{4j} = 0.9$. The other configuration defines each block as homogeneous; in this case, for each block j, the loadings are defined as $\pi_{1j} = 0.9$, $\pi_{2j} = 0.9$, $\pi_{3j} = 0.9$ and $\pi_{4j} = 0.9$.

Path Coefficients Configurations Another set of parameters that have been tested are the path coefficients. Similarly to the definitions presented for the loadings, two configurations have been used in order to build the simulation scenarios: one where all path coefficients $\beta_{jj'}$ are equal to 0.3 with exception for paths connected with η_4 that are equal to 0.5; in the second configuration, all path coefficients $\beta_{jj'}$ are set to 0.3.

Sample Size The simulations have been processed with four different sample sizes: $n = 50$, $n = 100$, $n = 200$ and $n = 500$.

Simulation Scenarios Definition Once all the configuration needed in order to assess several characteristics of the proposed algorithm are defined, it is fundamental to build a simulation structure composed by scenarios.

A scenario can be defined as a combination of the aforementioned configurations. In the end all scenarios must exhaustively cover all possible combinations between the model configurations.

The information presented in the previous paragraphs can be summarised as:

– **Sample Size Configurations**

  Configuration 1: $n = 50$;

  Configuration 2: $n = 100$;

  Configuration 3: $n = 200$;

  Configuration 4: $n = 500$.

– **Loadings Configurations**

Configuration 1: heterogeneous blocks;

Configuration 2: homogeneous blocks.

– **Path Coefficients Configurations**

Configuration 1: all path coefficients $\beta_{jj'}$ are equal to 0.3 with exception for paths connected with η_4 that are equal to 0.5;

Configuration 2: all path coefficients $\beta_{jj'}$ are set to 0.3.

The combination of the aforementioned configurations generate the 16 scenarios presented in table 3.1. For each one of the 16 scenarios it has been decided to generate 1000 repetitions.

Scenario Number	Sample Size	Loadings	Path Coefficients
1	50	Configuration 1	Configuration 1
2	50	Configuration 1	Configuration 2
3	50	Configuration 2	Configuration 1
4	50	Configuration 2	Configuration 2
5	100	Configuration 1	Configuration 1
6	100	Configuration 1	Configuration 2
7	100	Configuration 2	Configuration 1
8	100	Configuration 2	Configuration 2
9	200	Configuration 1	Configuration 1
10	200	Configuration 1	Configuration 2
11	200	Configuration 2	Configuration 1
12	200	Configuration 2	Configuration 2
13	500	Configuration 1	Configuration 1
14	500	Configuration 1	Configuration 2
15	500	Configuration 2	Configuration 1
16	500	Configuration 2	Configuration 2

Table 3.1: Simulation Scenarios

The following sections present a set of summarised results for each one of the simulation scenarios with the aim of analysing convergence and stability of the proposed algorithm.

3.3 Simulation Results: Analysis and Comments

The simulation results presented in this section are obtained by executing the proposed algorithm with the following configurations:

- Outer Weights Estimation Method: Mode A for all blocks
- Algorithm Convergence Tolerance: $1e - 05$
- Algorithm Convergence Maximum Number of Iterations: 100
- Nonlinear Polynomial Degree Selection Statistic: BIC

The next two subsections present a detailed analysis on the simulation results for each scenario tested and some thoughts on the results obtained for the proposed algorithm.

3.3.1 Results Analysis

This section presents the main finding related with the simulation analysis separated in three main blocks: Algorithm Convergence, Estimates Stability and Predictive In-Sample Assessment.

Algorithm Convergence

The 16 scenarios designed in the previous section generated 16000 samples (1000 samples per scenario). The main objective of this section is to study the convergence patterns for each scenario and analyse if there is a particular configuration causing lower convergence rates.

The results for this analysis are summarised in table 3.2.

Scenario Number	Sample Size	Loadings	Path Coefficients	Convergent Repetitions
1	50	Heterogeneous Blocks	0.3, 0.5	982 (98.2%)
2	50	Heterogeneous Blocks	0.3	979 (97.9%)
3	50	Homogeneous Blocks	0.3, 0.5	979 (97.9%)
4	50	Homogeneous Blocks	0.3	970 (97.0%)
5	100	Heterogeneous Blocks	0.3, 0.5	997 (99.7%)
6	100	Heterogeneous Blocks	0.3	995 (99.5%)
7	100	Homogeneous Blocks	0.3, 0.5	997 (99.7%)
8	100	Homogeneous Blocks	0.3	1000 (100.0%)
9	200	Heterogeneous Blocks	0.3, 0.5	1000 (100.0%)
10	200	Heterogeneous Blocks	0.3	1000 (100.0%)
11	200	Homogeneous Blocks	0.3, 0.5	1000 (100.0%)
12	200	Homogeneous Blocks	0.3	1000 (100.0%)
13	500	Heterogeneous Blocks	0.3, 0.5	1000 (100.0%)
14	500	Heterogeneous Blocks	0.3	1000 (100.0%)
15	500	Homogeneous Blocks	0.3, 0.5	1000 (100.0%)
16	500	Homogeneous Blocks	0.3	1000 (100.0%)

Table 3.2: Algorithm Convergence Analysis

The results presented in table 3.2 trigger two main warnings related with sample size and the path coefficients values hypothesised in the theoretical model. From the empirical tests emerges that (i) the proposed algorithm seems to reach convergence when the sample size is at least 100 and that (ii) the choice of similar path coefficients (instead of higher coefficients for the fourth latent variable η_4) leads to slightly worse convergence rates. For sample sizes lower than 100 the minimum convergence rate is 97%.

Estimates Stability

Another important characteristic to be tested for the proposed algorithm is the stability related with the estimation process. This study aims to analyse the distribution of the estimated loadings. The theoretical model shown in this chapter presents 16 loadings (4 for each block). The distributions are analysed using box plots and the loadings are named sequentially from 1 to 16 (where 1 to 4 are related to the first block and are placed on the first row, 5 to 8 to the second block and placed on the second row and so on).

In order to avoid redundancy in the results presented, this section only shows two examples considered as representative of the whole simulation analysis. The full set of results can be found in the appendix section A.3.

Case 1 Figure 3.2 presents the distribution of λ_{31} (loading that relates x_3 to ξ_1) for the simulation scenario number 1 (sample size = 50, heterogeneous blocks and path coefficients equal to 0.3 and 0.5 when connected to η_4).

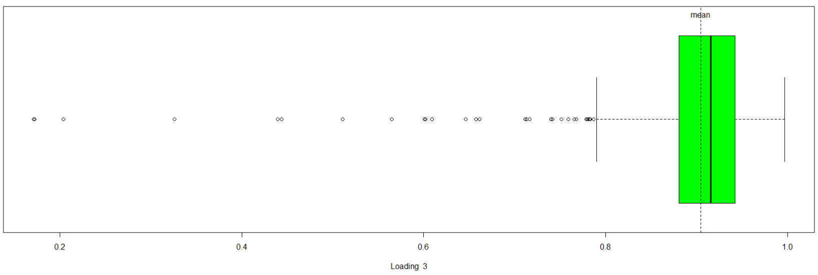


Figure 3.2: Simulation Scenario 1: Distribution of Loading related to ξ_1 using the proposed algorithm

The box plot shows some dispersion and presents several outliers between 0.2 and 0.8. The results obtained by all simulation study when sample size is equal to 50, present the same dispersion patterns.

In order to assess if the dispersion is related to the proposed algorithm, the same distribution analysis is presented for the standard PLS path modelling algorithm using the *plspm* package developed by Sánchez (2013) with Mode A for outer estimation and Factorial Scheme for inner weights estimation (see Figure 3.3).

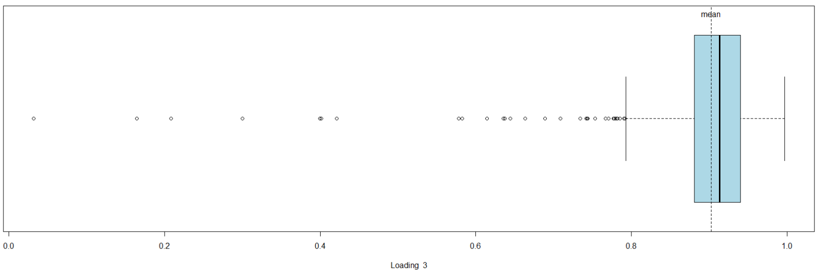


Figure 3.3: Simulation Scenario 1: Distribution of Loading related to ξ_1 using the standard PLSPM

Figure 3.3 highlights that the dispersion seen in figure 3.2 is not generated by the proposed algorithm since the results obtained by the standard PLSPM algorithm are very similar.

As referred above, all simulation scenario with sample size equal to 50 observations present distributions similar to the one presented in figure 3.2.

Case 2 The second case presents the distribution of λ_{31} (loading that relates x_3 to ξ_1) for the simulation scenario number 16 (sample size = 500, homogeneous blocks and all path coefficients equal to 0.3.

As presented in figure 3.4, the distribution is concentrated between 0.99 and 1.

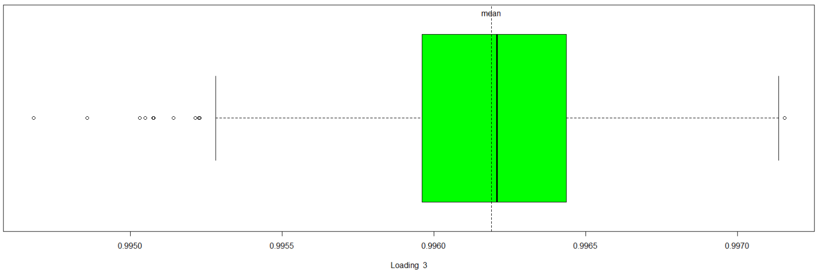


Figure 3.4: Simulation Scenario 16: Distribution of Loading related to ξ_1 using the proposed algorithm

All simulations executed with a sample dimension greater or equal to 100 present similar distributions where estimates have little variance.

Predictive In-Sample Assessment

The previous sections aimed to verify the algorithm convergence and the stability of its estimations. This section completes the simulation analysis by verifying the structural model performance.

As mentioned in the previous chapters, there are several ways to assess the structural model. Given that the proposed algorithm does not have the concept of path coefficient as known in the PLS path modelling, the inner model performance is analysed through the R^2. The R^2 has been calculated for both proposed and standard PLSPM algorithms and then compared.

The structural model used for the simulation exercise, presents 3 endogenous variables: η_2, η_3 and η_4 and the structural equations are summarised in equation 3.1.

The R^2 results obtained for the 16 simulation scenarios, are promising, in fact, the R^2 obtained for the Nonlinear PLSPM approach are always higher than the R^2 presented by the standard algorithm.

With the objective of avoiding redundancy in the results presented, this section only shows one of the 16 R^2 distributions for Nonlinear and standard PLSPM. The full set of results can be found in the appendix section A.4.

Figure 3.5 shows a comparison between the R^2 distributions obtained in the Nonlinear PLSPM (in green) and in the standard PLSPM algorithm (in blue). The dashed lines represent the average value for each one of the algorithms used in this study. The results are obtained using the data generated for the simulation scenario number 13 (sample size = 500, heterogeneous blocks and path coefficients equal to 0.3 and 0.5 when connected to η_4).

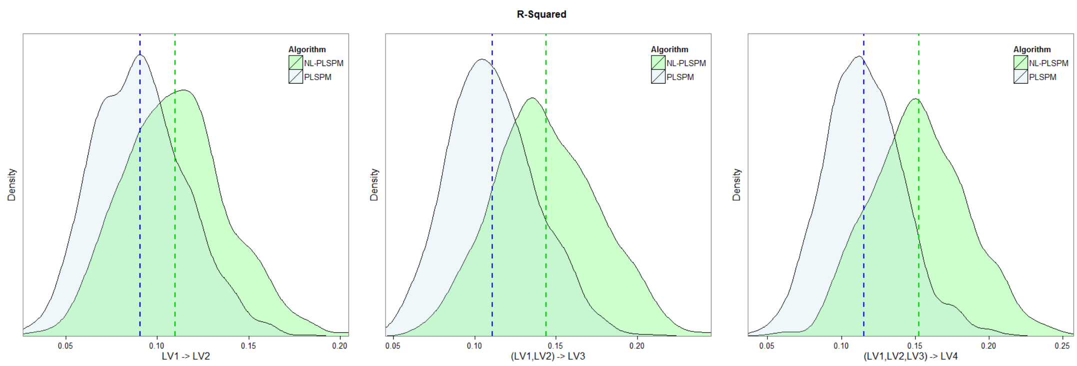


Figure 3.5: Simulation Scenario 13: R^2 Distribution Comparison: PLSPM vs. NL-PLSPM

Based on the results obtained for the R^2, it is possible to state that the proposed algorithm presents a better fit for the structural model estimation process.

3.3.2 Thoughts on Simulations Results

The simulation approach presented in this chapter aimed to assess convergence, inner and outer model estimated stability.
After analysing the results obtained in these three blocks, it seems clear that this approach is stable, becoming more consistent when the sample size is greater than or equal to 100 observations.
Even if the results are promising, there are several reflections that may lead to future developments and fine-tuning of the proposed algorithm.
The two main improvement points identified for future development are:

- **Analysis of Convergence**: in this topic, the main objective is to study the few non-convergence cases obtained when the sample size is equal to 50 observations. As an input for future developments, this sections presents one specific sample where the algorithm stopped reaching the maximum number of iterations defined by the user. This example is obtained using sample number 23 in the simulation scenario 1. The convergence criterion used is $\sum (w_t - w_{t+1})^2$ (where t represents the iteration number) and the convergence behaviour is presented in figure 3.6.

  Given to the scale used in figure 3.6 it is not possible to clearly identify the patterns characterising the convergence criterion. For this reason it has been decided to plot only the last 50 iterations obtained for this same sample (see figure 3.7).

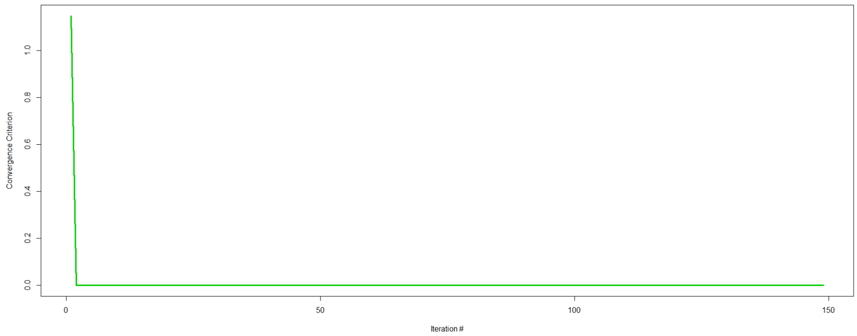


Figure 3.6: A non-convergence example: sample number 23 in Simulation Scenario 1

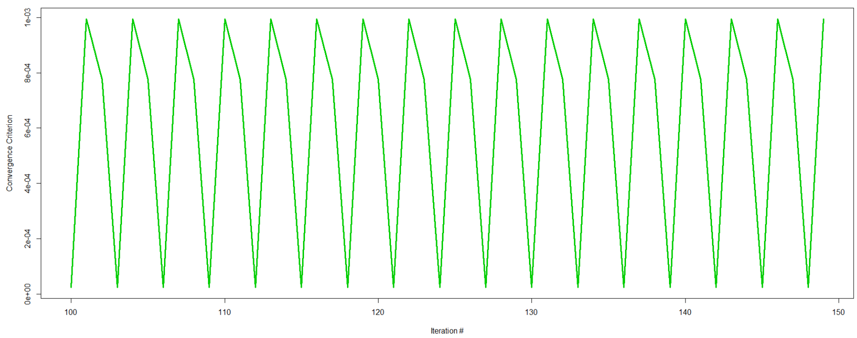


Figure 3.7: A non-convergence example: sample number 23 in Simulation Scenario 1 (last 50 iterations)

The previous plots show some instability that leads to non convergence. This case is similar to the other non convergence verified in the simulation analysis, mostly happening for $n = 50$.

This is a point that requires attention in further developments.

– **Misspecification Analysis**: another important topic that requires further simulation analysis is related to model misspecification. In more detail, the main objective would be to analyse how the model behaves when it is specified differently from the theoretical model.

Chapter 4

An Energy Customer Satisfaction Study

This chapter presents an application focussed on a Customer Satisfaction study on EDP Comercial, one of the top players of the Portuguese liberalised energy supply market.

4.1 Company and Market Overview

The data used in this document belongs to a customer satisfaction project conducted at EDP (Energias de Portugal).

EDP Group is an Energy Solutions Operator which operates in the business areas of generation, supply and distribution of electricity and supply and distribution of gas.

In the supply market, the process of liberalisation of the electricity sectors of most European countries was carried out in a phased manner, and started by including customers with higher consumptions and higher voltage levels.

In Portugal, an identical methodology was followed, and since the 4th of September 2006 all consumers in mainland Portugal have been able to choose their electricity supplier (ERSE). The evolution of the liberalised market is shown in figure 4.1 (Source: ERSE, 2007, 2008, 2009, 2010, 2011, 2012, 2013, 2014, 2015, 2016).

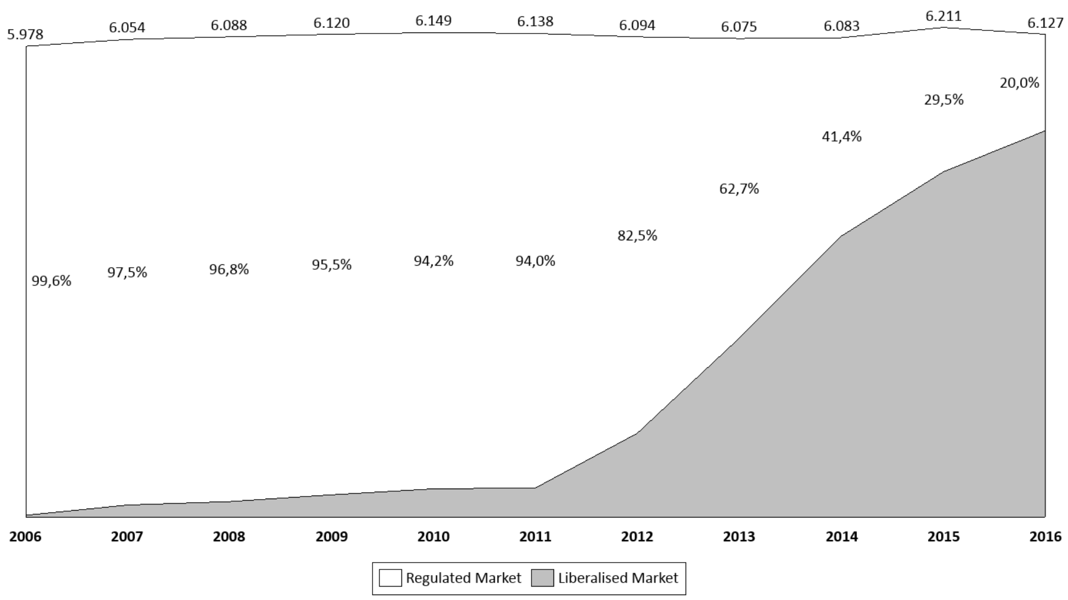


Figure 4.1: Evolution of the Number of Customers in the Portuguese Energy Supply Market (Regulated and Liberalised) between 2006 and 2016

Associated with the liberalisation and the construction of the internal electricity market there is an expected increase in competition, reflected in the level of prices and in the service quality improvement, which should lead to higher levels of customer satisfaction.

In Portugal, EDP Comercial is market leader in the liberalised electricity market. The company's leadership position is driven by its strat-

egy, which is focused on three business units: companies and institutions (B2B business unit), residential and small business customers (B2C business unit) and finally added value Energy Services business unit.
In Portugal, EDP supplies electricity to customers who decided to move to the liberalised market through EDP Comercial.
The application studied in this chapter is focussed on customers with at least one active electricity or gas contract in the liberalised market. More details are presented in the next sections.

4.2 Business Challenge

The business challenge is related to the change of paradigm driven by the liberalisation process. The first results after this process were promising, in fact, EDP was able to be considered as customer's first choice when these were leaving the regulated market to join the liberalised market.
As the years passed by EDP's competitors started increasing their pressure and built several strategies to gain a piece of the liberalised energy (electricity and gas) market.
The liberalised energy market is in a maturity growth process and, when compared to the telecommunications market, is evident that the path to a competitive and saturated market is still long and full of challenges.
Among the future challenges there are some related to what EDP represents for its customers and other energy customers with active contracts in the competition.
During the last years, EDP's strategy reinforced the need for a customer-centric approach where every product, service or action has to be made

around the customer needs.

EDP's ultimate goal is to be Portugal's favourite company due to its offering and service excellence, keeping the customer at the centre of its work.

One of the initiatives related to the customer-centric behaviour is the analysis and the monitoring of customer satisfaction and loyalty through market research studies.

In this direction, EDP started participating in an European project named ECSI Portugal[1]. Its objective is to measure quality and estimating customers satisfaction at several levels (i.e., company, sector, country, etc.)

The ECSI Portugal project follows a methodology based on PLSPM, where customers interviews are structured and used to estimate the satisfaction model (Anderson et al., 1994; Bayol et al., 2000; Fornell, 1992). The objective of this work is to propose an alternative estimation approach (see section 2.4) that breaks the linearity assumption made in the original PLSPM model (used in the ECSI Portugal project). This approach allows for nonlinear relations among latent variables (motivations can be found in section 2.1).

The application of a nonlinear approach aims to inform business decisions providing more details than the original PLSPM algorithm on the nature of the causal relations and guiding a set of targeted business strategy.

[1] More information at http://www.ecsiportugal.pt

4.3 Data and Model Description

This application focusses on the estimation of a Nonlinear PLSPM model for residential EDP customers with at least one active electricity or gas contract in the liberalised market. As referred above, EDP Group operates in the liberalised market through EDP Comercial (EDPC).
In the ECSI model a customer is defined as an individual (at least 18 years old at the moment of the interview) with exposure to consumption and acquisition of products and/or services provided by EDPC over the six months prior to the interview.

4.3.1 Sampling Plan

The sampling plan is composed by a stage where household phone number are selected through a plan comparable to random sampling with equal probabilities and without replacement. For each household the objective is to select the decision-maker in all matters related with the electricity contract. Once the individual is identified, it is classified as customer through a set of questions. In addition to the landline numbers, the sampling plan also used a set of mobile numbers randomly selected. The interviews were carried using CATI (Computer-Assisted Telephone Interviewing) surveying technique between April and June of 2016 and, by the end of that period EDPC had 750 respondents.

4.3.2 ECSI Model

The ECSI model follows the same notation used in the original methodology. In fact, the overall model is composed by structural and measurement models.

The structural or inner model is composed by eight latent variables connected as shown in figure 4.2.

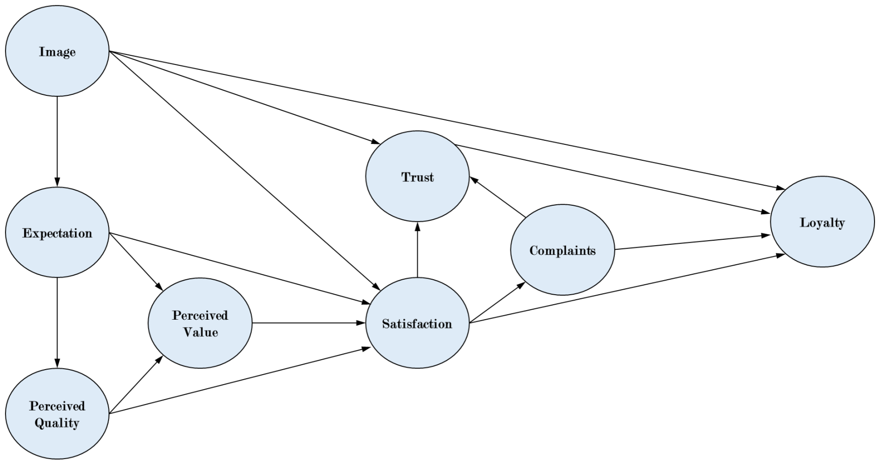


Figure 4.2: ECSI Model for EDPC: Structural Model

The measurement model presents eight blocks composed by the following indicators:

- **Image**

  Image 1: Trustworthy company in what it says and does

  Image 2: Stable and market-based company

  Image 3: Company with a positive contribution to society

  Image 4: Company that cares about customers

  Image 5: Innovative and forward-looking company

- **Expectations**

  Expectations 1: Overall expectations about the company

  Expectations 2: Expectations about the company's ability to offer products and services that meet customer needs

Expectations 3: Expectations regarding reliability, that is, how often things can go wrong

- **Perceived Quality**

  Perceived Quality 1: Overall perceived quality

  Perceived Quality 2: Quality of electricity supply

  Perceived Quality 3: Clarity and transparency in the information provided on safety, emergencies and consumption estimates

  Perceived Quality 4: Counselling and customer care

  Perceived Quality 5: Billing and payment services' reliability and quality

  Perceived Quality 6: Accessibility via digital channels to the provided services

  Perceived Quality 7: Stores and agents accessibility and availability

  Perceived Quality 8: Clarity and transparency in the information provided on contracting, billing and payment, complaints and commercial information

  Perceived Quality 9: Products and services' diversification

- **Perceived Value**

  Perceived Value 1: Evaluation of the price paid, given the quality of products and services

  Perceived Value 2: Evaluation of the quality of products and services, given the price paid

- **Satisfaction**

  Satisfaction 1: Overall satisfaction with the company

Satisfaction 2: Satisfaction compared to expectations (realisation of expectations)

Satisfaction 3: Distance to the ideal electricity company

- **Complaints**

  Complaints 1a: Identification of complaining customers

  Complaints 1b: Evaluation of last resolved complaint (for those who complained)

  Complaints 1c: Perceived evaluation of a potential complaint (for those who did not complain)

- **Trust**

  Trust 1: Overall trust

  Trust 2: Confidence in Company's performance

  Trust 3: Honesty in service providing

- **Loyalty**

  Loyalty 1: Intention to remain as a customer

  Loyalty 2: Price sensitivity

  Loyalty 3: Intention to recommend the company to colleagues and friends

4.3.3 Input Data

The input matrix X has 750 observations and 29 variables described in the previous paragraphs. Table 4.1 presents the summary statistics for the manifest variables.

With exception made for the variable Loyalty 2 (Price sensitivity), all the manifest variables present in this study show a negative skewed curve. A

	Sample Size	Mean	Standard Dev.	Median	Min	Max	Skewness	Kurtosis
Image 1	749	7.76	1.78	8.00	1.00	10.00	-0.96	4.30
Image 2	749	8.63	1.29	9.00	2.00	10.00	-0.83	3.66
Image 3	749	7.64	1.73	8.00	1.00	10.00	-0.90	4.34
Image 4	749	6.96	2.08	7.00	1.00	10.00	-0.74	3.53
Image 5	749	8.02	1.52	8.00	1.00	10.00	-0.90	4.47
Expectation 1	749	7.50	1.63	8.00	1.00	10.00	-0.72	4.36
Expectation 2	749	7.64	1.55	8.00	1.00	10.00	-0.61	3.78
Expectation 3	749	7.61	1.61	8.00	1.00	10.00	-0.91	4.81
Perceived Quality 1	749	7.71	1.72	8.00	1.00	10.00	-1.07	4.86
Perceived Quality 2	749	8.50	1.40	9.00	1.00	10.00	-1.31	6.13
Perceived Quality 3	749	7.10	2.02	7.04	1.00	10.00	-1.01	4.24
Perceived Quality 4	749	7.53	1.84	8.00	1.00	10.00	-1.07	4.83
Perceived Quality 5	749	7.95	1.84	8.00	1.00	10.00	-1.36	5.55
Perceived Quality 6	749	7.85	1.45	8.00	1.00	10.00	-1.51	7.92
Perceived Quality 7	749	7.16	1.83	7.16	1.00	10.00	-1.01	4.83
Perceived Quality 8	749	7.45	1.82	8.00	1.00	10.00	-0.93	4.29
Perceived Quality 9	749	7.51	1.62	8.00	1.00	10.00	-0.88	4.67
Perceived Value 1	749	5.48	2.24	6.00	1.00	10.00	-0.27	2.67
Perceived Value 2	749	6.50	2.01	7.00	1.00	10.00	-0.44	3.21
Satisfaction 1	749	7.56	1.65	8.00	1.00	10.00	-0.77	4.40
Satisfaction 2	749	7.20	1.93	8.00	1.00	10.00	-1.04	4.37
Satisfaction 3	749	7.07	2.04	7.00	1.00	10.00	-0.79	3.82
Complaints 1	749	6.71	2.39	7.00	1.00	10.00	-0.80	3.27
Trust 1	749	7.63	2.01	8.00	1.00	10.00	-1.02	4.18
Trust 2	749	7.71	1.91	8.00	1.00	10.00	-1.00	4.19
Trust 3	749	7.39	2.17	8.00	1.00	10.00	-0.94	3.74
Loyalty 1	749	7.57	2.41	8.00	1.00	10.00	-0.99	3.47
Loyalty 2	749	3.13	2.95	2.23	1.00	10.00	1.75	4.34
Loyalty 3	749	7.52	2.30	8.00	1.00	10.00	-0.95	3.54

Table 4.1: EDP's Input Data: Summary Statistics for the Manifest Variables

more detailed graphical analysis for the manifest variables is presented in the appendix A.5.

Another interesting analysis can be done by getting the correlations between manifest variables. Figure 4.3 presents graphically the correlations between all manifest variables; each block of variables is represented by a black outlined box.

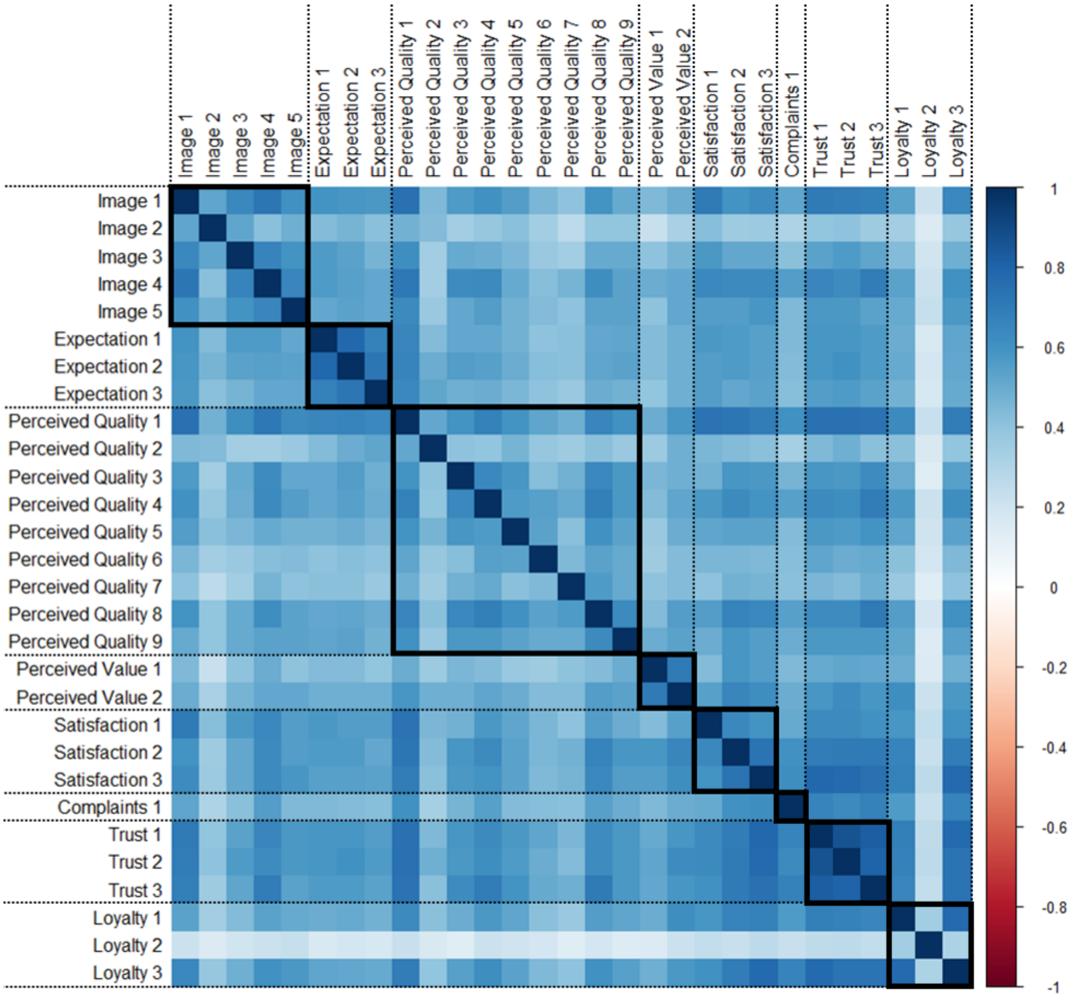


Figure 4.3: EDP's Input Data: Correlations between Manifest Variables

The correlation matrix presents high correlations for almost all variables in the eight block analysed. The lowest correlation appears to be the one between variable Loyalty 2 (Price sensitivity) and the other two variables in the same block. Given the fact that Loyalty 2 represents the percentage of price discount needed for the customer to switch to a competitor, it should present a positive correlation with the others belonging to the same group (i.e., the higher the price sensitivity score given by the customer, the less likely the customer will switch to a competitor). This variable's relevance and sign coherence will be analysed in the next section.

4.4 Results

Disclaimer *Due to confidentiality reasons, some results such as latent variables average values and other data that could jeopardise EDP's position can not be disclosed.*

The data presented in the previous sections has been used as input data for the proposed Nonlinear PLSPM algorithm using the inner model structure presented in figure 4.2 and with the following configurations:

- **Outer Weights Estimation Technique**: for all eight blocks present in the analysed model, it has been decided to set Mode A as outer estimations weights method;
- **Inner Weights Estimation Technique**: the structural weights have been estimated using piecewise inner weights estimation based on first and second degree polynomial functions. The best fit selection between first and second degree has been done using BIC (Bayesian Information Criterion, Schwarz (1978)). As presented in section 2.4.2, there are several ways to adapt the available weighting estimation techniques in a piecewise estimation process; for

this specific business case the method used is Piecewise Factorial Scheme (see equation 2.17);

- **Algorithm Convergence Details**: the algorithm stopping criteria are: (i) outer weights stopping criterion $< 1 \times 10^{-6}$; or (ii) the number of iterations becomes greater than 150.

As presented in chapter 1, when the outer estimation method is mode A, it is important to check the unidimensionality of the block. In this sense, before executing the proposed Nonlinear PLSPM alternative approach, follows an analysis of the three main techniques used to check the unidimensionality: Principal Component Analysis (PCA), Chronbach's α and Dillon-Goldstein's ρ.

Principal Component Analysis (PCA)

With this technique, a block can be considered unidimensional if the first eigenvalue of the correlation matrix built based on all the MVs related to the block is greater than 1 and the second one smaller than 1, or at least far enough from the first one.
Analysing the results in figure 4.4 it is possible to state that the block is unidimensional in the sense of the PCA.

Chronbach's α

This index can be used to check unidimensionality in a block of manifest variables, when they are all positively correlated. In practice, a block can be considered unidimensional when α is larger than 0.7.

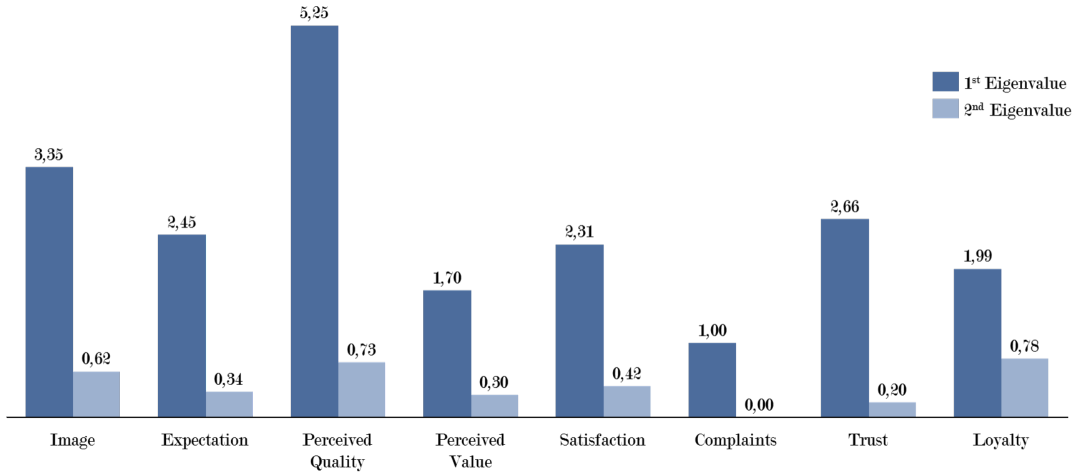


Figure 4.4: Unidimensionality Check: Principal Components

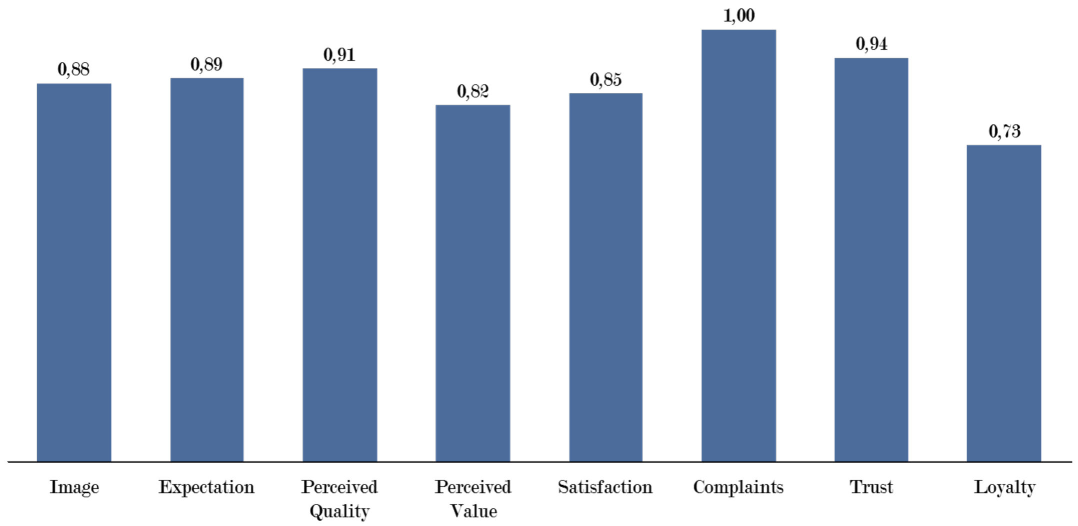


Figure 4.5: Unidimensionality Check: Chronbach's α

Analysing the results from figure 4.5 and crossing it with the Chronbach's α reference levels in table 1.1 it is possible to conclude that the blocks are unidimensional. The only block that presents a lower but acceptable α is Loyalty.

Dillon-Goldstein's ρ

For this index, by construction, the correlation signs between manifest variables and the latent variable have to be positive (i.e., all loadings are positive). A block can be defined unidimensional when all loadings are large. A block can be considered unidimensional when $\hat{\rho}$ is larger than 0.7. As mentioned in chapter 1, this statistics is considered to be the best option to check unidimensionality for a block of manifest variables (Chin, 1998a).

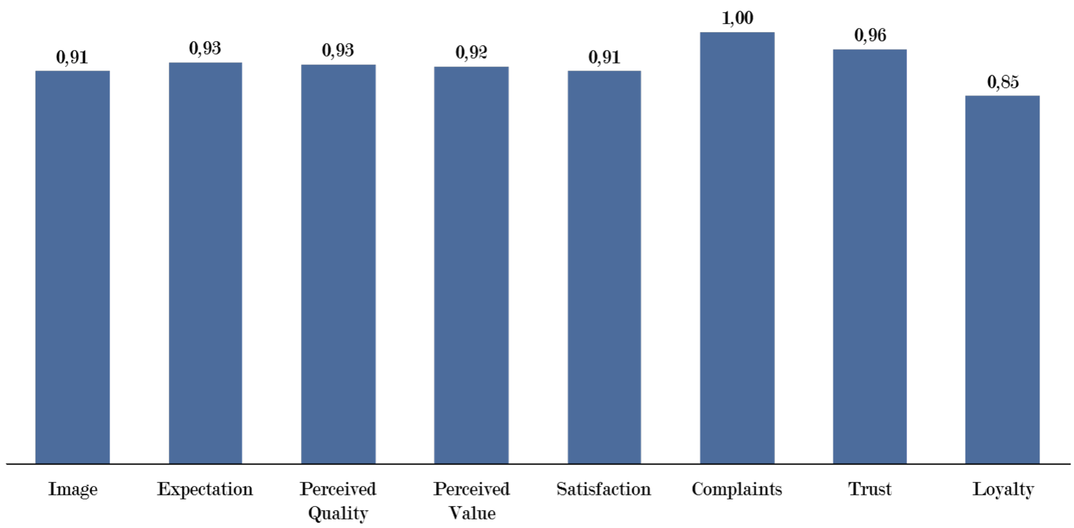


Figure 4.6: Unidimensionality Check: Dillon-Goldstein's ρ

Analysing the results related to Dillon-Goldstein's ρ is clear that all blocks can be considered as unidimensional.

The aforementioned analysis concludes that the manifest variables' blocks are unidimensional; the only change that could be applied is associated to the Loyalty block where the MV Loyalty 2 (Price sensitivity) could

be dropped in order to increase the block's unidimensionality.
After carefully analysing the variables and given the importance of price sensitivity for retention matters, it has been decided to keep all the initial manifest variables.

4.4.1 Outer Model Summary and Global Metrics

The outer model can be analysed through loadings and communalities. Another interesting measure commonly used in these studies is the redundancy.
A loading represents the strength of a relation between an observed variable and its component. The communality index measures the component's capability to explain the variance of its manifest variables. The redundancy represents the capability of a component belonging to an exogenous block to explain the variance of an endogenous block to which is connected. Given the fact that the calculation of the redundancy index takes into account both measurement and structural models, this measure can be used as a global metric in PLSPM applications.
The results presented in table 4.2 are useful to understand each manifest variable's contribution to the construction of the composite. As seen for the unidimensionality checks, the manifest variable Loyalty 2 presents the lowest loading (0.60) and the blocks presenting the highest loadings are Perceived Value, Trust and Expectation.
Appendix A.6 presents the cross-loadings obtained from the estimation of this model.

Manifest Variable	Loadings	Communality	Redundancy
Image 1	0.87	0.76	
Image 2	0.68	0.47	
Image 3	0.84	0.70	
Image 4	0.87	0.75	
Image 5	0.82	0.67	
Expectation 1	0.91	0.83	0.42
Expectation 2	0.93	0.86	0.43
Expectation 3	0.88	0.77	0.39
Perceived Quality 1	0.83	0.70	0.37
Perceived Quality 2	0.61	0.37	0.20
Perceived Quality 3	0.79	0.62	0.32
Perceived Quality 4	0.82	0.68	0.36
Perceived Quality 5	0.77	0.60	0.31
Perceived Quality 6	0.71	0.50	0.26
Perceived Quality 7	0.69	0.47	0.25
Perceived Quality 8	0.85	0.71	0.38
Perceived Quality 9	0.78	0.61	0.32
Perceived Value 1	0.92	0.84	0.38
Perceived Value 2	0.93	0.86	0.38
Satisfaction 1	0.84	0.71	0.51
Satisfaction 2	0.90	0.82	0.59
Satisfaction 3	0.89	0.79	0.57
Complaints 1	1.00	1.00	0.43
Trust 1	0.95	0.90	0.61
Trust 2	0.95	0.89	0.61
Trust 3	0.93	0.86	0.59
Loyalty 1	0.91	0.82	0.54
Loyalty 2	0.60	0.36	0.23
Loyalty 3	0.90	0.81	0.53

Table 4.2: Outer Model Summary: Loadings, Communality and Redundancy

4.4.2 Inner Model Summary

Up to this point the way results are calculated by the proposed approach is no different from the standard PLSPM algorithm.

The innovation related to the proposed nonlinear approach to PLSPM impacts directly on the results obtained in the structural model and on how they are presented; this alternative approach affects the outer model only in an indirect manner when the composites calculated as part of the inner estimation process are passed to the measurement model.

When analysing the results related to the structural model the most commonly used metric is the path coefficient that allows, through a numerical value, to get an idea about the strength (or intensity) of the linear relation among two latent variables. For example, if EDP wants to define actions in order to improve customer loyalty, it will look at all the composites connected to Loyalty and select the ones that present the largest path coefficient (this can be translated as selecting the composite with the biggest impact on customer loyalty).

This work's motivation is built on top of what in section 2.1 is defined as a potential flaw: the presence of a nonlinear relation. When the existing relation between two variables is nonlinear, a single number (path coefficient) may be insufficient or even misleading when defining business actions and setting priorities.

The next paragraphs present some of the examples obtained from this application (the causal relations omitted in this chapter can be found in appendix A.7).

Perceived Value explained by Perceived Quality

This section presents the relation between Perceived Value and Perceived Quality. The algorithm selected a second order polynomial function to fit the relation between these two latent variables.

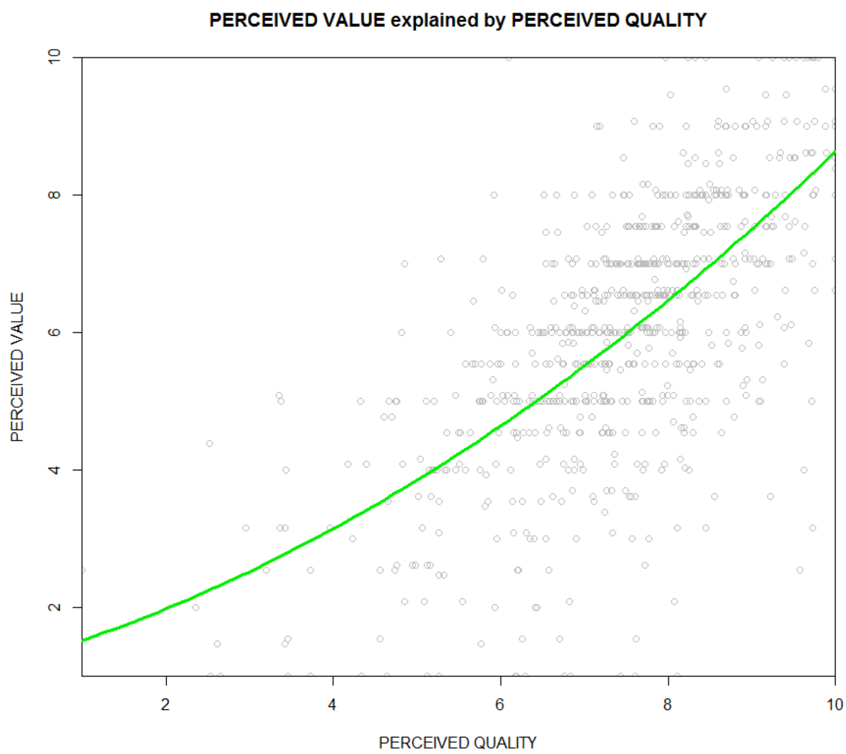


Figure 4.7: Inner Model Summary: Perceived Value explained by Perceived Quality

Figure 4.7 shows that there is no linear relationship between perceived Quality and Value dimensions. From positive evaluations in perceived Quality (≥ 6 on a scale of 1 to 10), the ratio is approximately 1.2 points (e.g., to a perceived Quality equal to 8 corresponds a perceived Value of 6.5), so EDP can bet on more targeted communications in order to optimise resources and obtain a more immediate potential. Some initiatives are proposed in this direction are:

– Take an active role in supporting energy savings, especially by advising contracted power and sending alerts when consumption approaches the predefined maximum value;

– Develop new tools and facilitate the use of consumer simulators (adjust contracted voltage level, tariffs, potential services adjusted to customer needs);

– Monitor the impact of energy efficiency measures through effective savings communication potentially reflected on the customer invoice.

Perceived Value explained by Expectation

This section presents the relation between Perceived Value and Expectation. The algorithm selected a second order polynomial function to fit the relation between these two latent variables.

Figure 4.8 presents high expectations compared to lower perceived value. Managing and meeting customer expectations can be challenging since they are not just related to price. In order to better handle customer expectations, EDP could present more information to the consumer, namely consumption curve and the possibility to compare the household consumption to households with similar characteristics.

Campaigns and promotions might be interesting drivers to improve the perceived value. EDP could better clarify the commercial offering, as well as information on the composition of the energy price. Some initiatives,

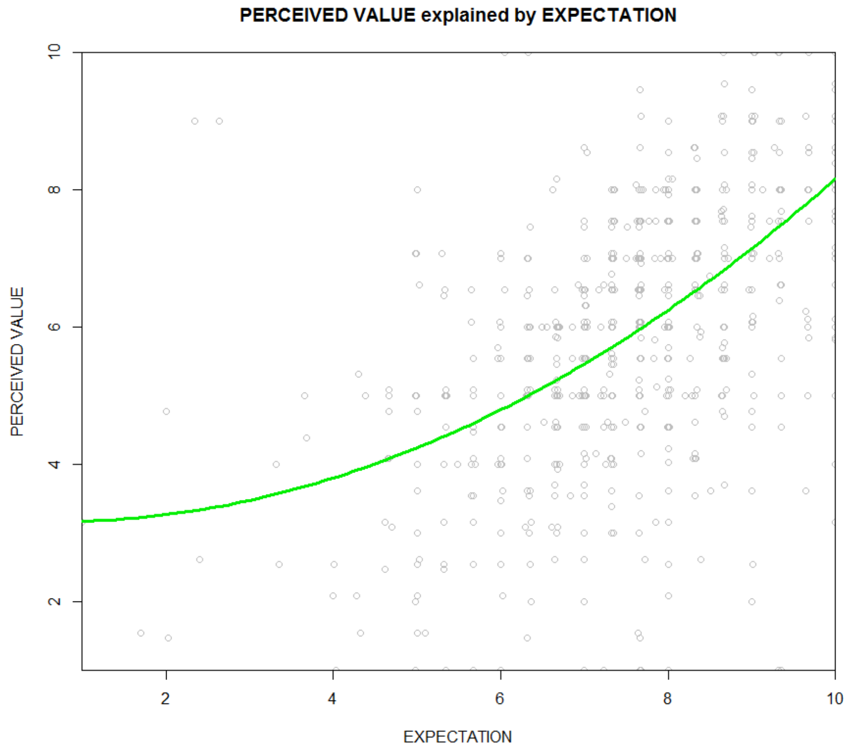


Figure 4.8: Inner Model Summary: Perceived Value explained by Expectation

such as launching a new invoice layout can have a strong impact on improving value perception.

Perceived Quality explained by Expectation

This section presents the relation between Perceived Quality and Expectation. The algorithm selected a second order polynomial function to fit the relation between these two latent variables.

Figure 4.7 shows a need to improve the expectations or guarantee delivery of high quality service. This could be achieved through a letter of commitments (e.g., resolution of problems in x hours, tracking customer

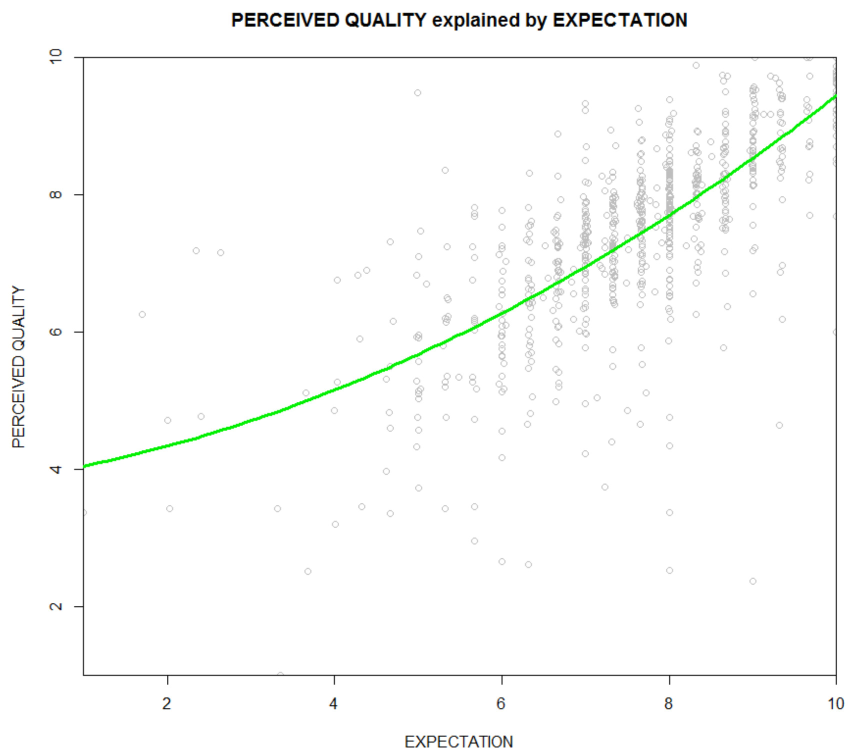


Figure 4.9: Inner Model Summary: Perceived Quality explained by Expectation

processes, inform about technical support team expected arrival time or other information useful to the customer).

EDP should also proactively offer customised solutions and facilitate contact with the company, namely through greater personalisation in the contact team (i.e., record of customer contacts history). Additionally, the relationship with the client can be improved by providing a high-quality customer management service (complaints, questions, etc.) through online channels.

Satisfaction explained by Expectation

This section presents the relation between Satisfaction and Expectation. The algorithm selected a second order polynomial function to fit the relation between these two latent variables.

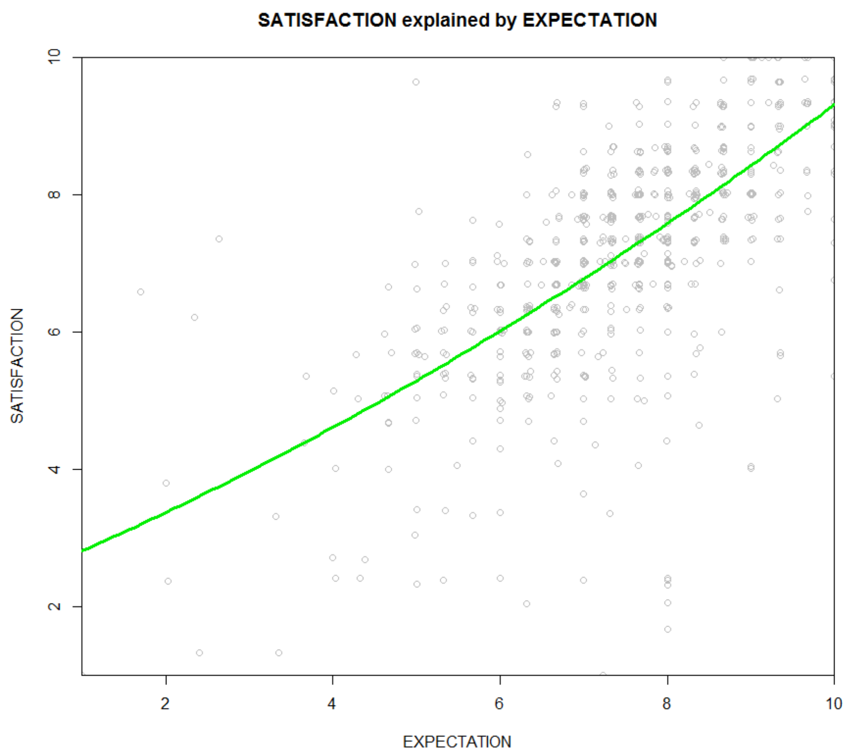


Figure 4.10: Inner Model Summary: Satisfaction explained by Expectation

Figure 4.10 presents an almost linear relation between the two composites. It is possible to conclude that Expectations are always above Satisfaction level.

Managing customer expectations can be challenging because of different factors. One of those factors is driven by the customer perception about EDP; they consider EDP an innovative and forward-looking organisation,

and as a consequence they expect a customised customer approach. In fact, customers are changing and they expect a lot from EDP mostly when it comes to information that the "new" customer wants to see.
From the data perspective, EDP needs to take advantage of the internal customer information and start sharing it with them in a collaborative, digital and useful manner.
Another important point is related to omni-channel management. EDP needs to ensure active listening and bet on responses homogenisation (i.e., ensuring the same answer independently from the channel used by the customer).
Expectations have to be met through a strong commitment made with the customers and making sure they play an active role in their relation with EDP.

Loyalty explained by Trust

This section presents the relation between Loyalty and Trust. The algorithm selected a second order polynomial function to fit the relation between these two latent variables.
Trust is a very present attribute in EDP's brand and it is partially "inherited" from the strong presence of EDP in the regulated market. In order to maintain and reinforce customer Trust, the company should bet on loyalty programs that could promote positive word of mouth among brand promoters.
Many companies drive internal activities focussed on empowering employees in order to become brand ambassadors.

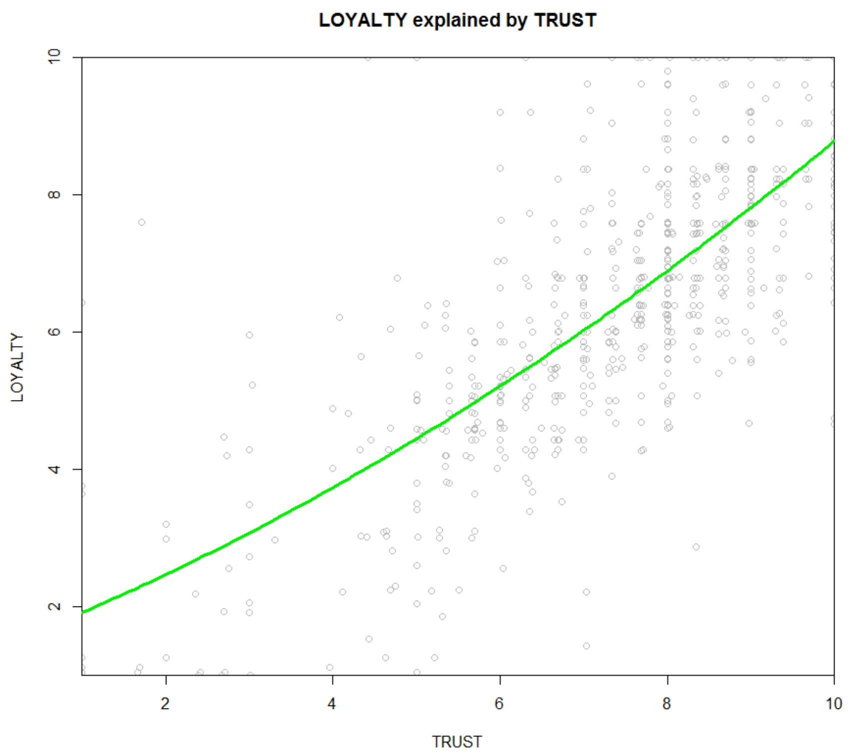


Figure 4.11: Inner Model Summary: Loyalty explained by Trust

4.4.3 Main Business Findings and Conclusions

The application detailed in this chapter represents a different approach to a common business issue. In fact, as previously mentioned, one of EDP's objectives is to get a better understanding on a set of latent variables (i.e., Satisfaction, Loyalty, Trust, etc.) and on the influential factors driving their changes (i.e., Image, Perceived Quality, Perceived Value, Complaints, etc.).

In order to get the most from the data retrieved and analysed by the ECSI Portugal project, it has been decided to use the proposed alternative composite based approach: Nonlinear PLSPM.

The results obtained are very promising and the causal relation defined in the theoretical model are free from the linearity assumption present in the original PLSPM algorithm.

When graphically presenting a nonlinear relation between two composites it is possible to define strategies for specific needs identified by the Nonlinear PLSPM (i.e., the relation between perceived quality and value presented two linear sub-behaviour: (i) one with a 1 to 1 relation between the two composites; and (ii) another with a 1 to approximately 1.2 ratio).

This application set the basis for new interpretation of the relation between composites based on the natural patterns present in the data.

Conclusions and Future Perspectives

Most real life statistical problems
have one or more nonstandard features.
There are no routine statistical question;
only questionable statistical routines.
David R. Cox

The PLSPM algorithm is characterised by a system of interdependent equations based on simple and multiple linear regressions. The algorithm estimates the dependence relationships among latent variables (inner or structural model) as well as the relationships between manifest variables and their own latent variable (outer or measurement model). All the relations present in both inner and outer models are estimated under the assumption of linearity.

This thesis proposes a flexible nonlinear alternative to the PLSPM algorithm which tackles two of the issues discussed in chapter 1 by: (i) breaking the linearity assumptions present in the inner model estimation phase; and (ii) accommodating path direction within the inner model estimation phase through a novel non-symmetrical approach for inner weights estimation.

This approach can be seen, when it comes to the inner model, as a data-driven estimation approach. In fact, the algorithm adapts to the form assumed by the inner relationships among composites by means of a piecewise estimation method. Its flexibility allows using different inner weights estimation methods taking advantage of the piecewise algorithm's architecture.

As detailed and motivated along this work, another added value is represented by the possibility of defining a non-symmetrical weighting system in the inner model estimation phase. This systems has been designed to accommodate a coherent path direction modelling among composites.

The results obtained in the simulation analysis show that, from an empirical perspective, the proposed approach is stable, becoming more consistent when the sample size is greater than or equal to 100 observations. The application to the energy supply market at EDP proved that the proposed approach adds value when it comes to analyse relations among composites.

The results obtained are very promising, and by using the Nonlinear PLSPM approach the causal relation defined in the theoretical model are free from the linearity assumption present in the original PLSPM algorithm.

Another advantage of this approach concerns its output; in fact, the

nonlinear polynomial function that relates two composites allows the definition of a more precise business strategy.
This application sets the basis for a more suitable interpretation of the relation between composites, based on the natural patterns present in the data.

Future Developments Even if the results are promising, there are several reflections that may lead to future developments and fine-tuning of the proposed algorithm.
The main improvement points identified are:

- **Comprehensive Business Framework**: to build a comprehensive business framework aiming at defining a customised business strategy. This framework should be able to combine results based on the following features: (i) prioritisation of business actions by measuring the impact of each exogenous variable on a connected endogenous variable by means of a multivariate nonlinear model; and (ii) understand company's maturity at a latent dimension level by identifying the company's position (in the sense of average dimension level) in the nonlinear curve, in order to anticipate the expected response in the endogenous dimension. This feature would allow to customise business actions based on the company's current situation.

- **Winsorisation-based Nonlinear Estimation**: to introduce a winsorisation (Dixon, 1960; Hastings Jr et al., 1947; Tukey, 1962) phase before fitting the polynomial function. This stage would estimate several polynomial functions by limiting extreme values in the input data in order to reduce the effect of possibly spurious outliers. This technique is named after the engineer turned biostatistician Charles P. Winsor (1895–1951). The analysed relations can be heavily influenced by outliers. A typical strategy is to set all outliers to a specified percentile of the data; for example, a 90% winsorisation would see all data below the 5-th percentile set to the 5-th percentile, and data above the 95-th percentile set to the 95-th percentile. Winsorised estimators are usually more robust to outliers than their more standard forms, although there are alternatives, such as trimming, that lead to a similar effect.

- **Nonlinear Measurement Model**: to apply the piecewise weighting estimation methodology to the measurement model.

- **Graphical Results**: to improve graphical outputs with the aim of supporting analysis and evaluation of the model's results. All the developed outputs should be focussed on improving the model's applicability to concrete business challenges.

- **Nonlinear PLSPM GUI**: to build a graphical user interface for the proposed Nonlinear PLPSM.

- **Analysis of Convergence**: in this topic, the main objective is to study the few non-convergence cases obtained when the sample size is equal to 50 observations. The instability example presented in chapter 3 represents a good starting point for further developments.

- **Misspecification Analysis**: another important topic that requires further simulation analysis is related to model misspecification. In more detail, the main objective would be to analyse how the model behaves when it is specified differently from the theoretical model.

Bibliography

Al-Nasser, Amjad D. Customer Satisfaction Measurement Models: Generalised Maximum Entropy Approach. *Pakistan Journal of Statistics*, 19(2):213–226, 2003.

Anderson, Eugene W. and Mittal, Vikas. Strengthening the Satisfaction-Profit Chain. *Journal of Service Research*, (July):22–25, 2000. ISSN 1094-6705. doi: 10.1177/109467050032001.

Anderson, Eugene W., Fornell, Claes, and Lehmann, Donald R. Customer satisfaction, market share, proftability - Findings from Sweden, 1994. ISSN 0022-2429.

Armstrong, J. Scott. Illusions in regression analysis. *International Journal of Forecasting*, 28(3):689–694, 2012. ISSN 01692070. doi: 10.1016/j.ijforecast.2012.02.001.

Astrachan, Claudia Binz, Patel, Vijay K., and Wanzenried, Gabrielle. A comparative study of CB-SEM and PLS-SEM for theory development in family firm research. *Journal of Family Business Strategy*, 5(1): 116–128, 2014. ISSN 18778585. doi: 10.1016/j.jfbs.2013.12.002. URL http://dx.doi.org/10.1016/j.jfbs.2013.12.002.

Baffi, G., Martin, E. B., and Morris, A. J. Non-linear projection to latent structures revisited: The quadratic PLS algorithm. *Computers and Chemical Engineering*, 23(3):395–411, 1999. ISSN 00981354. doi: 10.1016/S0098-1354(98)00283-X.

Baffi, G., Martin, E. B., and Morris, A. J. Non-linear dynamic projection to latent structures modelling. *Chemometrics and Intelligent Laboratory Systems*, 52(1):5–22, 2000. ISSN 01697439. doi: 10.1016/S0169-7439(00)00083-6.

Bagozzi, Richard P and Yi, Youjae. Advanced topics in structural equation models. *Advanced methods of marketing research*, 151, 1994.

Barclay, Donald, Higgins, Christopher, and Thompson, Ronald. The partial least squares (PLS) approach to causal modeling: Personal computer adoption and use as an illustration. *Technology studies*, 2 (2):285–309, 1995.

Bass, Bernard M., Avolio, Bruce J., Jung, Dong I., and Berson, Yair. Predicting unit performance by assessing transformational and transactional leadership. *The Journal of applied psychology*, 88(2):207–218, 2003. ISSN 0021-9010. doi: 10.1037/0021-9010.88.2.207.

Bayol, Marie-Paule, de la Foye, Anne, Tellier, Carole, and Tenenhaus, Michel. Use of PLS Path Modelling to estimate the European Consumer Satisfaction Index (ECSI) model. *Statistica Applicata*, 12(3): 361–375, 2000.

Becker, Jan-Michael, Rai, Arun, and Rigdon, Edward E. Predictive Validity and Formative Measurement in Structural Equation Modeling: Embracing Practical Relevance. *Thirty Fourth International Conference on Information Systems*, (January 2016):1–19, 2013. ISSN 02767783. doi: 10.1146/annurev.clinpsy.1.102803.144239. URL http://aisel.aisnet.org/cgi/viewcontent.cgi?article=2876{&}amp{%}5Cncontext=misq.

Bentler, Peter M. and Huang, Wenjing. On Components, Latent Variables, PLS and Simple Methods: Reactions to Rigdon's Rethinking of PLS. *Long Range Planning*, 47(3):138–145, 2014. ISSN 00246301. doi: 10.1016/j.lrp.2014.02.005. URL http://dx.doi.org/10.1016/j.lrp.2014.02.005.

Bentler, Peter M. and Wu, Eric J. C. EQS 6.1 for Windows User's Guide. (818):1–26, 1995.

Bollen, Kenneth A. Structural Equation Models That are Nonlinear in Latent Variables: A Least-Squares Estimator. *Sociological Methodology*, 25:223–251, 1995.

Bollen, Kenneth A. and Paxton, Pamela. Interactions of latent variables in structural equation models. *Structural Equation Modeling*, 5(3):267–293, 1998. ISSN 1070-5511. doi: 10.1080/10705519809540105. URL http://www.tandfonline.com/doi/full/10.1080/10705519809540105.

Bookstein, Fred L. Data analysis by partial least squares. *Evaluation of econometric models*, I:75–90, 1980. URL http://www.nber.org/chapters/c11694.pdf{%}5Cnpapers3://publication/uuid/87DB037B-0B82-436E-A691-9D3004554576.

Bookstein, Fred L. The geometric meaning of soft modeling, with some generalizations. *System under indirect observation*, 2:55–74, 1982.

Cataldo, Rosanna. *Developments in PLS-PM for the building of a System of Composite Indicators*. PhD thesis, 2016.

Chin, Wynne W. The Partial Least Squares Approach to Structural Equation Modeling. In Marcoulides, George A, editor, *Modern methods for business research*, volume 295, pages 295–336. 1998a.

Chin, Wynne W. *PLS - Graph User's Guide*. 1998b.

Chin, Wynne W. Commentary: Issues and Opinion on Structural Equation Modeling. *MIS Quarterly*, 22(1):1, 1998c. ISSN 02767783. doi: Editorial.

Chin, Wynne W. Bootstrap cross-validation indices for PLS path model assessment. In *Handbook of partial least squares*, pages 83–97. Springer, 2010.

Chin, Wynne W. and Newsted, Peter R. Structural Equation Modeling Analysis with Small Samples Using Partial Least Square. In Hoyle, Rick, editor, *Statistical Strategies for small sample research*, chapter 12. 1999.

Chin, Wynne W., Marcolin, Barbara L., and Newsted, Peter R. A Partial Least Squares Latent Variable Modeling Approach for Measuring Interaction Effects: Results from a Monte Carlo Simulation Study and an Electronic-Mail Emotion/ Adoption Study. *Informa-*

tion Systems Research, 14(2):189–217, 2003. ISSN 10477047. doi: 10.1287/isre.14.2.189.16018.

Cobb, Charles W. and Douglas, Paul H. A Theory of Production. *The American Economic Review*, 18(1):139–165, 1928. URL http://www.jstor.org/stable/1811556.

Cohen, Jacob. *Statistical Power Analysis for the Behavioral Sciences*. 1988.

Coolen, H.C., Van Rijckevorsel, J., and de Leeuw, Jan. An algorithm for nonlinear principal components analysis with B-splines by means of alternating least squares. *H. Caussinus and P. Ettinger amd JR Mathieu, editors, COMSTAT*, 2, 1982.

Cortina, José M. What is coefficient alpha? An examination of theory and applications. *Journal of Applied Psychology*, 78(1):98–104, 1993. ISSN 0021-9010. doi: 10.1037/0021-9010.78.1.98.

Crainer, Stuart and Dearlove, Des. *Financial Times: Handbook of Management*. Pearson Education, 2004.

Dana, Jason and Dawes, Robyn M. The Superiority of Simple Alternatives to Regression for Social Science Predictions. *Journal of Educational and Behavioral Statistics*, 29(3):317–331, 2004. ISSN 1076-9986. doi: 10.3102/10769986029003317.

Diamantopoulos, Adamantios and Winklhofer, H. M. Index construction with formative indicators: An alternative to scale development. *Jour-*

nal of Marketing Research, 38(2):269–277, 2001. ISSN 0022-2437. doi: 10.1509/jmkr.38.2.269.18845.

Dijkstra, Theo K. Some comments on maximum likelihood and partial least squares methods. *Journal of Econometrics*, 22(1):67–90, 1983.

Dijkstra, Theo K. Latent variables and indicies: Herman Wold's basic design and partial least squares. In Esposito Vinzi, Vincenzo, Chin, Wynne W., Henseler, Jörg, and Wang, Huiwen, editors, *Handbook of partial least squares*, number 1993, pages 23–46. Springer Berlin Heidelberg, 2010.

Dijkstra, Theo K. PLS' Janus Face - Response to Professor Rigdon's 'Rethinking Partial Least Squares Modeling: In Praise of Simple Methods'. *Long Range Planning*, 47(3):146–153, 2014. ISSN 00246301. doi: 10.1016/j.lrp.2014.02.004. URL http://dx.doi.org/10.1016/j.lrp.2014.02.004.

Dijkstra, Theo K. and Henseler, Jörg. Consistent and asymptotically normal PLS estimators for linear structural equations. *Computational Statistics and Data Analysis*, 81:10–23, 2015. ISSN 01679473. doi: 10.1016/j.csda.2014.07.008. URL http://dx.doi.org/10.1016/j.csda.2014.07.008.

Dixon, W. J. Simplified Estimation from Censored Normal Samples. *The Annals of Mathematical Statistics*, 31:385–391, 1960. ISSN 0003-4851. doi: 10.1214/aoms/1177705900.

Dolce, Pasquale. *Component-based Path Modeling Open Issues and*

Methodological Contributions. PhD thesis, Università degli Studi di Napoli Federico II, 2015.

Dolce, Pasquale and Lauro, Carlo. Comparing maximum likelihood and PLS estimates for structural equation modeling with formative blocks. *Quality and Quantity*, 49(3):891–902, 2015. ISSN 15737845. doi: 10.1007/s11135-014-0106-8.

Draper, Norman R., Smith, Harry, Draper, Norman R., and Smith, Harry. Fitting a Straight Line by Least Squares. *Applied Regression Analysis*, pages 15–46, 2014. ISSN 1118625595. doi: 10.1002/9781118625590.ch1. URL http://doi.wiley.com/10.1002/9781118625590.ch1.

Efron, Bradley. *The Future of Statistics.* Stanford University, 2009.

Eklof, Jan A., Hackl, Peter, and Westlund, Anders. On measuring interactions between customer satisfaction and financial results. *Total Quality Management*, 10(4-5):514–522, 1999. ISSN 0954-4127. doi: 10.1080/0954412997479.

Emancipator, Kenneth and Kroll, Martin H. A quantitative measure of nonlinearity. *Clinical Chemistry*, 39(5):766–772, 1993. ISSN 00099147. doi: 10.1002/prca.201090041.

ERSE. Liberalisation. URL http://www.erse.pt/eng/electricity/Liberalization/Paginas/default.aspx.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2007). Technical report, 2007.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2008). Technical report, 2008.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2009). Technical report, 2009.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2010). Technical report, 2010.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2011). Technical report, 2011.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2012). Technical report, 2012.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2013). Technical report, 2013.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2014). Technical report, 2014. URL http://www.erse.pt/pt/electricidade/liberalizacaodosector/informacaosobreomercadoliberalizado/2014/comunicados/201412{_}ml{_}elec{_}resinf.pdf.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Dezembro 2015). Technical report, 2015.

ERSE. Resumo Informativo: Mercado Liberalizado - Eletricidade (Novembro 2016). Technical report, 2016.

Esposito Vinzi, Vincenzo. The contribution of PLS regression to PLS path modelling: formative measurement model and causality network in the structural model. In *Joint Statistical Meetings (JSM) 2008*, 2008.

Esposito Vinzi, Vincenzo. PLS path modeling and PLS regression: a joint partial least squares component-based approach to structural equation modeling. *IFCS@ GFKL–Classification as a Tool for Research (IFCS 2009)*, 2009.

Esposito Vinzi, Vincenzo and Russolillo, Giorgio. Partial least squares algorithms and methods. *Wiley Interdisciplinary Reviews: Computational Statistics*, 5(1):1–19, 2013. ISSN 19395108. doi: 10.1002/wics.1239.

Esposito Vinzi, Vincenzo, Trinchera, Laura, Squillacciotti, Silvia, and Tenenhaus, Michel. REBUS-PLS:Aresponse-based procedure for detecting unit segments in PLS path modelling. *Applied Stochastic Models in Business and Industry*, 24:439–458, 2008. doi: 10.1002/asmb.728.

Evermann, Joerg and Tate, Mary. Comparing the Predictive Ability of Pls and Covariance Models. *ICIS*, pages 1–18, 2014.

Evermann, Joerg and Tate, Mary. Assessing the predictive performance of structural equation model estimators. *Journal of Business Research*, 69(10):4565–4582, 2016. ISSN 01482963. doi: 10.1016/j.jbusres.2016.03.050. URL http://dx.doi.org/10.1016/j.jbusres.2016.03.050.

Farooq, Omer, Merunka, Dwight, and Valette-Florence, Pierre. Employees' Response to Corporate Social Responsibility: An Application of a Non Linear Mixture REBUS Approach. *Springer Proceedings in Mathematics and Statistics*, 56:257–268, 2013. ISSN 21941009. doi: 10.1007/978-1-4614-8283-3_18.

Fornell, Claes. *A second generation of multivariate analysis. 2. Measurement and evaluation*, volume 2. Praeger Publishers, 1982.

Fornell, Claes. A National Customer Satisfaction Barometer: The Swedish Experience. *Journal of Marketing*, 56(1):6–21, 1992.

Fornell, Claes and Bookstein, Fred L. Two structural equation models: LISREL and PLS applied to consumer exit-voice theory. *Journal of marketing research*, 19(4):440–452, 1982.

Fornell, Claes and Larcker, David F. Evaluating structural equation models with unobservable variables and measurement error. *Journal of marketing research*, 18(1):39–50, 1981. ISSN 0022-2437. doi: 10.2307/3151312. URL http://www.jstor.org/stable/3151312{%}5Cnhttp://www.jstor.org/stable/10.2307/3151312.

Fornell, Claes and Larcker, David F. A second generation of multivariate analysis: Classification of methods and implications for marketing research, 1987. ISSN 1098-6596.

Geisser, Seymour. The predictive sample reuse method with applications. *Journal of The American Statistical Association*, 70(350), 1975.

Gelman, Andrew and Park, David K. Splitting a Predictor at the

Upper Quarter or Third and the Lower Quarter or Third. *The American Statistician*, 63(1):1–8, 2009. ISSN 0003-1305. doi: 10.1198/tast.2009.0001. URL http://www.tandfonline.com/doi/abs/10.1198/tast.2009.0001{%}5Cnhttp://www.tandfonline.com/doi/abs/10.1198/tast.2009.0001{#}.UqIfhsRDuCQ.

Gerlach, Robert W., Kowalski, Bruce R., and Wold, Herman. Partial Least Squares Path Modelling with Latent Variables. *Analytics Chimica Acta*, 1979.

Gregor, Shirley. The nature of theory in Information Systems. *MIS Quarterly*, 30(3):611–642, 2006. ISSN 02767783. doi: 10.1080/0268396022000017725. URL http://www.scopus.com/inward/record.url?eid=2-s2.0-33846102423{&}partnerID=40{&}md5=e999cc9b09812ffe3192acf4b90d3e96.

Hahn, Carsten, Johnson, Michael D., Herrmann, Andreas, and Huber, Frank. Capturing Customer Heterogeneity Using a Finite Mixture PLS Approach. *Schmalenbach Business Review*, 54(July):243 – 269, 2002. ISSN 1556-5068. doi: 10.2139/ssrn.321004.

Hair, Joe, Hollingsworth, Carole L., Randolph, Adriane B., and Chong, Alain Yee Loong. An updated and expanded assessment of PLS-SEM in information systems research. *Industrial Management & Data Systems*, 117(3):442–458, apr 2017. ISSN 0263-5577. doi: 10.1108/IMDS-04-2016-0130. URL http://www.emeraldinsight.com/doi/pdfplus/10.1108/IMDS-02-2014-0069http://www.emeraldinsight.com/doi/10.1108/IMDS-04-2016-0130.

Hair, Joseph F., Ringle, Christian M., and Sarstedt, Marko. PLS-SEM: Indeed a Silver Bullet. *The Journal of Marketing Theory and Practice*, 19(2):139–152, 2011. ISSN 1069-6679. doi: 10.2753/MTP1069-6679190202.

Hair, Joseph F., Sarstedt, Marko, Pieper, Torsten M., and Ringle, Christian M. The Use of Partial Least Squares Structural Equation Modeling in Strategic Management Research: A Review of Past Practices and Recommendations for Future Applications. *Long Range Planning*, 45(5-6):320–340, 2012a. ISSN 00246301. doi: 10.1016/j.lrp.2012.09.008. URL http://dx.doi.org/10.1016/j.lrp.2012.09.008.

Hair, Joseph F., Sarstedt, Marko, Ringle, Christian M., and Mena, Jeannette A. An assessment of the use of partial least squares structural equation modeling in marketing research. *Journal of the Academy of Marketing Science*, 40(3):414–433, 2012b. ISSN 00920703. doi: 10.1007/s11747-011-0261-6.

Hair, Joseph F. Jr., Hult, G. Tomas M., Ringle, Christian M., and Sarstedt, Marko. *A Primer on Partial Least Squares Structural Equation Modeling (PLS-SEM)*, volume 46. Sage Publications, 2014. ISBN 9781452217444.

Hanafi, Mohamed. PLS Path modelling: Computation of latent variables with the estimation mode B. *Computational Statistics*, 22(2):275–292, 2007. ISSN 09434062. doi: 10.1007/s00180-007-0042-3.

Harrell, Frank. Problems caused by categorizing continuous variables,

2008. URL http://biostat.mc.vanderbilt.edu/twiki/bin/view/Main/CatContinuous.

Hastie, Trevor, Tibshirani, Robert, and Friedman, Jerome. *The Elements of Statistical Learning*, volume 20 of *Springer Series in Statistics*. Springer New York, New York, NY, jan 2009. ISBN 978-0-387-84857-0. doi: 10.1007/978-0-387-84858-7. URL http://www.tandfonline.com/doi/full/10.1080/01443610062940http://link.springer.com/10.1007/978-0-387-84858-7.

Hastings Jr, Cecil, Mosteller, Frederick, Tukey, John W., and Winsor, Charles P. Low moments for small samples: A comparative study of order statistics. *The Annals of Mathematical Statistics*, pages 413–426, 1947. ISSN 0003-4851. doi: 10.1214/aoms/1177730388.

Henseler, Jörg. On the convergence of the partial least squares path modeling algorithm. *Computational Statistics*, 25(1):107–120, 2010. ISSN 09434062. doi: 10.1007/s00180-009-0164-x.

Henseler, Jörg and Chin, Wynne W. A Comparison of Approaches for the Analysis of Interaction Effects Between Latent Variables Using Partial Least Squares Path Modeling. *Structural Equation Modeling: A Multidisciplinary Journal*, 17(1):82–109, 2010. ISSN 1070-5511. doi: 10.1080/10705510903439003. URL http://www.informaworld.com/openurl?genre=article{&}doi=10.1080/10705510903439003{&}magic=crossref{%}7C{%}7CD404A21C5BB053405B1A640AFFD44AE3.

Henseler, Jörg and Sarstedt, Marko. Goodness-of-fit indices for partial least squares path modeling. *Computational Statistics*, 28(2):565–580, apr 2013. ISSN 0943-4062. doi: 10.1007/s00180-012-0317-1. URL http://link.springer.com/10.1007/s00180-012-0317-1.

Henseler, Jörg, Fassott, Georg, and Dijkstra, Theo K. Analyzing Curvilinear Effects Through Partial Least Squares Path Modeling : A Simulation-based Comparison of Available Approaches. pages 1–57, 2008.

Henseler, Jörg, Ringle, Christian M., and Sinkovics, Rudolf R. *The Use of Partial Least Squares Path Modeling in International Marketing*, volume 20 of *Advances in International Marketing*. Emerald Group Publishing, 2009. ISBN 978-1-84855-468-9. doi: 10.1108/S1474-7979(2009)0000020014. URL http://search.ebscohost.com/login.aspx?direct=true{&}db=ufh{&}AN=6250585{&}site=ehost-livehttp://www.emeraldinsight.com/10.1108/S1474-7979(2009)0000020014.

Henseler, Jörg, Fassott, Georg, Dijkstra, Theo K., and Wilson, Bradley. Analysing quadratic effects of formative constructs by means of variance-based structural equation modelling. *European Journal of Information Systems*, 21(1):99–112, 2012. ISSN 0960-085X. doi: 10.1057/ejis.2011.36.

Henseler, Jörg, Dijkstra, Theo K., Sarstedt, Marko, Ringle, Christian M., Diamantopoulos, Adamantios, Straub, Detmar W., Ketchen, David J., Hair, Joseph F., Hult, G. Tomas M., and Calantone, Roger J. Common Beliefs and Reality about Partial Least Squares: Comments on

Rönkkö & Evermann (2013),. *Organizational Research Methods*, 17 (2):in print, 2014. ISSN 1094-4281. doi: 10.1177/1094428114526928.

Hotelling, Harold. Relations Between Two Sets of Variates. *Biometrika*, 28(3/4):321, dec 1936. ISSN 00063444. doi: 10.2307/2333955. URL http://www.jstor.org/stable/2333955?origin=crossref.

Hulland, John, Ryan, Michael J., and Rayner, Robert K. Modeling Customer Satisfaction: A Comparative Performance Evaluation of Covariance Structure Analysis Versus Partial Least Squares. In Esposito Vinzi, Vincenzo, Chin, Wynne W, Henseler, Jörg, and Wang, Huiwen, editors, *Handbook of Partial Least Squares: Concepts, Methods and Applications*, pages 307–325. Springer Berlin Heidelberg, Berlin, Heidelberg, 2010. ISBN 978-3-540-32827-8. doi: 10.1007/978-3-540-32827-8_15. URL http://dx.doi.org/10.1007/978-3-540-32827-8{_}15.

Hwang, Heungsun and Takane, Yoshio. Generalized structured component analysis. *Psychometrika*, 69(1):81–99, 2004. ISSN 0033-3123. doi: 10.1007/BF02295841.

Ingrassia, Salvatore and Trinchera, Laura. Some Remarks on Nonlinear Relationships. *Statistica Applicata*, 20(3-4), 2008.

Jaccard, James and Turrisi, Robert. Interaction Effects in Multiple Regression, 2003.

Jakobowicz, Emmanuel. Latent variable transformation using monotonic B-splines in PLS Path Modeling. In *IASC '07*, pages 1–7, 2007a.

Jakobowicz, Emmanuel. *Contributions aux modèles d'équations structurelles à variables latentes.* PhD thesis, Conservatoire national des arts et metiers-CNAM, 2007b.

Jakobowicz, Emmanuel and Saporta, Gilbert. A nonlinear PLS path modeling based on monotonic B-spline transformations. In *Causalities explored by indirect observations-PLSŠ07, 5th International symposium on PLS and related methods*, 2007.

Johnson, Norman L. and Kotz, Samuel. *Leading Personalities in Statistical Science.* 1998. ISBN 0471163813. doi: 10.1002/9781118150719. URL http://www.tandfonline.com/doi/pdf/10.1080/00401706.1998.10485221.

Johnston, Robert. The Determinants of Service Quality - Satisfiers and Dissatisfiers. *International Journal of Service Industry Management*, 6(5):53–71, 1995. ISSN 0956-4233. doi: 10.1108/09564239510101536. URL http://wrap.warwick.ac.uk/19244/.

Jöreskog, Karl G. A general method for analysis of covariance structure, 1970.

Jöreskog, Karl G. and Sorbom, Dag. LISREL 8: Structural equation modeling with the SIMPLIS command language, 1993.

Jöreskog, Karl G. and Yang, Fan. Nonlinear Structural Equation Models: The Kenny-Judd Model with Interaction Effects. In Marcoulides, G A and Schumacker, R E, editors, *Advanced structural equation modeling: Issues and techniques*, number 3, chapter 3, pages 57–88. 1996.

Kano, Noriaki, Seraku, Nobuhiku, Takahashi, Fumio, and Tsuji, Shinichi. Attractive quality and must-be quality. 1984.

Kenny, David A. and Judd, Charles M. Estimating the Nonlinear and Interactive Effects of Latent Variables. *Psychological Bulletin*, 96(1): 201–210, 1984. ISSN 0033-2909. doi: 10.1037/0033-2909.96.1.201.

Klein, Andreas G and Muthén, Bengt O. Quasi-Maximum Likelihood Estimation of Structural Equation Models With Multiple Interaction and Quadratic Effects. *Multivariate Behavioral Research*, 42(4):647–673, dec 2007. ISSN 0027-3171. doi: 10.1080/00273170701710205. URL http://www.tandfonline.com/doi/abs/10.1080/00273170701710205.

Krämer, Nicole. Nonlinear partial least squares path models. In *3rd World conference of the IASC, Cyprus*, volume 99, page 100, 2005.

Krämer, Nicole. *Analysis of High-Dimensional Data with Partial Least Squares and Boosting*. PhD thesis, Technischen Universität Berlin, 2007.

Kroll, Martin H. and Emancipator, Kenneth. A theoretical evaluation of linearity. *Clinical Chemistry*, 39(3):405–413, 1993. ISSN 00099147.

Kuhn, Max and Johnson, Kjell. *Applied Predictive Modeling*. 2013. ISBN 1461468485. doi: 10.1007/978-1-4614-6849-3. URL http://www.amazon.com/Applied-Predictive-Modeling-Max-Kuhn/dp/1461468485/ref=pd{_}bxgy{_}b{_}img{_}z.

Kumar, Niraj Rakesh Jaiswal Anand. Examining the Nonlinear Effects in Satisfaction-Loyalty-Behavioral Intentions Model. 2007.

Kutner, Michael H, Nachtsheim, Christopher J., Neter, John, and Li, William. *Applied Linear Statistical Models*. 2005. ISBN 9780071122214. URL http://books.google.fr/books?id=0xqCAAAACAAJ{&}dq=intitle:Applied+linear+statistical+models+djvu{&}hl={&}cd=1{&}source=gbs{_}api.

Lee, Sik-Yum, Song, Xin-Yuan, and Poon, Wai-Yin. Comparison of approaches in estimating interaction and quadratic effects of latent variables. *Multivariate Behavioral Research*, 39(1):37–67, 2004. ISSN 0027-3171. doi: 10.1207/s15327906mbr3901. URL https://shelob.ocis.temple.edu:2343/login?url=http://search.ebscohost.com/login.aspx?direct=true{&}db=aph{&}AN=13435892{&}site=ehost-live.

Lee, Sik-Yum, Song, Xin-Yuan, and Tang, Nian-Sheng. Bayesian Methods for Analyzing Structural Equation Models With Covariates, Interaction, and Quadratic Latent Variables. *Structural Equation Modeling: A Multidisciplinary Journal*, 14(3):404–434, 2007. ISSN 1070-5511. doi: 10.1080/10705510701301511. URL http://www.tandfonline.com/doi/abs/10.1080/10705510701301511.

Little, Todd D., Bovaird, James A., and Widaman, Keith F. On the Merits of Orthogonalizing Powered and Product Terms: Implications for Modeling Interactions Among Latent Variables. *Structural Equation*

Modeling: A Multidisciplinary Journal, 13(4):497–519, 2006. ISSN 1070-5511. doi: 10.1207/s15328007sem1304_1.

Lohmöller, Jan-Bernd. *LVPLS 1.6 program manual: latent variables path analysis with partial least-squares estimation; mit 2 Disketten Version 1.8*. Zentralarchiv für empirische Sozialforschung, 1984.

Lohmöller, Jan-Bernd. *Latent Variable Path Modeling with Partial Least Squares*, volume 1. Springer-Verlag Berlin Heidelberg, Heidelberg, 1989. ISBN 978-3-642-52514-8. doi: 10.1007/978-3-642-52512-4. URL http://link.springer.com/10.1007/978-3-642-52512-4.

Marcoulides, George A. and Saunders, Carol. Editor's comments: PLS: a silver bullet? *MIS Quarterly*, 30(2):iii–ix, 2006. ISSN 0276-7783. doi: 10.2307.25148727. URL citeulike-article-id:10723370{%}5Cnhttp://portal.acm.org/citation.cfm?id=2017308.

Marcoulides, George A., Chin, Wynne W., and Saunders, Carol. A critical look at partial least squares modeling. *MIS Quarterly*, 33(1):171–175, 2009. ISSN 0276-7783. doi: Article.

Martínez-Ruiz, Alba and Aluja-Banet, Tomas. Two-step PLS path modeling MODE B: Nonlinear and interaction effects between formative constructs. *Springer Proceedings in Mathematics and Statistics*, 56: 187–199, 2013. ISSN 21941009. doi: 10.1007/978-1-4614-8283-3_12.

Mateos-Aparacio, Gregoria. Partial least squares (PLS) methods: Origins, evolution, and application to social sciences. *Communications* *in Statistics-Theory and Methods*, 40(13):1–18, 2011. ISSN 0361-0926. doi: 10.1080/03610921003778225.

Matzler, Kurt, Hinterhuber, Hans H., Bailom, Franz, and Sauerwein, Elmar. How to delight your customers. *Journal of Product & Brand Management*, 5(2):6–18, 1996. ISSN 1061-0421. doi: 10.1108/10610429610119469. URL http://www.emeraldinsight.com/doi/abs/10.1108/10610429610119469.

Matzler, Kurt, Bailom, Franz, Hinterhuber, Hans H., Renzl, Birgit, and Pichler, Johann. The Asymmetric Relationship Between Attribute-Level Performance and Overall Customer Satisfaction: A Reconsideration of the Importance-Performance Analysis. *Industrial Marketing Management*, 33(4):271–277, 2004. ISSN 00198501. doi: 10.1016/S0019-8501(03)00055-5.

Mittal, Vikas, Ross, William T., and Baldasare, Patrick M. The Asymmetric Impact of Negative and Positive Attribute-Level Performance on Overall Satisfaction and Repurchase Intentions. *Journal of Marketing*, 62(1):33–47, 1998.

Mooijaart, Ab and Bentler, Peter M. An Alternative Approach for Nonlinear Latent Variable Models. *Structural Equation Modeling*, 17(3): 357–373, 2010. ISSN 1070-5511. doi: 10.1080/10705511.2010.488997.

Moosbrugger, Helfried, Schermelleh-engel, Karin, Kelava, Augustin, and Klein, Andreas G. Testing Multiple Nonlinear Effects In Structural Equation Modeling: A Comparison of Alternative Estimation. *Struc-*

tural Equation Modeling in Educational Research: Concepts and Applications, pages 103–136, 2006.

Noonan, Richard and Wold, Herman. NIPALS Path Modelling with Latent Variables, 1977. ISSN 0031-3831.

Paulssen, Marcel and Sommerfeld, Angela. Modeling the Nonlinear Relationship Between Satisfaction and Loyalty with Structural Equation Models. In Spiliopoulou, Myra, Kruse, Rudolf, Borgelt, Christian, Nürnberger, Andreas, and Gaul, Wolfgang, editors, *Data and Information Analysis to Knowledge Engineering: Proceedings of the 29th Annual Conference of the Gesellschaft f{ü}r Klassifikation e.V. University of Magdeburg, March 9–11, 2005*, pages 574–581. Springer Berlin Heidelberg, Berlin, Heidelberg, 2006. ISBN 978-3-540-31314-4. doi: 10.1007/3-540-31314-1_70. URL http://dx.doi.org/10.1007/3-540-31314-1{_}70.

Paxton, Pamela, Curran, Patrick J., Bollen, Kenneth a., Kirby, Jim, and Chen, Feinian. Monte Carlo Experiments: Design and Implementation. *Structural Equation Modeling: A Multidisciplinary Journal*, 8(2): 287–312, 2001. ISSN 1070-5511. doi: 10.1207/S15328007SEM0802_7.

Pedhazur, Elazar J. *Multiple Regression in Behavioral Research*, volume 3. 1997. ISBN 9780030728310. doi: 10.2307/2285468.

Ping Jr., Robert A. Latent Variable Interaction and Quadratic Effect Estimation: A Two-Step Technique Using Structural Equation Analysis. *Psychological Bulletin*, 119(1):166–175, 1996.

Rigdon, Edward E. Rethinking Partial Least Squares Path Modeling: In Praise of Simple Methods. *Long Range Planning*, 45(5-6):341–358, 2012. ISSN 00246301. doi: 10.1016/j.lrp.2012.09.010. URL http://dx.doi.org/10.1016/j.lrp.2012.09.010.

Rigdon, Edward E. Rethinking Partial Least Squares Path Modeling: Breaking Chains and Forging Ahead. *Long Range Planning*, 47(3): 161–167, 2014. ISSN 00246301. doi: 10.1016/j.lrp.2014.02.003. URL http://dx.doi.org/10.1016/j.lrp.2014.02.003.

Rigdon, Edward E. Choosing PLS path modeling as analytical method in European management research: A realist perspective. *European Management Journal*, 34(6):598–605, 2016. ISSN 02632373. doi: 10.1016/j.emj.2016.05.006. URL http://dx.doi.org/10.1016/j.emj.2016.05.006.

Ringle, Christian M., Wende, Sven, and Will, Alexander. Customer segmentation with FIMIX-PLS. In *Proceedings of PLS-05 International Symposium, SPAD Test&go, Paris*, pages 507–514, 2005a.

Ringle, Christian M., Wende, Sven, and Will, Alexander. Smart-PLS Version 2.0 M3. *University of Hamburg*, 2005b.

Ringle, Christian M., Sarstedt, Marko, and Mooi, Erik A. Response-Based Segmentation Using Finite Mixture Partial Least Squares. In *International Journal of Research in Marketing*, volume 14, pages 19–49. 2010a. ISBN 9781441912794. doi: 10.1007/978-1-4419-1280-0_2. URL http://www.springerlink.com/

index/10.1007/978-1-4419-1280-0http://link.springer.com/10.1007/978-1-4419-1280-0{_}2.

Ringle, Christian M., Will, Alexander, and Wende, Sven. The Finite Mixture Partial Least Squares Approach: Methodology and Application. *Handbook of Partial Least Squares*, pages 195–218, 2010b.

Ringle, Christian M., Sarstedt, Marko, and Straub, Detmar W. A critical look at the use of PLS-SEM in MIS Quarterly. *MIS Quarterly*, 36(1), 2012.

Ronkko, Mikko and Evermann, Joerg. A critical examination of common beliefs about partial least squares path modeling. *Organizational Research Methods*, 16(3):425–448, 2013. ISSN 1094-4281. doi: 10.1177/1094428112474693.

Rönkkö, Mikko, McIntosh, Cameron N., Antonakis, John, and Edwards, Jeffrey R. Partial least squares path modeling: Time for some serious second thoughts. *Journal of Operations Management*, jun 2016. ISSN 02726963. doi: 10.1016/j.jom.2016.05.002. URL http://dx.doi.org/10.1016/j.jom.2016.05.002http://linkinghub.elsevier.com/retrieve/pii/S0272696316300237.

Rosipal, Roman. Nonlinear partial least squares: An overview. *Chemoinformatics and Advanced Machine Learning Perspectives: Complex Computational Methods and Collaborative Techniques*, pages 169–189, 2011. doi: 10.4018/978-1-61520-911-8.ch009. URL http://aiolos.um.savba.sk/{~}roman/Papers/

npls{_}book11.pdf{%}5Cnpapers2://publication/uuid/55966E8F-2346-4326-B57E-3A1F47835189.

Rosipal, Roman and Trejo, Leonard J. Kernel partial least squares regression in Reproducing Kernel Hilbert Space. *Journal of Machine Learning Research*, 2(2):97–123, 2002. ISSN 1532-4435. doi: 10.1162/15324430260185556.

Royston, Patrick, Altman, Douglas G., and Sauerbrei, Willi. Dichotomizing continuous predictors in multiple regression: A bad idea. *Statistics in Medicine*, 25(1):127–141, 2006. ISSN 02776715. doi: 10.1002/sim.2331.

Sánchez, Gastón. PLS Path Modeling with R. *R Package Notes*, page 235, 2013. ISSN 01679473. doi: citeulike-article-id:13341888. URL http://gastonsanchez.com/PLS{_}Path{_}Modeling{_}with{_}R.pdf.

Sánchez, Gastón and Aluja-Banet, Tomas. PATHMOX: A PLS-PM Segmentation Algorithm. *Proceedings of the IASC Symposium on Knowledge Extraction by Modelling (KNEMO 2006)*, 2006. URL http://www.stat.unipg.it/iasc/Proceedings/2006/COMPSTAT{_}Satellites/KNEMO/Lavori/PapersCD/SanchezAluja.pdf.

Sarstedt, Marko, Ringle, Christian M., Henseler, Jörg, and Hair, Joseph F. On the Emancipation of PLS-SEM: A Commentary on Rigdon (2012). *Long Range Planning*, 47(3):154–160, 2014. ISSN

00246301. doi: 10.1016/j.lrp.2014.02.007. URL http://dx.doi.org/10.1016/j.lrp.2014.02.007.

Sarstedt, Marko, Hair, Joseph F., Ringle, Christian M., Thiele, Kai O., and Gudergan, Siegfried P. Estimation issues with PLS and CBSEM: Where the bias lies! *Journal of Business Research*, 69(10):3998–4010, 2016. ISSN 01482963. doi: 10.1016/j.jbusres.2016.06.007. URL http://dx.doi.org/10.1016/j.jbusres.2016.06.007.

Schwarz, Gideon. Estimating the dimension of a model. *The Annals of Statistics*, 6(2):461–464, 1978. ISSN 0090-5364. doi: 10.1214/aos/1176344136. URL http://projecteuclid.org/euclid.aos/1176344136.

Sharma, Pratyush Nidhi, Sarstedt, Marko, Shmueli, Galit, and Kim, Kevin H. Predictive model selection in partial least squares path modeling (PLS-PM). In *Proceedings of the 2nd International Symposium on Partial Least Squares Path Modeling - The Conference for PLS Users*, volume 18, pages 1–50. University of Twente, jun 2015. ISBN 9789036540568. doi: 10.3990/2.336. URL http://dx.doi.org/10.1016/j.jclepro.2009.10.014{%}5Cnhttp://dx.doi.org/10.1016/j.autcon.2012.04.015{%}5Cnhttp://scholar.google.com/scholar?hl=en{&}btnG=Search{&}q=intitle:The+Cross+Section+of+Common+Stock+Returns:+A+Review+of+the+Evidence+and+Some+New+Findings{#}0{%}25.

Shmueli, Galit and Koppius, Otto R. What is Predictive about Partial

Least Squares? *Sixth Symposium on Statistical Challenges in eCommerce Research (SCECR)*, 2010.

Shmueli, Galit and Koppius, Otto R. Predictive analytics in information systems research. *MIS Quarterly*, 35(3):553–572, 2011. ISSN 0276-7783.

Shmueli, Galit, Ray, Soumya, Velasquez Estrada, Juan Manuel, and Chatla, Suneel Babu. The elephant in the room: Predictive performance of PLS models. *Journal of Business Research*, 69(10): 4552–4564, oct 2016. ISSN 01482963. doi: 10.1016/j.jbusres.2016.03.049. URL http://linkinghub.elsevier.com/retrieve/pii/S0148296316301217.

Stone, Mervyn. Cross-Validatory Choice and Assessment of Statistical Predictions. *American Sociological Review*, 40(1):37–47, 1974. ISSN 00359246. doi: 10.2307/2984809.

Tenenhaus, Arthur and Tenenhaus, Michel. Regularized Generalized Canonical Correlation Analysis. *Psychometrika*, 76(2):257–284, apr 2011. ISSN 0033-3123. doi: 10.1007/s11336-011-9206-8. URL http://link.springer.com/10.1007/s11336-011-9206-8.

Tenenhaus, Michel. *La Régression PLS: Théorie et Pratique*. Editions Technip, 1998.

Tenenhaus, Michel and Hanafi, Mohamed. A bridge between PLS Path Modeling and Multi-Block data analysis. In Esposito Vinzi, Vincenzo, Chin, Wynne W., Henseler, Jörg, and Wang, Huiwen, editors, *Handbook of partial least squares*, pages 99–123. Springer Berlin Heidelberg,

2010. ISBN 978-3-540-32825-4. doi: 10.1007/978-3-540-32827-8. URL http://link.springer.com/10.1007/978-3-540-32827-8.

Tenenhaus, Michel, Amato, Silvano, and Esposito Vinzi, Vincenzo. A global goodness-of-fit index for PLS structural equation modelling. *The XLII SIS Scientific Meeting*, pages 739–742, 2004.

Tenenhaus, Michel, Esposito Vinzi, Vincenzo, Chatelin, Yves Marie, and Lauro, Carlo. PLS path modeling. *Computational Statistics and Data Analysis*, 48(1):159–205, 2005. ISSN 01679473. doi: 10.1016/j.csda.2004.03.005.

Trinchera, Laura. *Unobserved Heterogeneity in Structural Equation Models: A New Approach to Latent Class Detection in PLS Path Modeling*. PhD thesis, Università degli Studi di Napoli Federico II, 2008.

Tukey, John W. The Future of Data Analysis. *The Annals of Mathematical Statistics*, 33(1):1–67, 1962. URL www.jstor.org/stable/2237638.

Tuu, Ho Huy and Olsen, Svein Ottar. Nonlinear effects between satisfaction and loyalty: An empirical study of different conceptual relationships. *Journal of Targeting, Measurement and Analysis for Marketing*, 18(3):239–251, 2010. ISSN 1479-1862. doi: 10.1057/jt.2010.19. URL http://dx.doi.org/10.1057/jt.2010.19.

Vale, C. David and Maurelli, Vincent A. Simulating multivariate nonnormal distributions. *Psychometrika*, 48(3):465–471, 1983. ISSN 00333123. doi: 10.1007/BF02293687.

Vilares, Manuel J. and Coelho, Pedro S. Likelihood and PLS Estimators for Structural Equation Modeling: An Assessment of Sample Size, Skewness and Model Misspecification Effects. In *Advances in Regression, Survival Analysis, Extreme Values, Markov Processes and Other Statistical Applications*, pages 11–33. Springer Berlin Heidelberg, Berlin, Heidelberg, 2013. ISBN 9783642349034. doi: 10.1007/978-3-642-34904-1_2. URL http://link.springer.com/10.1007/978-3-642-34904-1{_}2.

Vilares, Manuel J., Almeida, Maria H., and Coelho, Pedro S. Comparison of Likelihood and PLS Estimators for Structural Equation Modeling: A Simulation with Customer Satisfaction Data. In *Handbook of Partial Least Squares*, number July, pages 289–305. Springer Berlin Heidelberg, Berlin, Heidelberg, 2010. ISBN 978-3-540-32825-4. doi: 10.1007/978-3-540-32827-8_14. URL http://link.springer.com/10.1007/978-3-540-32827-8{_}14.

Wall, Melanie M and Amemiya, Yasuo. A method of moments technique for fitting interaction effects in structural equation models. *The British journal of mathematical and statistical psychology*, 56(Pt 1):47–63, 2003. ISSN 0007-1102. doi: 10.1348/000711003321645331. URL http://www.ncbi.nlm.nih.gov/pubmed/12803821.

Wilson, D. J. H., Irwin, G. W., and Lightbody, G. Nonlinear PLS modelling using radial basis functions. *American Control Conference, 1997. Proceedings of the 1997*, (June):3275–3276, 1997.

Wold, Herman. A fix-point theorem with econometric background.

Arkiv för Matematik, 6(3):221–240, jan 1965. ISSN 0004-2080. doi: 10.1007/BF02592031. URL http://link.springer.com/10.1007/BF02592031.

Wold, Herman. Nonlinear estimation by iterative least squares procedures. *Research Papers in Statistics*, 630, 1966a.

Wold, Herman. Estimation of Principal Components and Related Models by Iterative Least squares. In *Multivariate Analysis.*, pages 391–420. Academic Press, New York, 1966b.

Wold, Herman. Nonlinear Iterative Partial Least Squares (NIPALS) Modelling: Some Current Developments. In Krishnaiah, Paruchuri Rama, editor, *Multivariate Analysis–III*, pages 383–407. Academic Press, 1973.

Wold, Herman. Causal flows with latent variables: partings of the ways in the light of NIPALS modelling. *European Economic Review*, 5(1): 67–86, 1974.

Wold, Herman. *Path models with latent variables: The NIPALS approach.* Acad. Press, 1975a.

Wold, Herman. Soft modeling by latent variables: the nonlinear iterative partial least squares approach. *Perspectives in probability and statistics, papers in honour of MS Bartlett*, pages 520–540, 1975b.

Wold, Herman. Model Construction and Evaluation When Theoretical Knowledge Is Scarce. In Kmenta, Jan and Ramsey, James B., editors, *Evaluation of Econometric Models*, pages 47–74. Academic Press,

1980. ISBN 9780124165502. URL http://www.nber.org/chapters/c11693.

Wold, Herman. Soft Modeling: Intermediate between Traditional Model Building and Data Analysis. In *Mathematical Statistics*, volume 6, pages 333–346, 1982a.

Wold, Herman. Models for Knowledge. In *The Making of Statisticians*, pages 189–212. Springer New York, New York, NY, 1982b. doi: 10.1007/978-1-4613-8171-6_14. URL http://link.springer.com/10.1007/978-1-4613-8171-6{_}14.

Wold, Herman. Soft modelling: The Basic Design and Some Extensions. *Systems Under Indirect Observation, Part II*, pages 36–37, 1982c. URL http://ci.nii.ac.jp/naid/10006132197/en/.

Wold, Svante, Martens, Harald, and Wold, Herman. The multivariate calibration problem in chemistry solved by the PLS method. In Kågström, Bo and Ruhe, Axel, editors, *Matrix Pencils*, pages 286–293. Springer Berlin Heidelberg, 1983. doi: 10.1007/BFb0062108. URL http://link.springer.com/10.1007/BFb0062108.

Woodside, Arch G. Moving beyond multiple regression analysis to algorithms: Calling for adoption of a paradigm shift from symmetric to asymmetric thinking in data analysis and crafting theory. *Journal of Business Research*, 66(4):463–472, apr 2013. ISSN 01482963. doi: 10.1016/j.jbusres.2012.12.021. URL http://linkinghub.elsevier.com/retrieve/pii/S014829631200375X.

Wright, Sewall. Correlation and Causation. *Journal of Agricultural Research*, 20(7):557–585, 1921.

Wright, Sewall. The Method of Path Coefficients. *The annals of mathematical statistics*, 5(3):161–215, 1934.

Zhang, Yueli and Li, Wenchuan. The Nonlinear Relationship Among Brand Satisfaction, Brand Trust and Brand Loyalty. 2009.

Appendix

A.1 Nonlinear PLS Path Modelling: R Code

```
#================================================|
# Nonlinear PLS Path Modelling
# Author: Francesco Costigliola
#================================================|

#------------------------------------------------|
# Install all required packages
#------------------------------------------------|
installRequiredPackages <- function() {
if (!require(GGally)) {install.packages("GGally")}
if (!require(polynom)) {install.packages("polynom")}
if (!require(plyr)) {install.packages("plyr")}
if (!require(earth)) {install.packages("earth")}
if (!require(plyr)) {install.packages("grid")}
if (!require(earth)) {install.packages("ggplot2")}
}

#------------------------------------------------|
# Load all required packages
#------------------------------------------------|
loadRequiredPackages <- function() {
library(GGally)
library(polynom)
library(plyr)
library(earth)
library(grid)
library(ggplot2)
}

#------------------------------------------------|
# Given a dependent and an independent variable,
# fits a set of polynomial functions returned in
```

```
# a list
#------------------------------------------------|
fitPolynomial <- function (Dep,Ind) {

Poly.1 <- lm(Dep ~ Ind)                          #1st degree
Poly.2 <- lm(Dep ~ poly(Ind,2,raw=TRUE))         #2nd degree
#Poly.3 <- lm(Dep ~ poly(Ind,3,raw=TRUE))        #3nd degree

out <- list("firstDegree" = Poly.1, "secondDegree" = Poly.2) #, "thirdDegree"
    ↪ = Poly.3)
return(out)
}
#------------------------------------------------|
# Given a list with all the fitted polynomials,
# return the one with the best fit based on input
# criterion
#------------------------------------------------|
evaluatePolynomial <- function (Poly.List,criterion,ind_i,ind_j,iter) {
n.Poly <- length(Poly.List)
assign("Assess",matrix(0,n.Poly,7), envir = .GlobalEnv)
assign("Selected",matrix(0,1,4), envir = .GlobalEnv)
Assess[,1] = iter
Assess[,3] = ind_i
Assess[,4] = ind_j
Selected[1,1] = iter
Selected[1,2] = ind_i
Selected[1,3] = ind_j

for (k in 1:n.Poly) {
Assess[k,2] <- k
Assess[k,5] <- BIC(Poly.List[[k]])
Assess[k,6] <- AIC(Poly.List[[k]])
Assess[k,7] <- summary(Poly.List[[k]])[["adj.r.squared"]]
}

if (criterion == "BIC") {
Selected[1,4] <- which.min(Assess[,5])
out <- list("bestPolynomial" = Poly.List[[which.min(Assess[,5])]],"
    ↪ polynomialDegree" = which.min(Assess[,5]),"Assess" = Assess,"Selected"
    ↪ = Selected)
}
else if (criterion =="AIC") {
Selected[1,4] <- which.min(Assess[,6])
out <- list("bestPolynomial" = Poly.List[[which.min(Assess[,6])]],"
    ↪ polynomialDegree" = which.min(Assess[,6]),"Assess" = Assess,"Selected"
    ↪ = Selected)
}
else if (criterion =="RSQ") {
Selected[1,4] <- which.max(Assess[,7])
```

```
out <- list("bestPolynomial" = Poly.List[[which.max(Assess[,7])]],"
    ↪ polynomialDegree" = which.max(Assess[,7]),"Assess" = Assess,"Selected"
    ↪ = Selected)
}
else {
stop("ERROR: No Polynomial assesment criteria defined!")
}
return(out)
}
#-----------------------------------------------|
# Given the best fitting polynomial, return
# stationary points
#-----------------------------------------------|
stationaryPoints <- function (Poly) {

formattedPoly <- polynomial(Poly[[1]][["coefficients"]])

out <- summary(formattedPoly)[["stationaryPoints"]]

return(out)
}

#-----------------------------------------------|
# Given a matrix with two latent variables and a
# grouping variable returns the correlation
#-----------------------------------------------|
corrByGroup <- function(rawLV){
#return(data.frame(COR = sign(cor(rawLV[,1],rawLV[,2]))))
return(data.frame(COR = cor(rawLV[,1],rawLV[,2])))
}

#-----------------------------------------------|
# Given the estimated Latent Variables returns
statistics about prediction power and fit
#-----------------------------------------------|
GetRSquared <- function(Tbl,n.lvs,IDMat,n) {
Rsqd <- matrix(0,nrow=n.lvs,ncol=4)
for (rw in 2:n.lvs) {
# Get number of exogenous variables
n.exog <- sum(IDMat[rw,])
if (n.exog != 0) {
# Create a matrix that will contain data fom endogenous and exogenous
    ↪ variables
data.for.LM <- matrix(NA, nrow = n, ncol = n.exog+1)
# Place the endogenous variable in the first column
data.for.LM[,1] <- Tbl[,rw]
# Initialize an index to get the exogenous variables
ind.col <- 1
lim.diag <- rw-1
```

```
for (cl in 1:lim.diag){
if (IDMat[rw,cl] == 1){
# Collect all exogenous variables
data.for.LM[,ind.col+1] <- Tbl[,cl]
ind.col <- ind.col + 1
}
}
y <- data.for.LM[,1]
x <- data.for.LM[,-1]
# Estimate regression model
lm.fit <- lm(y~x)
# Get R-Squared
Rsqd[rw,4] <- summary(lm.fit)$r.squared
# Get Residuals Sum of Squares
Rsqd[rw,3] <- sum(summary(lm.fit)$residuals^2)
# Calculate Total Sum of Squares
Rsqd[rw,1] <- - (Rsqd[rw,3] / (Rsqd[rw,4] - 1))
# Get an estimate of the predictive power of the model
Rsqd[rw,2] <- Rsqd[rw,1] - Rsqd[rw,3]
}
}
return (Rsqd)
}

#-----------------------------------------------|
# Assess Unidimensionality for each block of
# manifest variables
#-----------------------------------------------|
AssessUnidim <- function(dts, blk_set, blk_len)
{
dts <- scale(dts)
lvs = length(blk_set)

Alpha = rep(1, lvs)
Rho = rep(1, lvs)
eig.1st = rep(1, lvs)
eig.2nd = rep(0, lvs)

for (aux in 1:lvs)
{
dts_part = dts[,blk_set[[aux]]]
if (blk_len[aux] != 1)
{
# PCA depending on block dimensions
if (nrow(dts_part) < ncol(dts_part)) {
# more columns than rows
X_pca = princomp(t(dts_part))
X_rho = t(dts_part)
} else {
```

```
# more rows than columns
X_pca = princomp(dts_part)
X_rho = dts_part
}
# Cronbach's alpha
p = ncol(dts_part)
correction = sqrt((nrow(dts_part)-1) / nrow(dts_part))
alpha_denom = var(rowSums(dts_part))
alpha_numer = 2 * sum(cor(dts_part)[lower.tri(cor(dts_part))])
alpha = (alpha_numer / alpha_denom) * (p / (p - 1))
Alpha[aux] <- ifelse(alpha < 0, 0, alpha)

# Rho
p = ncol(X_rho)
rho_numer = colSums(cor(X_rho, X_pca$scores[,1]))^2
rho_denom = rho_numer + (p - colSums(cor(X_rho, X_pca$scores[,1])^2) )
Rho[aux] = rho_numer / rho_denom

# Eigenvalues
eig.1st[aux] = X_pca$sdev[1]^2
eig.2nd[aux] = X_pca$sdev[2]^2
}
}

# output
data.frame(C.alpha = Alpha,
DG.rho = Rho,
eig.1st,
eig.2nd)
}

#-----------------------------------------------|
# Collect Path Coefficients
#-----------------------------------------------|
getPathCoeff <- function(paths, scores)
{
scores <- scale(scores)
n.lvs <- ncol(paths)
checkEndo <- as.logical(rowSums(paths))
Path = paths

for (aux in 1:n.lvs)
{
if (checkEndo[aux] == 1) {
X <- scores[,which(paths[aux,]==1)]
Y <- scores[,aux]
Path[aux,which(paths[aux,]==1)] = solve(t(X)%*%X) %*% t(X)%*%Y
}
}
```

```
return(Path)
}



#------------------------------------------------|
# Plot Path Model with Nonlinear fit
#------------------------------------------------|
plotPaths <- function(IDM, LVScores) {
dim <- nrow(IDM)

for (i in 1:dim) {
print (paste0("i = ",i))
for (j in 1:i) {
print(paste0("j = ",j))
if (j <= i & IDM[i,j]==1){
print ("inside")
Dep <- 1 +(LVScores[,i] - min(LVScores[,i])) / (max(LVScores[,i]) - min(
    ↪ LVScores[,i])) * 9
Ind <- 1 +(LVScores[,j] - min(LVScores[,j])) / (max(LVScores[,j]) - min(
    ↪ LVScores[,j])) * 9
Polys <- fitPolynomial(Dep,Ind)
Poly <- evaluatePolynomial(Polys,"BIC",1,1,1)
FinalPoly <- polynomial(Poly$bestPolynomial$coefficients)
plot(Ind,
Dep,
main=paste0(colnames(LVScores)[i], " explained by ", colnames(LVScores)[j]),
col="grey",
xlab = colnames(LVScores)[j],
ylab = colnames(LVScores)[i],
xlim = c(0,10),
xaxs ="i",
yaxs ="i",
ylim = c(0,10)
)
lines(FinalPoly,col="green2",lwd=3)
}
}

}
}


#------------------------------------------------|
# THIS FUNCTION RUNS THE NONLINEAR PARTIAL LEAST
# SQUARES PATH MODELLING
#
# INPUTS ARE:
#     inData:          INPUT DATA
```

```
#     IDM:               INNER DESIGN MATRIX
#     tolerance          TOLERANCE VALUE FOR CONVERGENCE
#     iterLimit          MAXIMUM NUMBER OF ITERATION FOR
#                        CONVERGENCE
#     lvs.names:         LATENT VARIABLES NAMES
#     mvs.names:         MANIFEST VARIABLES NAMES
#     sets:              SET OF MANIFEST VARIABLES FOR
#                        EACH BLOCK
#     modes:             SET OF MEASUREMENT MODEL
#                        ESTIMATION MODES
#     NLselCrit:         NONLINEAR SELECTION CRITERION
#                        (AIC,BIC,RSQ)
#     activateLVplots:   ACTIVATES SCATTER PLOT MATRIX
#                        BETWEEN LATENT VARIABLES FOR
#                        EVERY MODEL ITERATION
#---------------------------------------------------|

NLPLSPM <- function(inData,IDM,tolerance,iterLimit,lvs.names,mvs.names,sets,
   ↪ modes,NLselCrit, activateLVplots) {

# Verify and Install all required packages
installRequiredPackages()
# Load all required packages
loadRequiredPackages()
# Get number of observations
n.obs = nrow(inData)
#X = scale(as.data.frame(inData), center=TRUE, scale=TRUE)
# Scale input data
X <- apply(inData, MARGIN=2,
FUN = function(X) (X - mean(X))/(sd(X) * sqrt((n.obs-1)/n.obs)))
# Get number of manifest variables
mvs = ncol(X)
# Set column and row names to the Inner Design Matrix
dimnames(IDM) = list(lvs.names, lvs.names)
# Get number of latent variables
lvs = nrow(IDM)
# Create variables blocks
blocks = unlist(lapply(sets, length))
# Create empty Outer Design Matrix structure
ODM = matrix(0, mvs, lvs)
# Set Outer Design Matrix variables names
colnames(ODM)=lvs.names
# Initialize index variable
aux = 1
# -> Start loop on 'k' to create the Outer Design Matrix (ODM)
for (k in 1:lvs){
# Set initial weights with values equal to 1
ODM[aux:sum(blocks[1:k]),k] = rep(1,blocks[k])
# Increase index
```

```
aux = sum(blocks[1:k]) + 1
# -| End loop on 'k'
}
# Define first set of outer weights
W = ODM %*% diag(1/((apply(X %*% ODM,2,sd)*sqrt((n.obs-1)/n.obs))),lvs,lvs)
test.w <- t(matrix(as.list(W[which(W!=0)],1,16)))
test.c <- t(matrix(0,1,1))
# Store outer weights for future comparison
w.old = rowSums(W)
# Initialize a scalar for checking weights convergence
w.dif = 1
# Initialize an index of number of iterations
itermax = 1
# Initialize historical weights convergence criterion matrix
w.hist = matrix(c(0,w.dif),ncol=2,nrow=1)
# Initialize matrix to store historical polynomial assessments
AssessPolySel.hist = matrix(NA,nrow=1,ncol=7)
# Initialize matrix to store historical polynomial assessments
SelectedPoly.hist = matrix(NA,nrow=1,ncol=4)
# -> Start while loop on weight and number of iterations criteria
while (w.dif > tolerance && itermax < iterLimit){
# Perform external estimation of latent variables 'Y'
Y = X %*% W
# Set column names for latent variables matrix 'Y'
colnames(Y)=lvs.names
# [NEW] Build the full IDM matrix based on the expression: IDM + IDM'
fullIDM <- IDM + t(IDM)
# [NEW] Create an empty matrix that will contain the inner estimations
Z = matrix(NA, nrow(Y), lvs)
# [NEW] -> Start a loop on 'i' to go trough all endogenous variables
for (i in 1:lvs){
# [NEW] Create a temporary vector containing the inner estimation done by row
tempLV <- matrix(0,nrow(Y),1)
# [NEW] -> Start a loop on 'j' to go trough all exogenous variables
for (j in 1:lvs){
# [NEW] Goes through if IDM presents a relation between 'i' and 'j'
if (fullIDM[i,j] == 1) {
# [NEW] Checks whether (i,j) position is in the lower triangular matrix
if (i <= j) {
# [NEW] If (i,j) in lower triangular matrix then Y[,i] is endogenous
ii = i
# [NEW] If (i,j) in lower triangular matrix then Y[,j] is exogenous
jj = j
# [NEW] Close IF
}
# [NEW] Checks whether (i,j) position is in the upper triangular matrix
else {
# [NEW] If (i,j) in upper triangular matrix then Y[,j] is endogenous (
    ↪ SYMMETRIC APPROACH)
```

```
ii = j
# [NEW] If (i,j) in upper triangular matrix then Y[,i] is exogenous (SYMMETRIC
    ↪ APPROACH)
jj = i
# [NEW] Close ELSE
}
# [NEW] Fit polynomial function to inner relations
assign(paste("Poly",i,j,sep="."),fitPolynomial(Y[,ii],Y[,jj]))
# [NEW] Selects the polynomial degree that presents the best fit
assign(paste("bestPoly",i,j,sep="."),
evaluatePolynomial(get(paste("Poly",i,j,sep=".")),
criterion = NLselCrit,
ind_i = i, ind_j = j,
iter = itermax))
# [NEW] SIMULATION: Get values for all statistics and all polynomial degrees
AssessPolySel.hist <- rbind(AssessPolySel.hist,
get(paste("bestPoly",i,j,sep="."))[[3]])
# [NEW] SIMULATION: Get the degree for the selected polynomial
SelectedPoly.hist <- rbind(SelectedPoly.hist,
get(paste("bestPoly",i,j,sep="."))[[4]])
# [NEW] Get inflection and stationary points for the polynomial functions
    ↪ fitted
assign(paste("statPoints",i,j,sep="."),
stationaryPoints(get(paste("bestPoly",i,j,sep="."))))
# [NEW] Splits variables to calculate correlation matrix
assign(paste("preCorrData",i,j,sep="."),
cbind(Y[,ii],Y[,jj],
findInterval(Y[,ii],
get(paste("statPoints",i,j,sep=".")))))
if (min(table(get(paste("preCorrData",i,j,sep="."))[,3])) == 1) {
temp.preCorrData <- get(paste("preCorrData",i,j,sep="."))
temp.preCorrData[,3][temp.preCorrData[,3] == 1] <- 0
assign(paste("preCorrData",i,j,sep="."),temp.preCorrData)
}
# [NEW] Prepares the structure to calculate correlation matrix
LV0 <- data.frame(get(paste("preCorrData",i,j,sep="."))[,1],
get(paste("preCorrData",i,j,sep="."))[,2],
group = get(paste("preCorrData",i,j,sep="."))[,3])
# [NEW] Calculates correlations by group
assign(paste("Correlations",i,j,sep="."), ddply(LV0, .(group), corrByGroup))
# [NEW] Join correlations based on the group defined above
assign(paste("LV",i,j,sep="."), join(as.data.frame(LV0),
as.data.frame(get(paste("Correlations",i,j,sep="."))), by="group"))
# [NEW] Latent variable inner estimation
tempLV[,1] <- tempLV[,1] + (Y[,jj] *
get(paste("LV",i,j,sep="."))[,length(get(paste("LV",i,j,sep=".")))])
# [NEW] Close IF to check if IDM presents a relation between 'i' and 'j'
}
# [NEW] -| End a loop on 'j'
```

```
}
# [NEW] Add estimated latent variable to the final matrix Z
Z[,i] <- apply(tempLV, MARGIN=2,FUN = function(X) (X - mean(X))/(sd(X) * sqrt
    ↪ ((n.obs-1)/n.obs)))
# [NEW] -| End a loop on 'i'
}
# Initialize index 'aux'
aux = 1
# -> Start loop to calculate outer weights 'W'
for (k in 1:lvs){
# Check whether selected mode for latent variable 'k' is Mode A
if (modes[k]=="A"){
# Calculate outer weights as simple linear regression
ODM[aux:sum(blocks[1:k]),k] =
solve(t(Z[,k])%*%Z[,k])%*%Z[,k] %*% X[,aux:sum(blocks[1:k])]
# Close IF Mode A
}
# Check whether selected mode for latent variable 'k' is Mode B
else if (modes[k]=="B"){
# Build block of variables for multiple linear regression
X.blok = X[,aux:sum(blocks[1:k])]
# Calculate outer weights as multiple linear regression
ODM[aux:sum(blocks[1:k]),k] = solve(t(X.blok)%*%X.blok)%*%t(X.blok) %*% Z[,k]
# Close ELSE
}
# Increase index 'aux'
aux = sum(blocks[1:k]) + 1
# -| End loop on 'k'
}
# Standardise Outer Weights (three types but using standard approach)
W = ODM %*% diag(1/((apply(X %*% ODM,2,sd)*sqrt((n.obs-1)/n.obs))),lvs,lvs)
#W = ODM %*% diag(1/as.data.frame(lapply(as.data.frame(X %*% ODM),function(x)
    ↪ Matrix::norm(as.matrix(x),"F"))),lvs,lvs)
#W = ODM / norm(X %*% ODM,"F")
# Store weights in column in order to perform a comparison with previous
w.new = rowSums(W)
test.w = rbind(test.w,t(matrix(as.list(W[which(W!=0)],1,mvs))))
test.c = rbind(test.c,(sum(cor(Z)^2)-lvs)/2)
# Compute outer weights difference
w.dif = sum((w.old - w.new)^2)
# Update last weights for next iteration
w.old = w.new
# Add a new row with the updated convergence criterion
w.hist = rbind(w.hist,matrix(c(itermax,w.dif),nrow=1,ncol=2))
# Increase index for the number of iterations 'itermax'
itermax = itermax + 1
# [NEW] Checks whether is asked to produce a scatter plot matrix for latent
    ↪ variables
if (activateLVplots == TRUE){
```

```
# [NEW] Define latent variables names
colnames(Z)=lvs.names
# [NEW] Plot scatter plot matrix for latent variables
print(ggpairs(data=Z, title="Latent Variables: Inner Model"))
# [NEW] Close IF
}
# -| End while loop on weight and number of iterations criteria
}
#-----------------------------------------------|
BUILD OUTPUT VARIABLES
#-----------------------------------------------|
# OUTPUT 1: Iteration to Convergence
IterToConvergence <- itermax
# OUTPUT 2: Get all weights in one column
OuterWeights <- matrix(rowSums(W),mvs,1)
# OUTPUT 2: Define rows names
rownames(OuterWeights) <- mvs.names
# OUTPUT 2: Define column names
colnames(OuterWeights) <- "Outer Weights"
# OUTPUT 3: Collect convergence criterion historical values
Convergence <- w.hist
# OUTPUT 3: Define columns names
colnames(Convergence) <- c("Iteration #","Convergence Criterion")
# OUTPUT 4: Polynomial Degree Choice
PolynomialAssessment <- AssessPolySel.hist[2:nrow(AssessPolySel.hist),]
# OUTPUT 4: Define columns names
colnames(PolynomialAssessment) <- c("Iteration #",
"Polynomial Degree",
"Endogenous LV",
"Exogenous LV",
"BIC",
"AIC",
"Adjusted R2")
# OUTPUT 5: Get estimated Latent Variables
LatentVariables <- scale(X %*% W)
# OUTPUT 5: Define columns names
colnames(LatentVariables) <- lvs.names
# OUTPUT 6: Calculate R Squared and other Predictive Power Statistics
RSquared <- GetRSquared(LatentVariables, lvs, IDM, n.obs)
# OUTPUT 6: Define rows names
rownames(RSquared) <- lvs.names
# OUTPUT 6: Define columns names
colnames(RSquared) <- c("SSTotal",
"SSModel",
"SSError",
"Rsquared")
# OUTPUT 7: Get Standardized Manifest Variables
StdMVs <- X
# OUTPUT 7: Define columns names
```

```
colnames(StdMVs) <- mvs.names
# OUTPUT 8: Copy structure from ODM matrix containing initial weights
ODMatrix <- ODM
# OUTPUT 8: Set all initial weights to 1 to get the clean matrix with outer
    ↪ relations
ODMatrix[ODMatrix != 0] = 1
# OUTPUT 8: Get all Loadings using correlation because variables are
    ↪ standardized
Loadings <- matrix(rowSums(ODMatrix*cor(StdMVs,LatentVariables)),mvs,1)
# OUTPUT 8: Define rows names
rownames(Loadings) <- mvs.names
# OUTPUT 9: Get Cross Loadings
CrossLoadings <- cor(StdMVs,LatentVariables)
# OUTPUT 10: Selected Polynomial Degree
SelectedPoly.hist <- SelectedPoly.hist[2:nrow(SelectedPoly.hist),]
# OUTPUT 10: Define columns names
colnames(SelectedPoly.hist) <- c("Iteration #",
"Endogenous LV",
"Exogenous LV",
"Selected Polynomial")
# OUTPUT 11: Calculate communality
Communality <- Loadings^2
# OUTPUT 11: Define rows names
rownames(Communality) <- mvs.names
# OUTPUT 12: Calculate redundancy
Redundancy <- Loadings^2 * rowSums(ODMatrix%*%RSquared[,4])
# OUTPUT 12: Define rows names
rownames(Redundancy) <- mvs.names
# OUTPUT 13: Calculate Average Communality
Av.Communality <- t(colSums(matrix(rep(Communality,lvs),mvs,lvs) *
ODMatrix)/colSums(ODMatrix))
# OUTPUT 14: Calculate Average Redundancy
Av.Redundancy <- t(colSums(matrix(rep(Redundancy,lvs),mvs,lvs) *
ODMatrix)/colSums(ODMatrix))
# OUTPUT 15: Calculate GoF
GoF <- sqrt(mean(Communality)*mean(RSquared[,4]))
# OUTPUT 16: Assess Unidimensionality
Unidim <- AssessUnidim(inData, sets, blocks)
# OUTPUT 17: Get Path Coefficients
PathCoeff <- getPathCoeff(IDM, LatentVariables)
# OUTPUT 17: Define columns names
colnames(PathCoeff) <- lvs.names
# OUTPUT 17: Define rows names
rownames(PathCoeff) <- lvs.names

# Build list of output to return
output <- list("IterConv"    = IterToConvergence,
"Weights"    = OuterWeights,
"ConvCrit"    = Convergence,
```

```
"PolyAssess"  = PolynomialAssessment,
"LatentVars"  = LatentVariables,
"RSquared"    = RSquared,
"StdMVs"      = StdMVs,
"Loadings"    = Loadings,
"xLoadings"   = CrossLoadings,
"SelPoly"     = SelectedPoly.hist,
"Commun"      = Communality,
"Redund"      = Redundancy,
"AvCommun"    = Av.Communality,
"AvRedund"    = Av.Redundancy,
"GoF"         = GoF,
"Unidim"      = Unidim,
"PathCoeff"   = PathCoeff,
"HistWgts"    = test.w,
"HistCorr"    = test.c
)
# Return output list
plotPaths(IDM, LatentVariables)
return (output)
# End function
}
#==================================|
```

A.2 EQS Code for Generating Simulated Data

Simulation Scenario 1

```
/TITLE Simulation Scenario # 1
/SPECIFICATIONS VARIABLES=16; CASES=50; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;  V2  = .5*F1 + E2;  V3  = .7*F1 + E3;
V4  = .9*F1 + E4;  V5  = .3*F2 + E5;  V6  = .5*F2 + E6;
V7  = .7*F2 + E7;  V8  = .9*F2 + E8;  V9  = .3*F3 + E9;
V10 = .5*F3 + E10; V11 = .7*F3 + E11; V12 = .9*F3 + E12;
V13 = .3*F4 + E13; V14 = .5*F4 + E14; V15 = .7*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM1'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 2

```
/TITLE Simulation Scenario # 2
/SPECIFICATIONS VARIABLES=16; CASES=50; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;  V2  = .5*F1 + E2;  V3  = .7*F1 + E3;
V4  = .9*F1 + E4;  V5  = .3*F2 + E5;  V6  = .5*F2 + E6;
V7  = .7*F2 + E7;  V8  = .9*F2 + E8;  V9  = .3*F3 + E9;
V10 = .5*F3 + E10; V11 = .7*F3 + E11; V12 = .9*F3 + E12;
V13 = .3*F4 + E13; V14 = .5*F4 + E14; V15 = .7*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM2'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 3

```
/TITLE Simulation Scenario # 3
/SPECIFICATIONS VARIABLES=16; CASES=50; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .9*F1 + E1;  V2  = .9*F1 + E2;  V3  = .9*F1 + E3;
V4  = .9*F1 + E4;  V5  = .9*F2 + E5;  V6  = .9*F2 + E6;
V7  = .9*F2 + E7;  V8  = .9*F2 + E8;  V9  = .9*F3 + E9;
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM3'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 4

```
/TITLE Simulation Scenario # 4
/SPECIFICATIONS VARIABLES=16; CASES=50; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .9*F1 + E1;  V2  = .9*F1 + E2;  V3  = .9*F1 + E3;
V4  = .9*F1 + E4;  V5  = .9*F2 + E5;  V6  = .9*F2 + E6;
V7  = .9*F2 + E7;  V8  = .9*F2 + E8;  V9  = .9*F3 + E9;
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM4'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 5

```
/TITLE Simulation Scenario # 5
/SPECIFICATIONS VARIABLES=16; CASES=100; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;  V2  = .5*F1 + E2;  V3  = .7*F1 + E3;
V4  = .9*F1 + E4;  V5  = .3*F2 + E5;  V6  = .5*F2 + E6;
V7  = .7*F2 + E7;  V8  = .9*F2 + E8;  V9  = .3*F3 + E9;
V10 = .5*F3 + E10; V11 = .7*F3 + E11; V12 = .9*F3 + E12;
V13 = .3*F4 + E13; V14 = .5*F4 + E14; V15 = .7*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM5'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 6

```
/TITLE Simulation Scenario # 6
/SPECIFICATIONS VARIABLES=16; CASES=100; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;  V2  = .5*F1 + E2;  V3  = .7*F1 + E3;
V4  = .9*F1 + E4;  V5  = .3*F2 + E5;  V6  = .5*F2 + E6;
V7  = .7*F2 + E7;  V8  = .9*F2 + E8;  V9  = .3*F3 + E9;
V10 = .5*F3 + E10; V11 = .7*F3 + E11; V12 = .9*F3 + E12;
V13 = .3*F4 + E13; V14 = .5*F4 + E14; V15 = .7*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM6'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 7

```
/TITLE Simulation Scenario # 7
/SPECIFICATIONS VARIABLES=16; CASES=100; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
```

```
/EQUATIONS
V1  = .9*F1 + E1;  V2  = .9*F1 + E2;  V3  = .9*F1 + E3;
V4  = .9*F1 + E4;  V5  = .9*F2 + E5;  V6  = .9*F2 + E6;
V7  = .9*F2 + E7;  V8  = .9*F2 + E8;  V9  = .9*F3 + E9;
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM7'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 8

```
/TITLE Simulation Scenario # 8
/SPECIFICATIONS VARIABLES=16; CASES=100; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .9*F1 + E1;  V2  = .9*F1 + E2;  V3  = .9*F1 + E3;
V4  = .9*F1 + E4;  V5  = .9*F2 + E5;  V6  = .9*F2 + E6;
V7  = .9*F2 + E7;  V8  = .9*F2 + E8;  V9  = .9*F3 + E9;
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM8'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 9

```
/TITLE Simulation Scenario # 9
/SPECIFICATIONS VARIABLES=16; CASES=200; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;  V2  = .5*F1 + E2;  V3  = .7*F1 + E3;
```

```
V4  = .9*F1 + E4;   V5  = .3*F2 + E5;   V6  = .5*F2 + E6;
V7  = .7*F2 + E7;   V8  = .9*F2 + E8;   V9  = .3*F3 + E9;
V10 = .5*F3 + E10;  V11 = .7*F3 + E11;  V12 = .9*F3 + E12;
V13 = .3*F4 + E13;  V14 = .5*F4 + E14;  V15 = .7*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM9'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 10

```
/TITLE Simulation Scenario # 10
/SPECIFICATIONS VARIABLES=16; CASES=200; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;   V2  = .5*F1 + E2;   V3  = .7*F1 + E3;
V4  = .9*F1 + E4;   V5  = .3*F2 + E5;   V6  = .5*F2 + E6;
V7  = .7*F2 + E7;   V8  = .9*F2 + E8;   V9  = .3*F3 + E9;
V10 = .5*F3 + E10;  V11 = .7*F3 + E11;  V12 = .9*F3 + E12;
V13 = .3*F4 + E13;  V14 = .5*F4 + E14;  V15 = .7*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM10'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 11

```
/TITLE Simulation Scenario # 11
/SPECIFICATIONS VARIABLES=16; CASES=200; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .9*F1 + E1;   V2  = .9*F1 + E2;   V3  = .9*F1 + E3;
V4  = .9*F1 + E4;   V5  = .9*F2 + E5;   V6  = .9*F2 + E6;
V7  = .9*F2 + E7;   V8  = .9*F2 + E8;   V9  = .9*F3 + E9;
```

```
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM11'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 12

```
/TITLE Simulation Scenario # 12
/SPECIFICATIONS VARIABLES=16; CASES=200; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .9*F1 + E1;  V2  = .9*F1 + E2;  V3  = .9*F1 + E3;
V4  = .9*F1 + E4;  V5  = .9*F2 + E5;  V6  = .9*F2 + E6;
V7  = .9*F2 + E7;  V8  = .9*F2 + E8;  V9  = .9*F3 + E9;
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM12'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 13

```
/TITLE Simulation Scenario # 13
/SPECIFICATIONS VARIABLES=16; CASES=500; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;  V2  = .5*F1 + E2;  V3  = .7*F1 + E3;
V4  = .9*F1 + E4;  V5  = .3*F2 + E5;  V6  = .5*F2 + E6;
V7  = .7*F2 + E7;  V8  = .9*F2 + E8;  V9  = .3*F3 + E9;
V10 = .5*F3 + E10; V11 = .7*F3 + E11; V12 = .9*F3 + E12;
V13 = .3*F4 + E13; V14 = .5*F4 + E14; V15 = .7*F4 + E15;
```

```
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM13'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 14

```
/TITLE Simulation Scenario # 14
/SPECIFICATIONS VARIABLES=16; CASES=500; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .3*F1 + E1;  V2  = .5*F1 + E2;  V3  = .7*F1 + E3;
V4  = .9*F1 + E4;  V5  = .3*F2 + E5;  V6  = .5*F2 + E6;
V7  = .7*F2 + E7;  V8  = .9*F2 + E8;  V9  = .3*F3 + E9;
V10 = .5*F3 + E10; V11 = .7*F3 + E11; V12 = .9*F3 + E12;
V13 = .3*F4 + E13; V14 = .5*F4 + E14; V15 = .7*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM14'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 15

```
/TITLE Simulation Scenario # 15
/SPECIFICATIONS VARIABLES=16; CASES=500; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .9*F1 + E1;  V2  = .9*F1 + E2;  V3  = .9*F1 + E3;
V4  = .9*F1 + E4;  V5  = .9*F2 + E5;  V6  = .9*F2 + E6;
V7  = .9*F2 + E7;  V8  = .9*F2 + E8;  V9  = .9*F3 + E9;
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
```

```
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .5*F2 + .5*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM15'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

Simulation Scenario 16

```
/TITLE Simulation Scenario # 16
/SPECIFICATIONS VARIABLES=16; CASES=500; METHOD=ML; ANALYSIS=COV; MATRIX=RAW;
/EQUATIONS
V1  = .9*F1 + E1;  V2  = .9*F1 + E2;  V3  = .9*F1 + E3;
V4  = .9*F1 + E4;  V5  = .9*F2 + E5;  V6  = .9*F2 + E6;
V7  = .9*F2 + E7;  V8  = .9*F2 + E8;  V9  = .9*F3 + E9;
V10 = .9*F3 + E10; V11 = .9*F3 + E11; V12 = .9*F3 + E12;
V13 = .9*F4 + E13; V14 = .9*F4 + E14; V15 = .9*F4 + E15;
V16 = .9*F4 + E16;
F2 = .3*F1 + D2;
F3 = .3*F1 + .3*F2 + D3;
F4 = .5*F1 + .3*F2 + .3*F3 + D4;
/VARIANCES F1 = 1*; E1 TO E16 = 0.01; D2 TO D4 = 1*;
/COVARIANCES
/SIMULATION
POPULATI/OUTPUT ALL; ON=MODEL; SEED=987654321;
REP=1000; DATA='SIM16'; SAVE=CONCATENATE;
/TECHNICAL CON=.0001;
/PRINT FIT=ALL; COVA=YES; TABLE=EQUATION; DIGITS=4;
/END
```

A.3 Simulation Results: Loadings Distributions

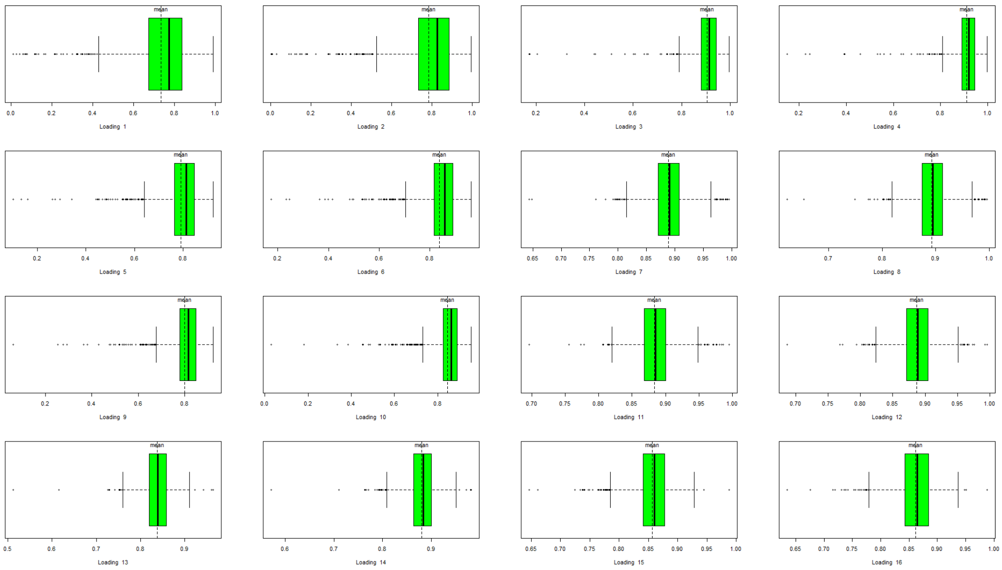


Figure A.3.1: Simulation Scenario 1 - Loadings Estimates Distribution

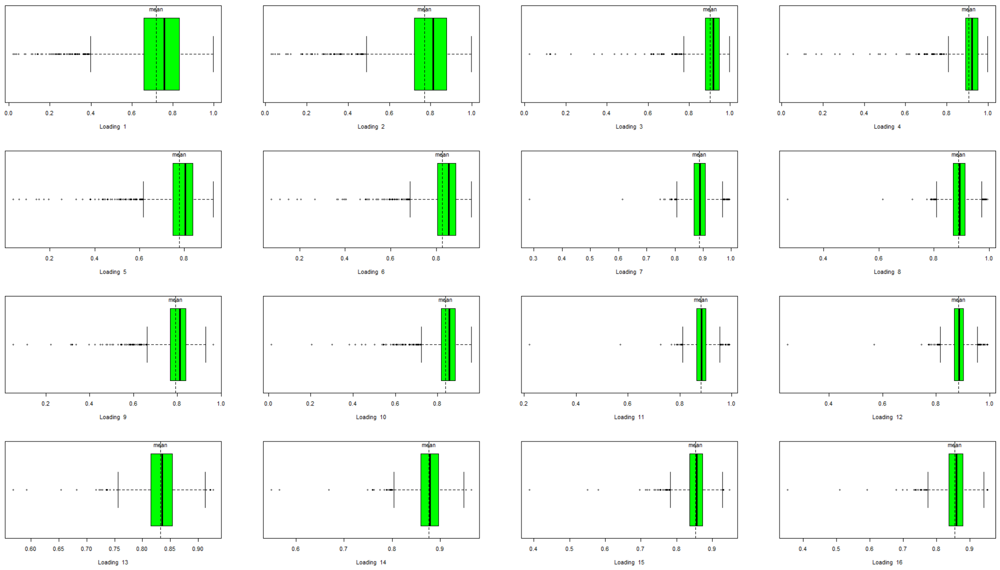


Figure A.3.2: Simulation Scenario 2 - Loadings Estimates Distribution

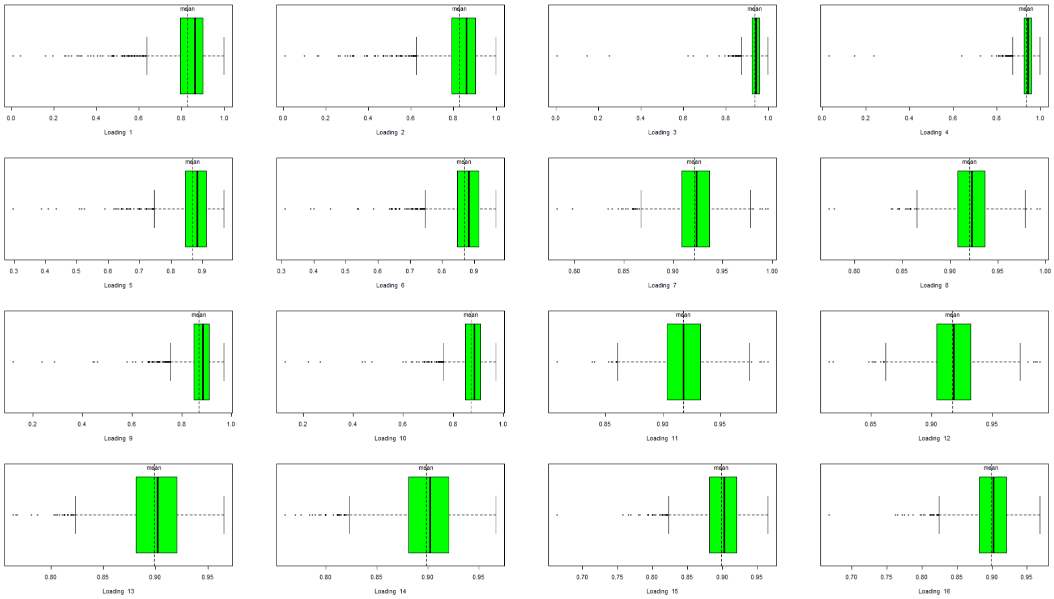


Figure A.3.3: Simulation Scenario 3 - Loadings Estimates Distribution

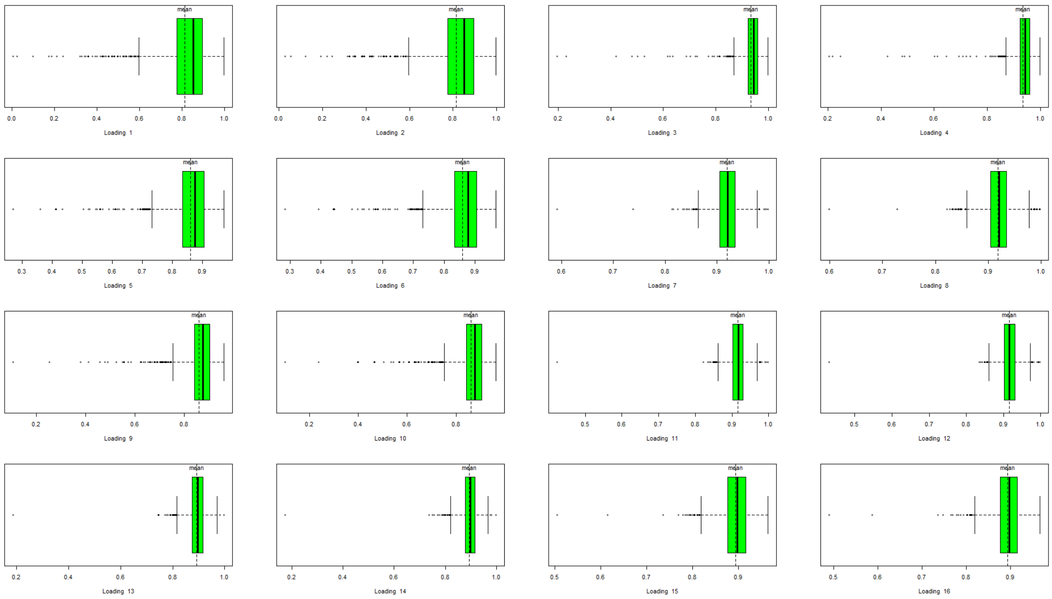


Figure A.3.4: Simulation Scenario 4 - Loadings Estimates Distribution

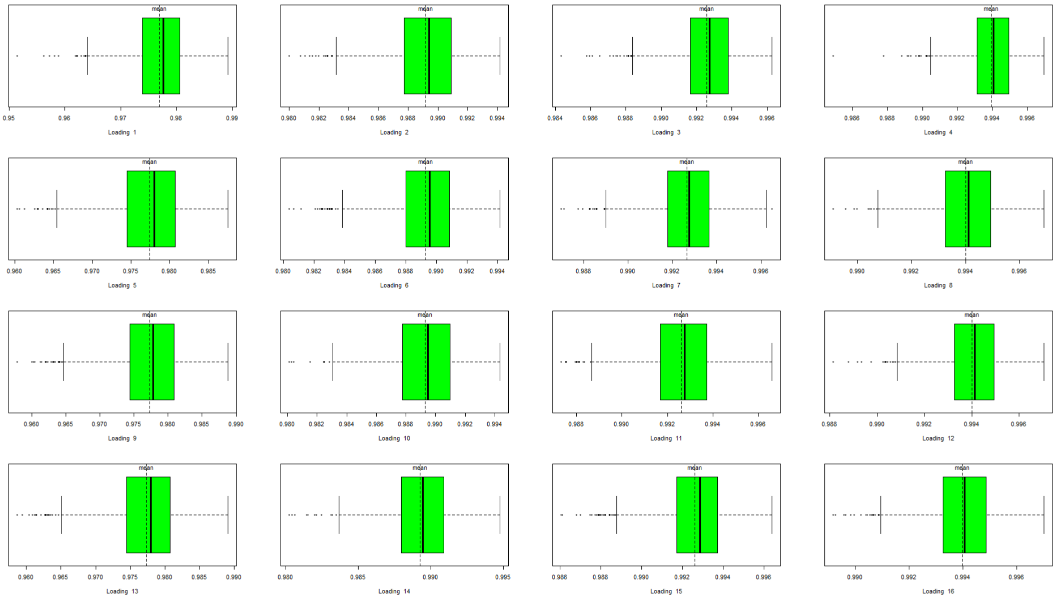


Figure A.3.5: Simulation Scenario 5 - Loadings Estimates Distribution

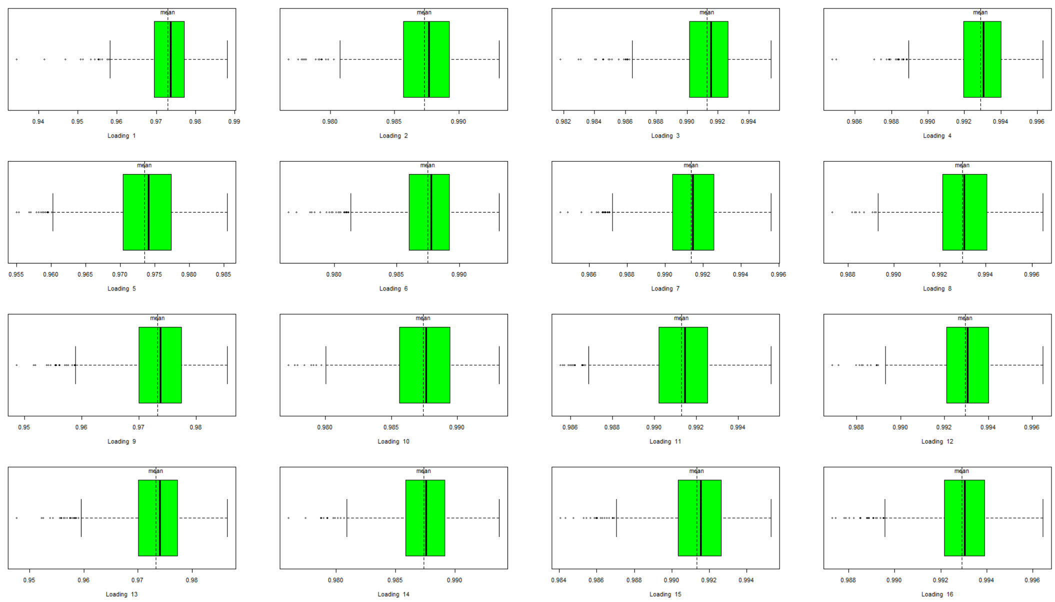


Figure A.3.6: Simulation Scenario 6 - Loadings Estimates Distribution

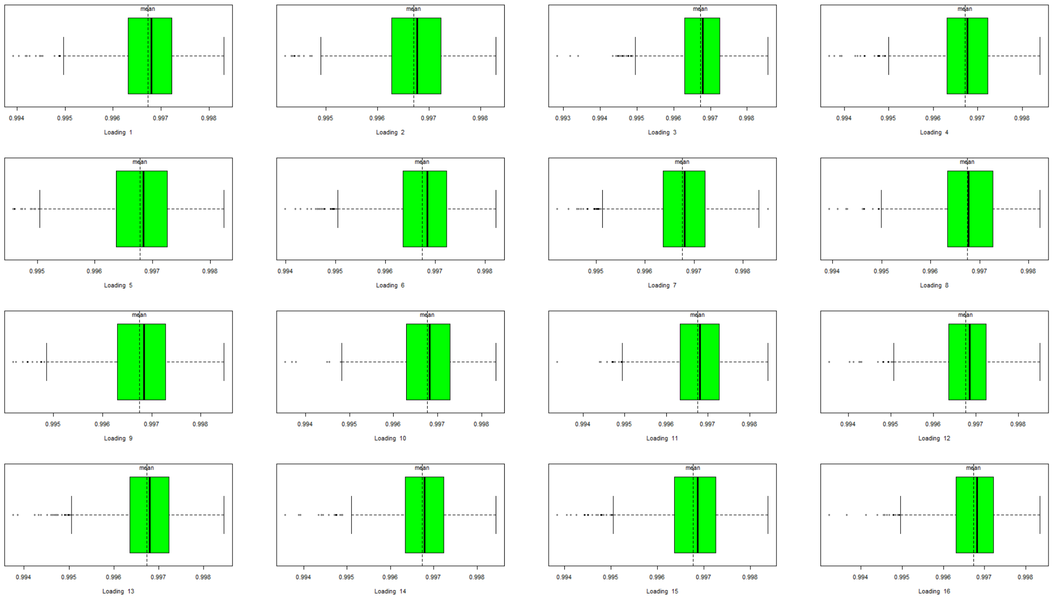


Figure A.3.7: Simulation Scenario 7 - Loadings Estimates Distribution

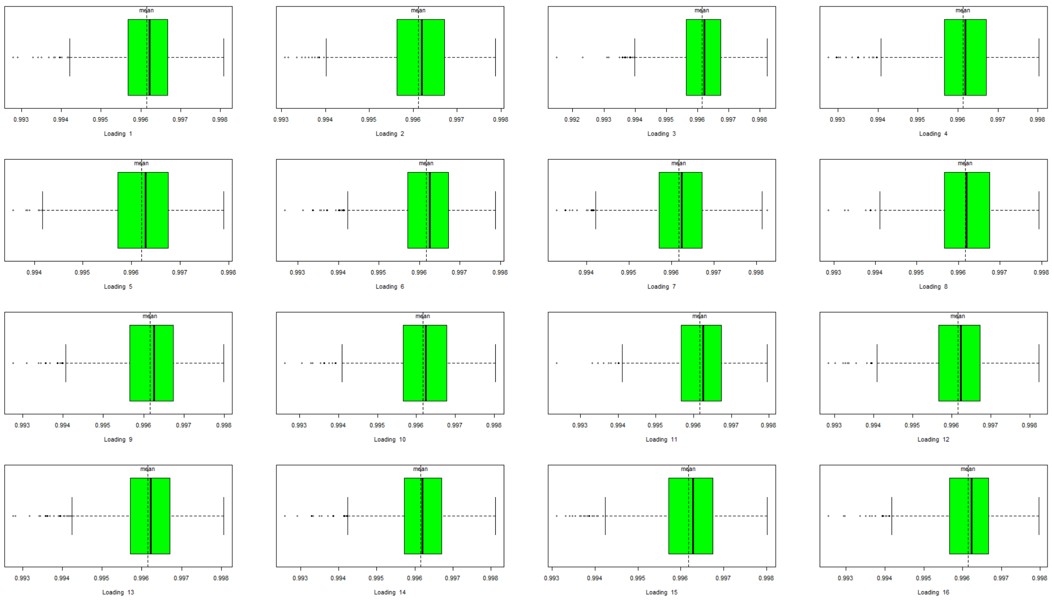


Figure A.3.8: Simulation Scenario 8 - Loadings Estimates Distribution

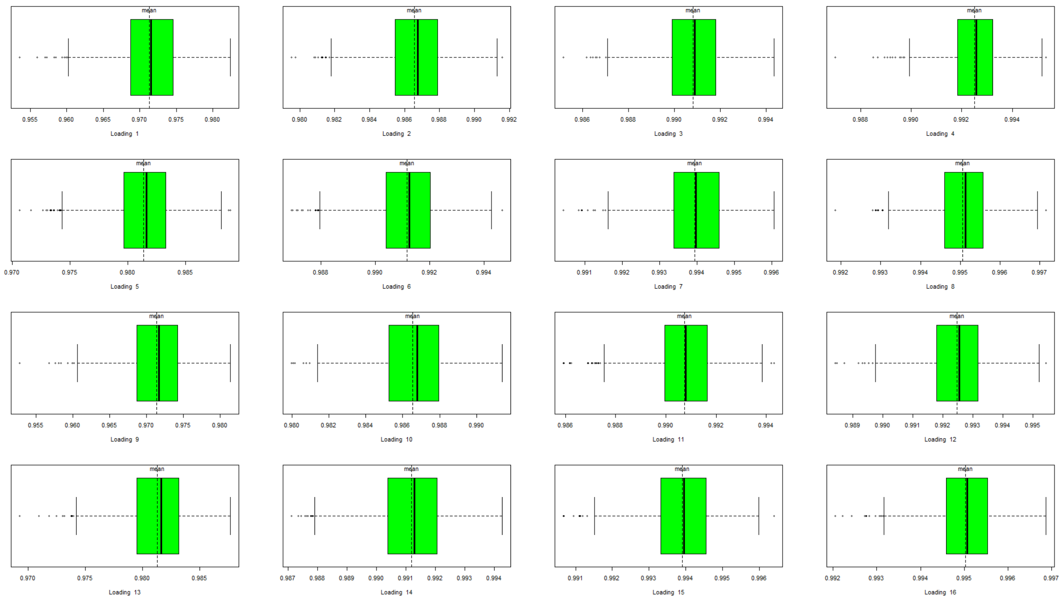


Figure A.3.9: Simulation Scenario 9 - Loadings Estimates Distribution

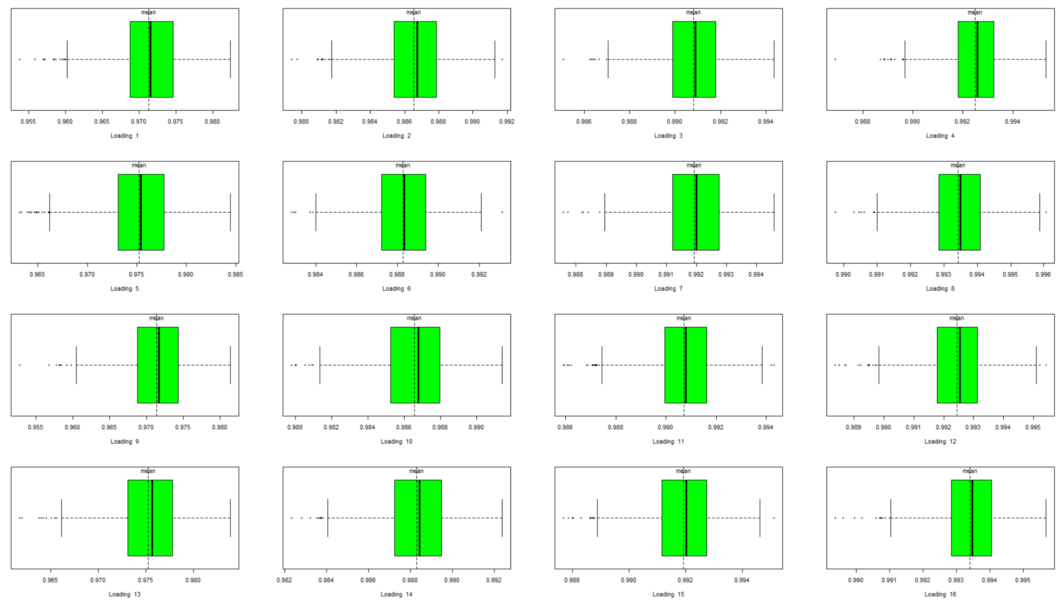


Figure A.3.10: Simulation Scenario 10 - Loadings Estimates Distribution

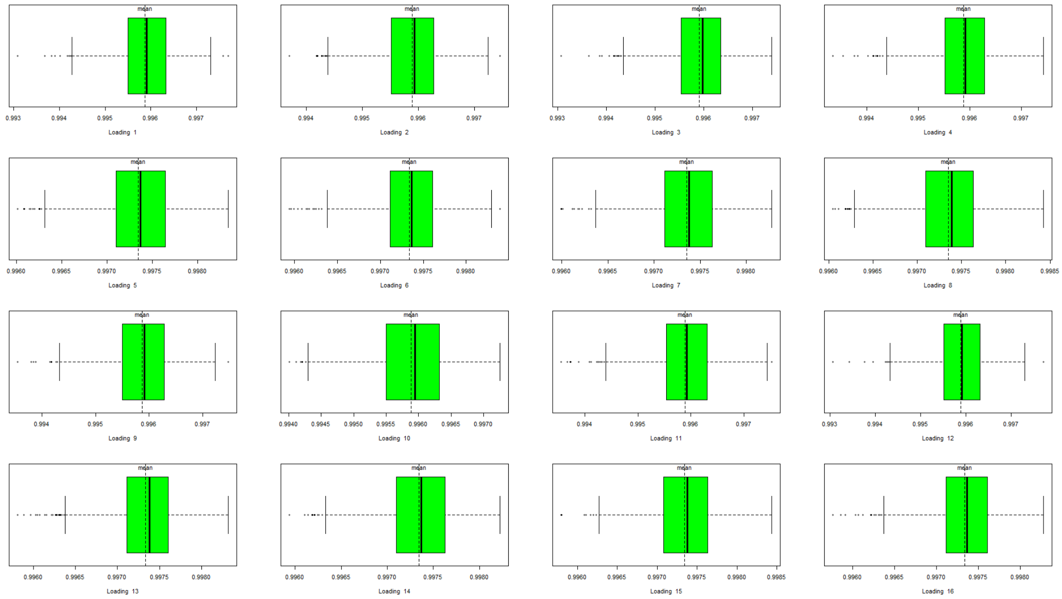


Figure A.3.11: Simulation Scenario 11 - Loadings Estimates Distribution

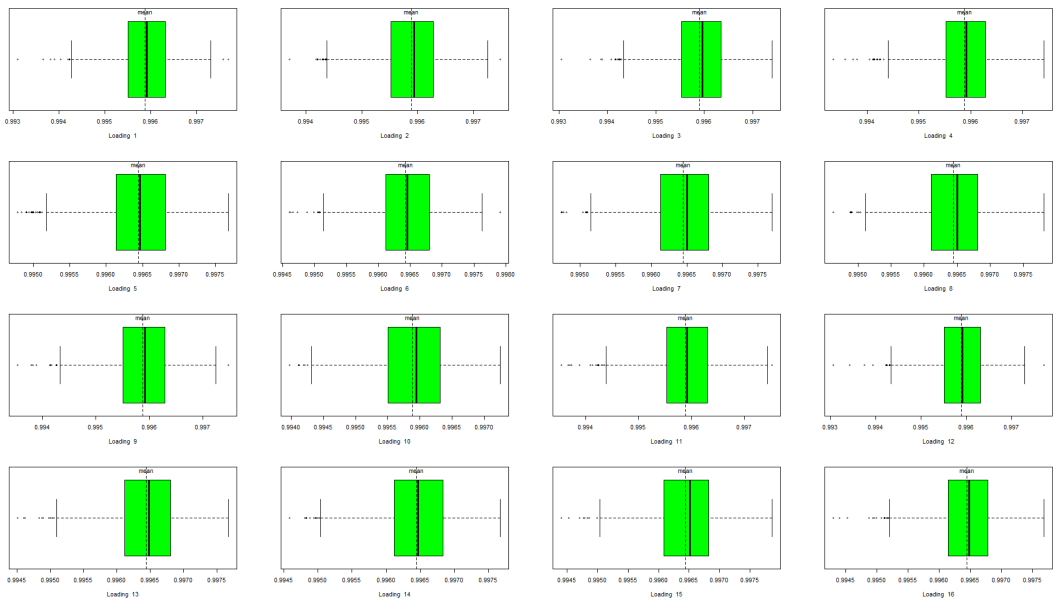


Figure A.3.12: Simulation Scenario 12 - Loadings Estimates Distribution

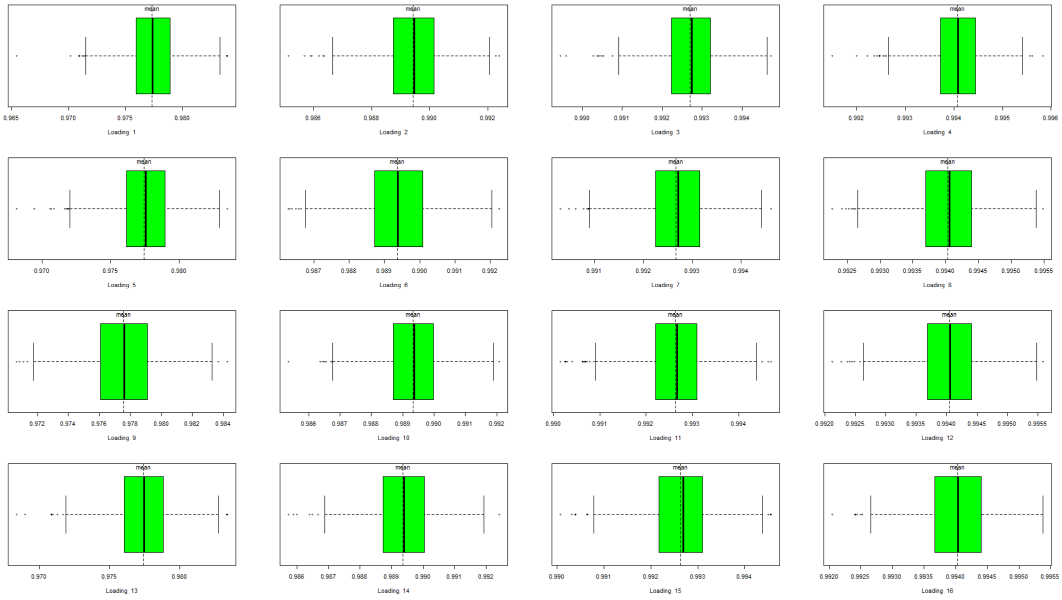


Figure A.3.13: Simulation Scenario 13 - Loadings Estimates Distribution

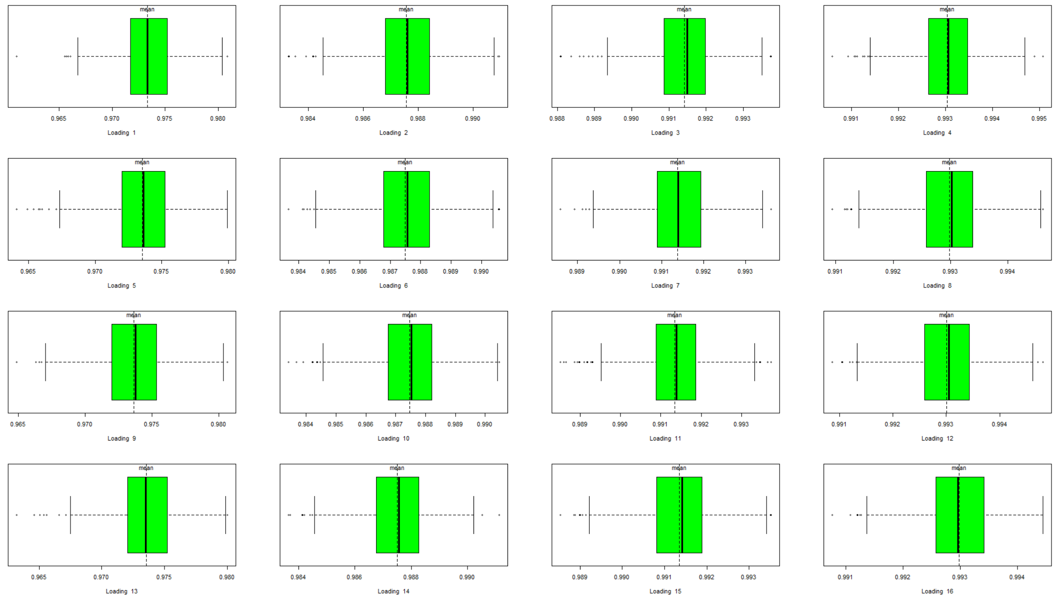


Figure A.3.14: Simulation Scenario 14 - Loadings Estimates Distribution

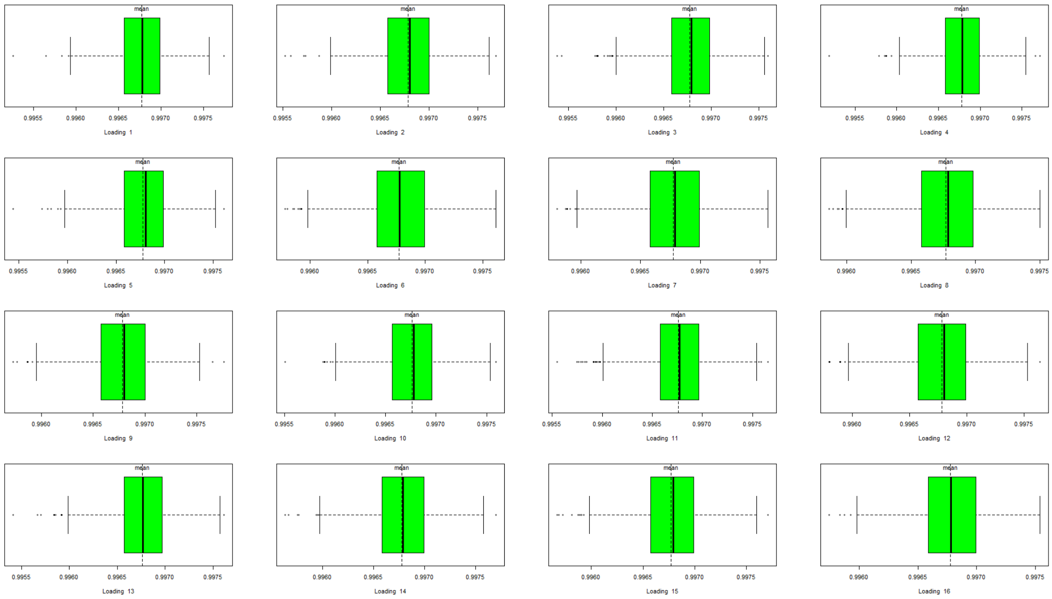


Figure A.3.15: Simulation Scenario 15 - Loadings Estimates Distribution

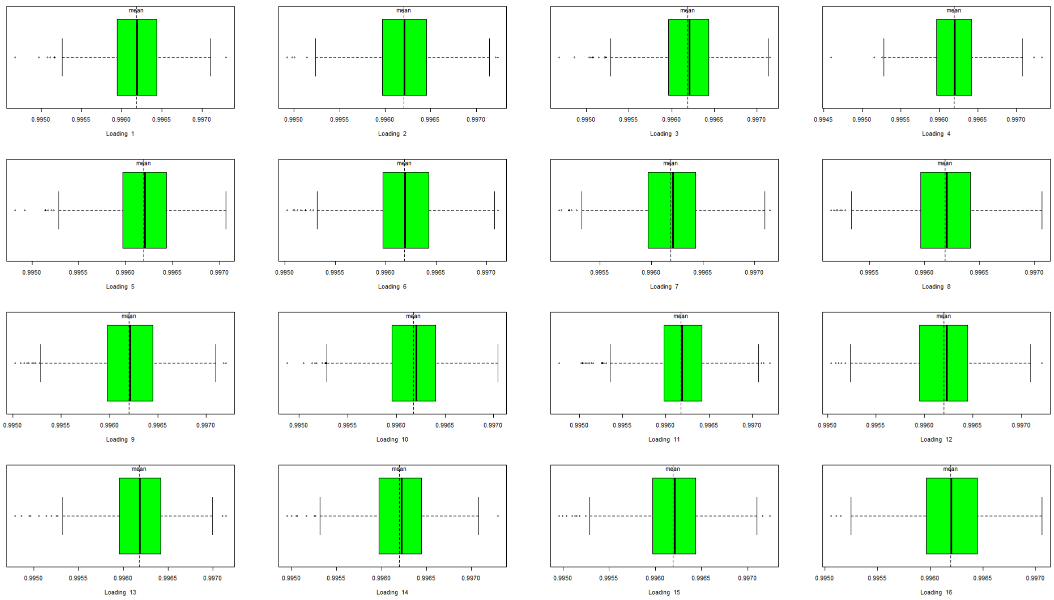


Figure A.3.16: Simulation Scenario 16 - Loadings Estimates Distribution

A.4 Simulation Results: In-Sample Predictive Power Distributions

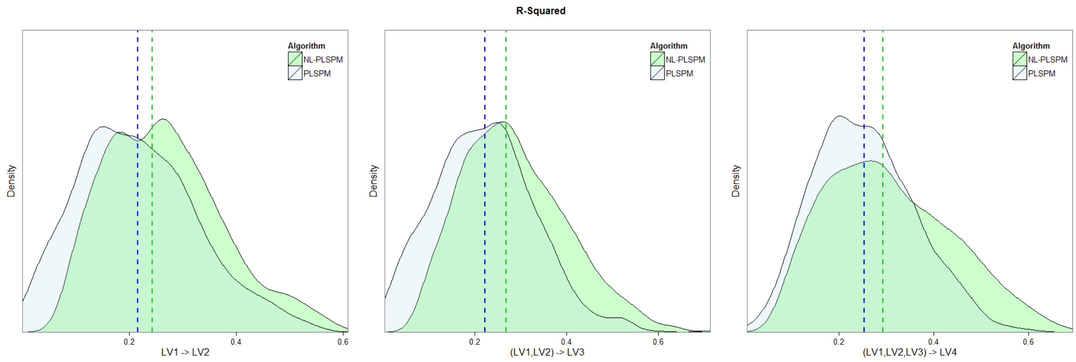


Figure A.4.1: Simulation Scenario 1 - R^2 Distribution Comparison

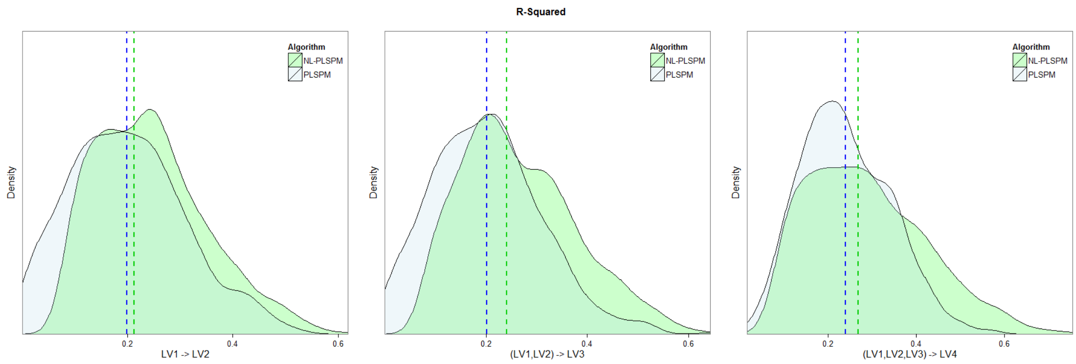


Figure A.4.2: Simulation Scenario 2 - R^2 Distribution Comparison

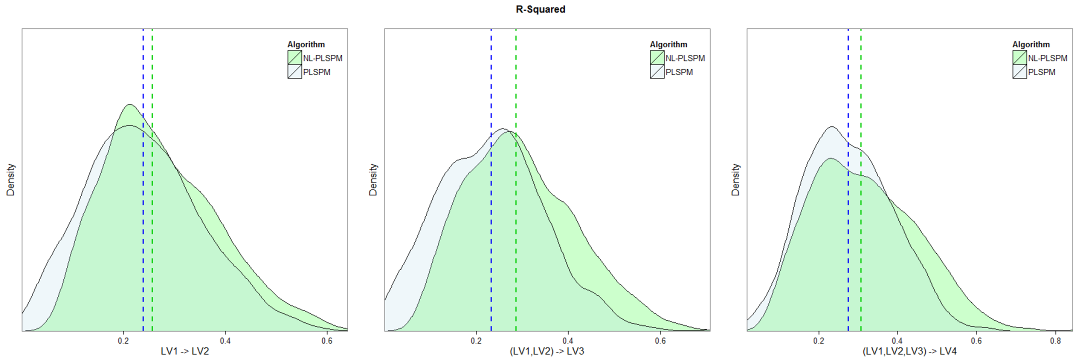


Figure A.4.3: Simulation Scenario 3 - R^2 Distribution Comparison

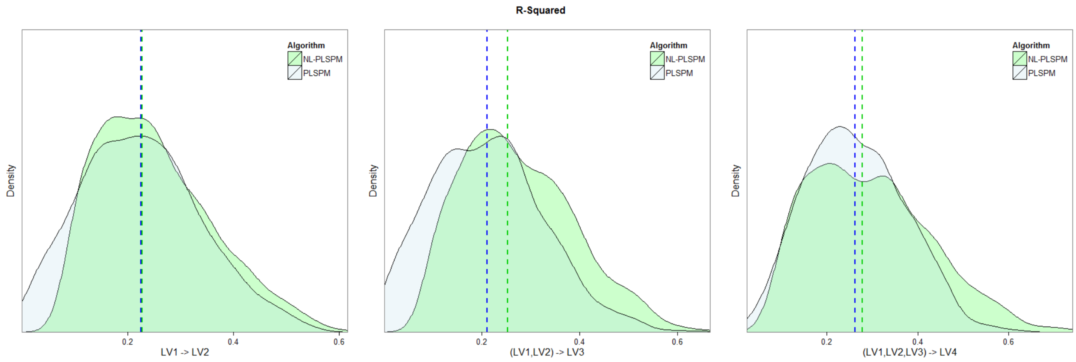


Figure A.4.4: Simulation Scenario 4 - R^2 Distribution Comparison

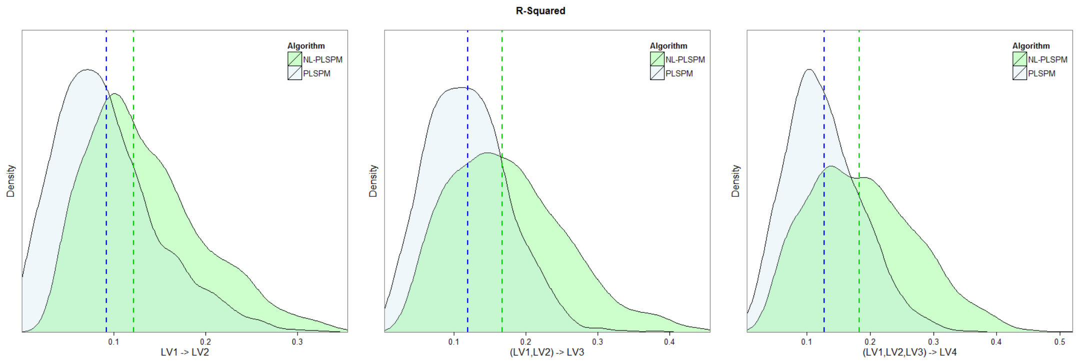


Figure A.4.5: Simulation Scenario 5 - R^2 Distribution Comparison

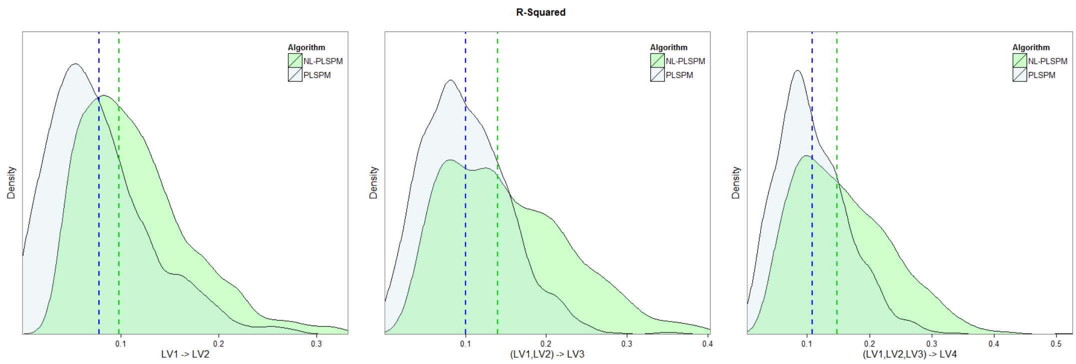


Figure A.4.6: Simulation Scenario 6 - R^2 Distribution Comparison

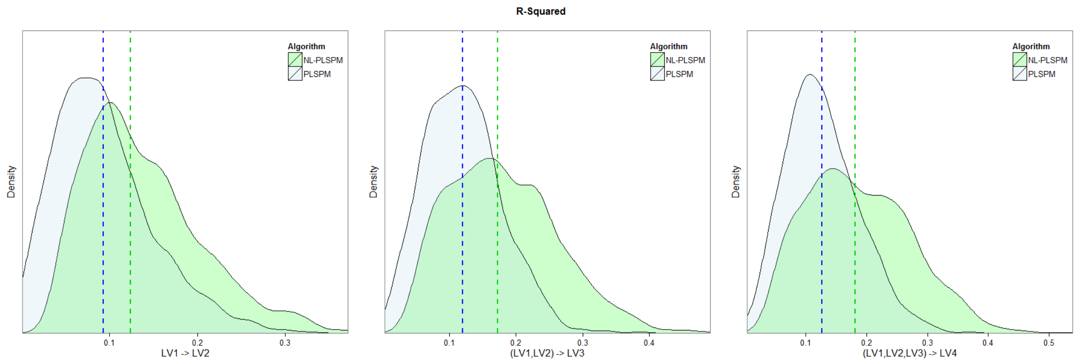


Figure A.4.7: Simulation Scenario 7 - R^2 Distribution Comparison

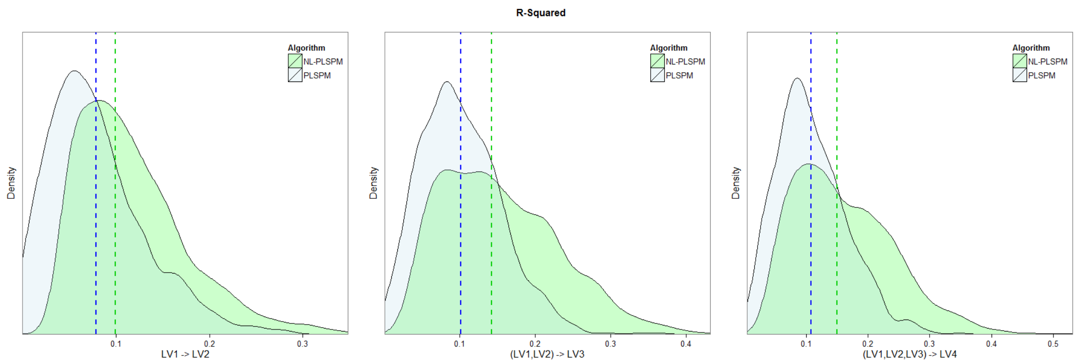


Figure A.4.8: Simulation Scenario 8 - R^2 Distribution Comparison

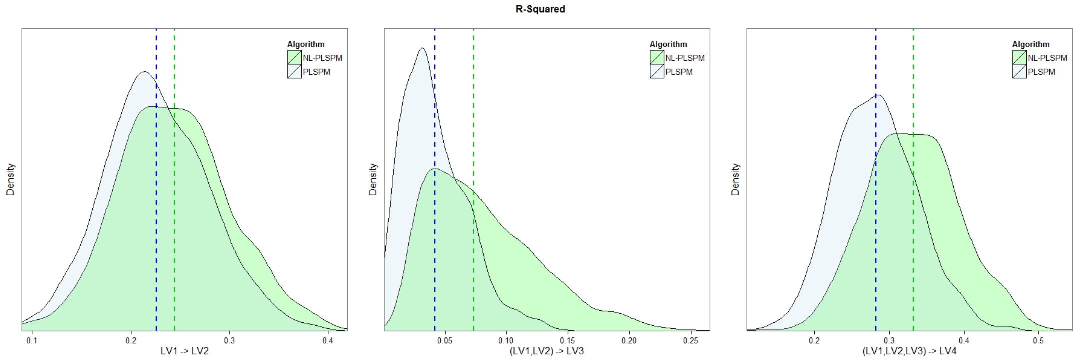


Figure A.4.9: Simulation Scenario 9 - R^2 Distribution Comparison

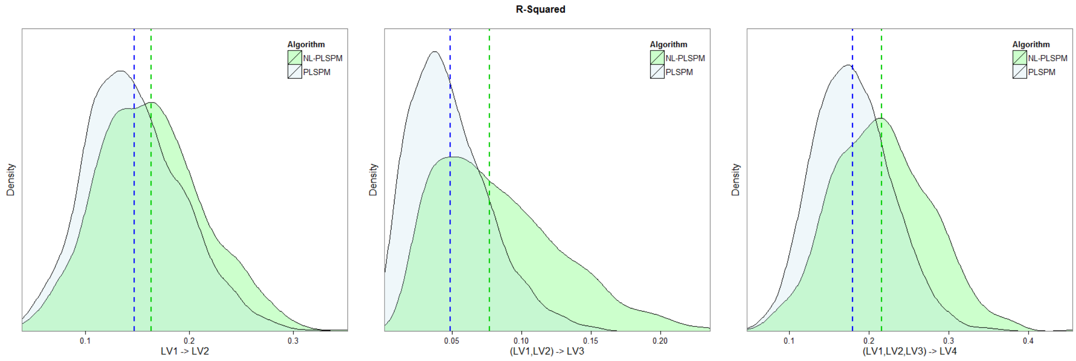


Figure A.4.10: Simulation Scenario 10 - R^2 Distribution Comparison

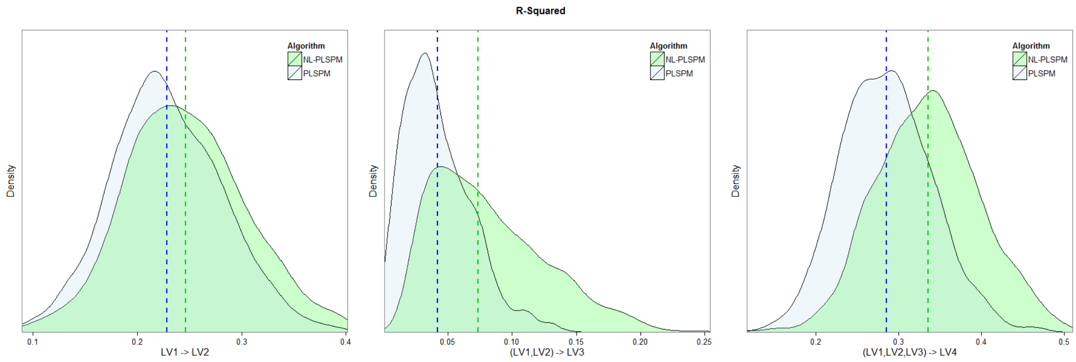


Figure A.4.11: Simulation Scenario 11 - R^2 Distribution Comparison

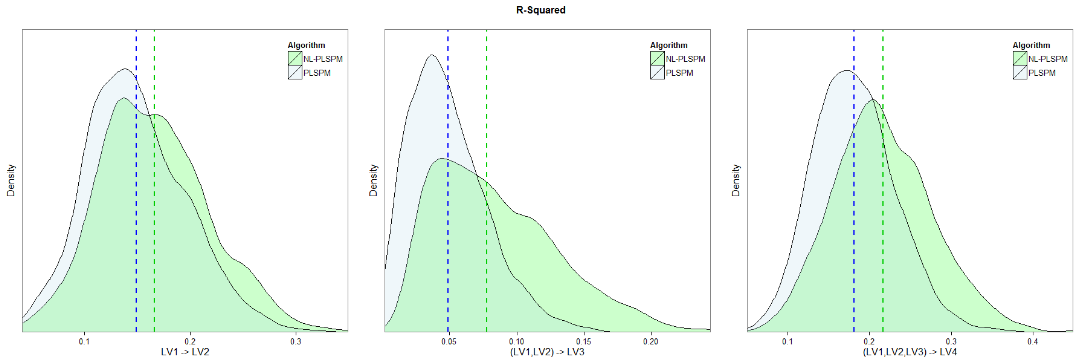


Figure A.4.12: Simulation Scenario 12: R^2 Distribution Comparison

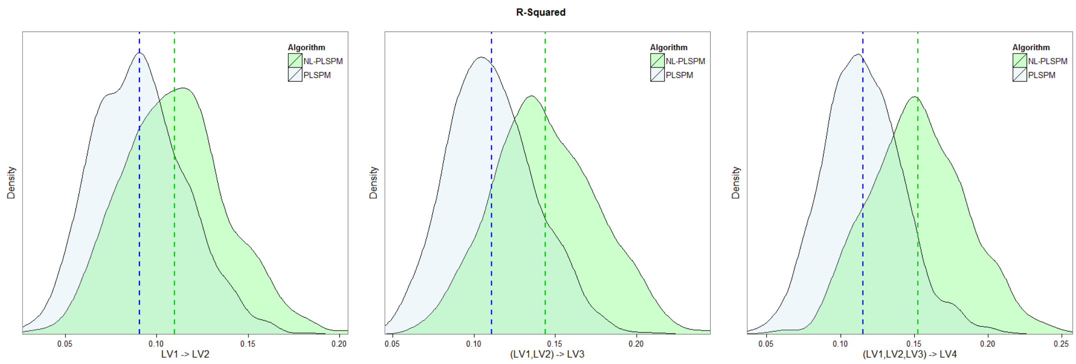


Figure A.4.13: Simulation Scenario 13 - R^2 Distribution Comparison

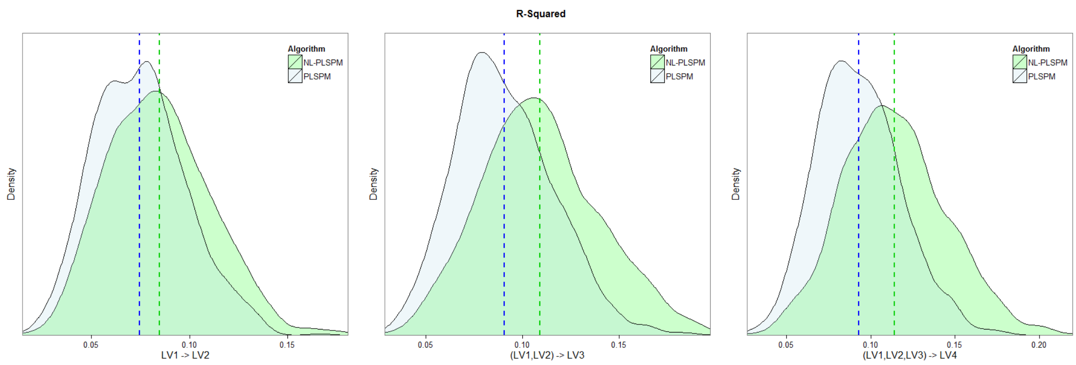


Figure A.4.14: Simulation Scenario 14 - R^2 Distribution Comparison

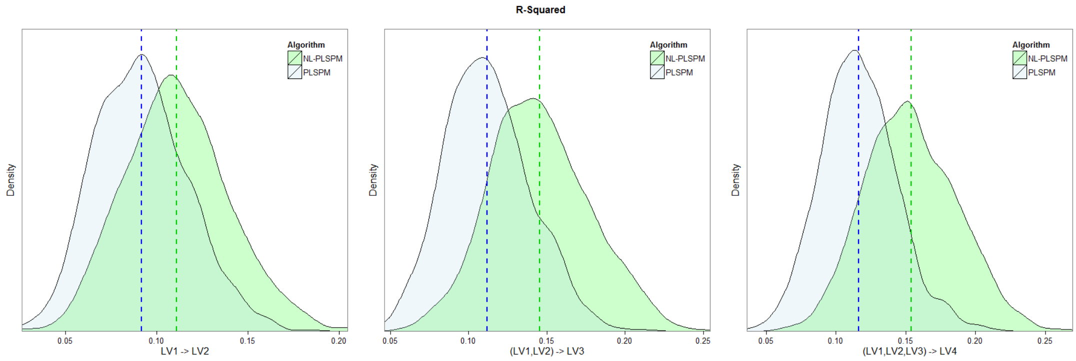


Figure A.4.15: Simulation Scenario 15 - R^2 Distribution Comparison

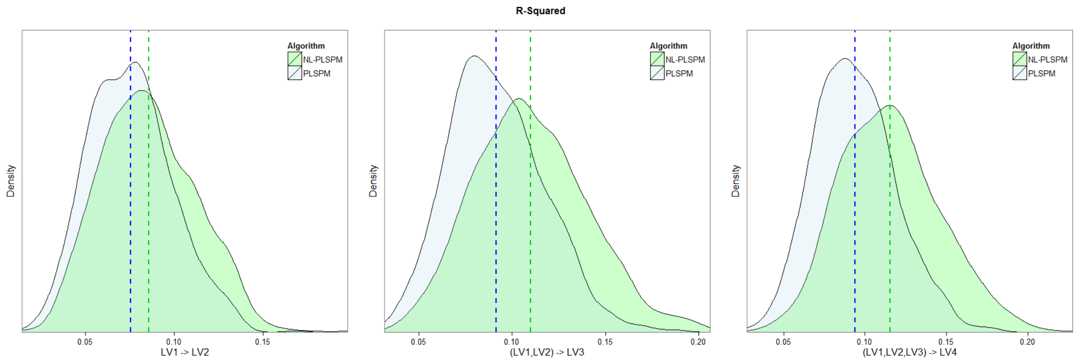


Figure A.4.16: Simulation Scenario 16 - R^2 Distribution Comparison

A.5 Application: Input Data Distribution

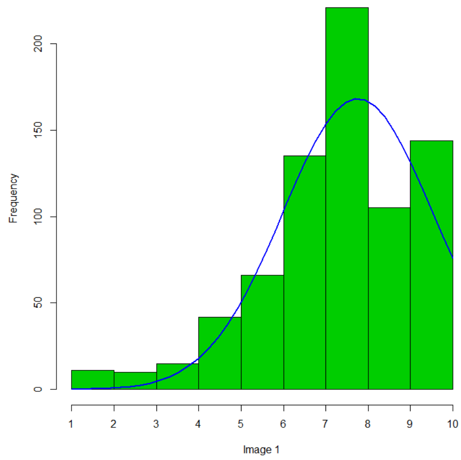


Figure A.5.1: Density Plot: Trustworthy company in what it says and what it does (Image 1)

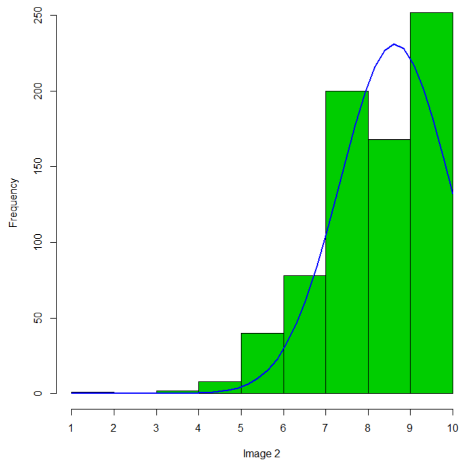


Figure A.5.2: Density Plot: Stable and market-based company (Image 2)

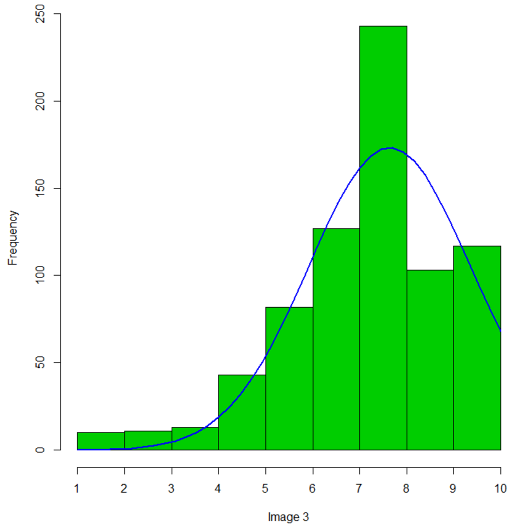


Figure A.5.3: Density Plot: Company with a positive contribution to society (Image 3)

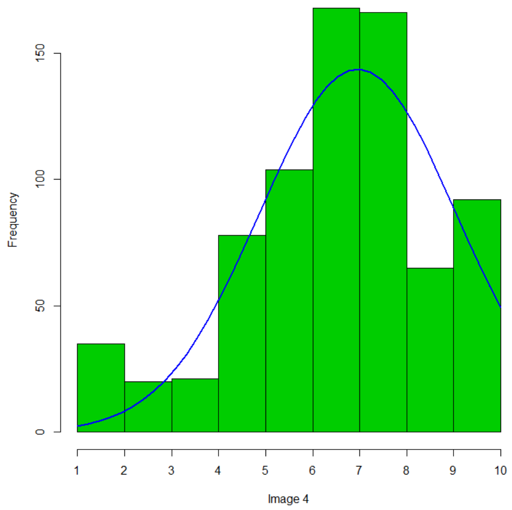


Figure A.5.4: Density Plot: Company that cares about customers (Image 4)

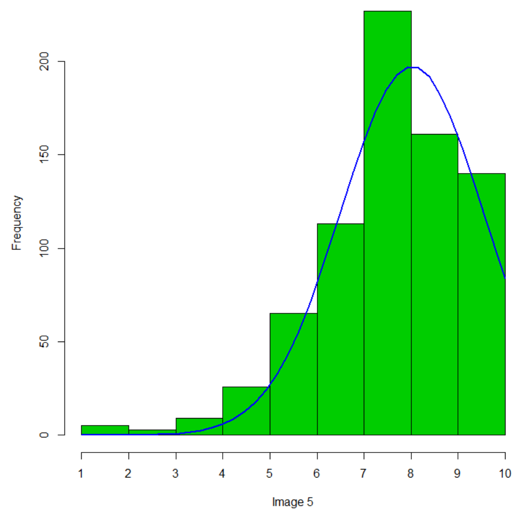


Figure A.5.5: Density Plot: Innovative and forward-looking company (Image 5)

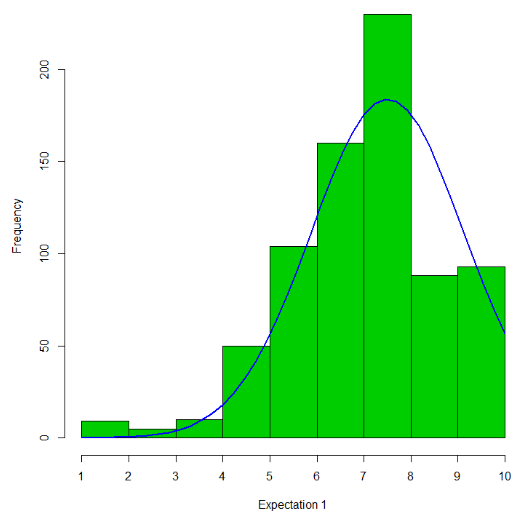


Figure A.5.6: Density Plot: Overall expectations about the company (Expectations 1)

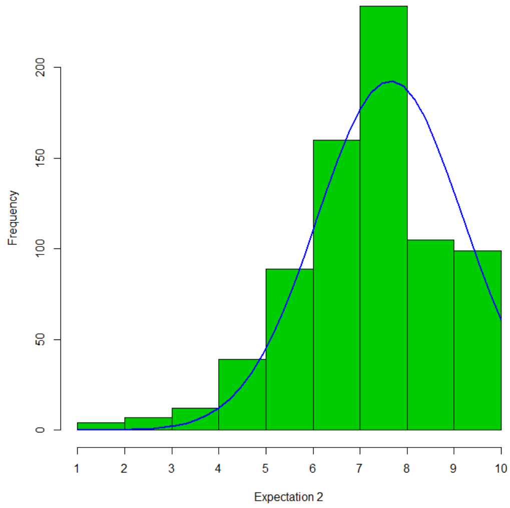


Figure A.5.7: Density Plot: Expectations about the company's ability to offer products and services that meet customer needs (Expectations 2)

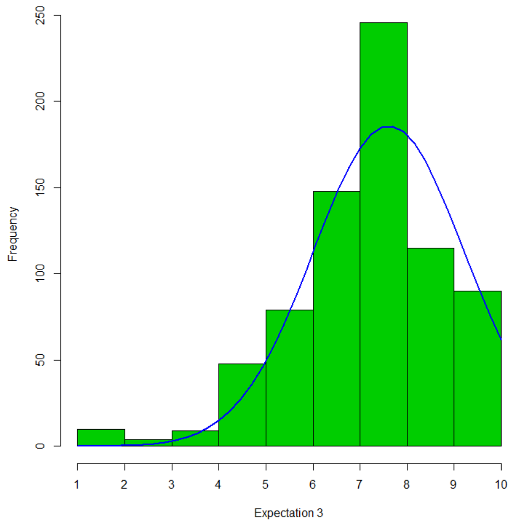


Figure A.5.8: Density Plot: Expectations regarding reliability, that is, how often things can go wrong (Expectations 3)

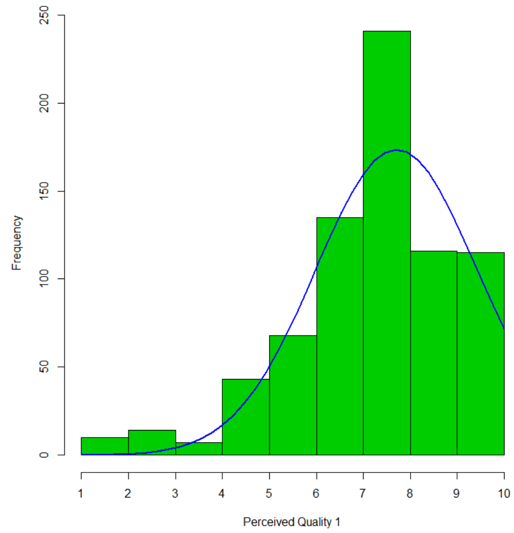


Figure A.5.9: Density Plot: Overall perceived quality (Perceived Quality 1)

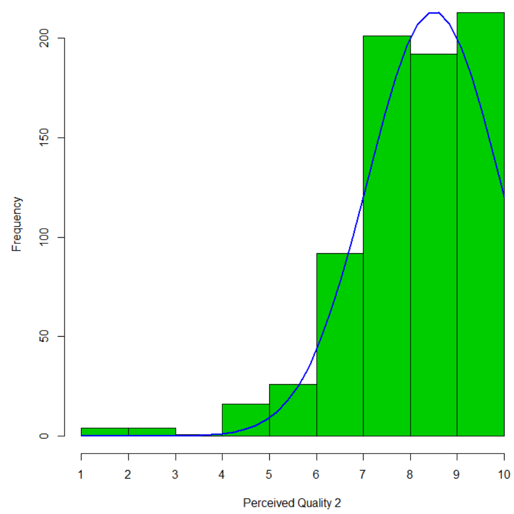


Figure A.5.10: Density Plot: Quality of electricity supply (Perceived Quality 2)

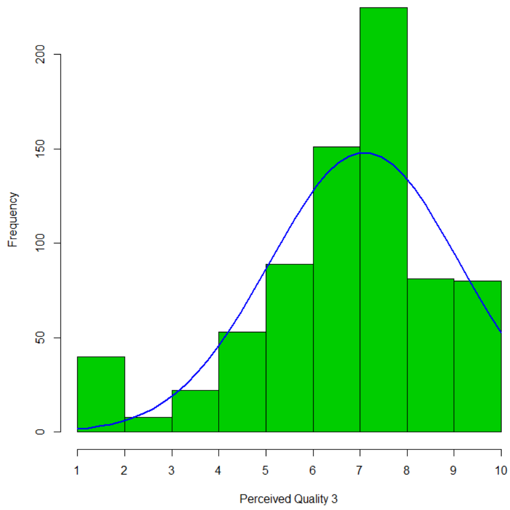


Figure A.5.11: Density Plot: Clarity and transparency in the information provided on safety, emergencies and consumption estimates (Perceived Quality 3)

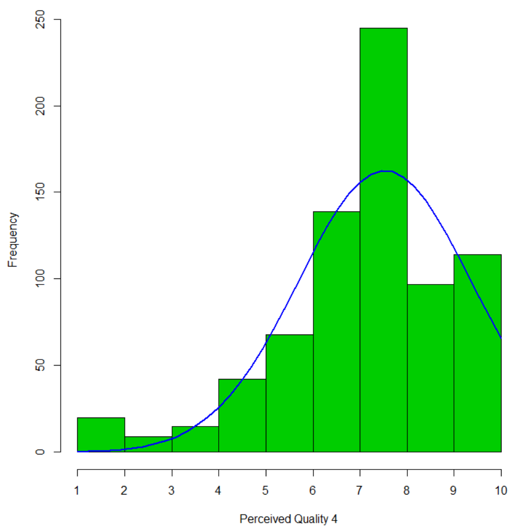


Figure A.5.12: Density Plot: Counselling and customer care (Perceived Quality 4)

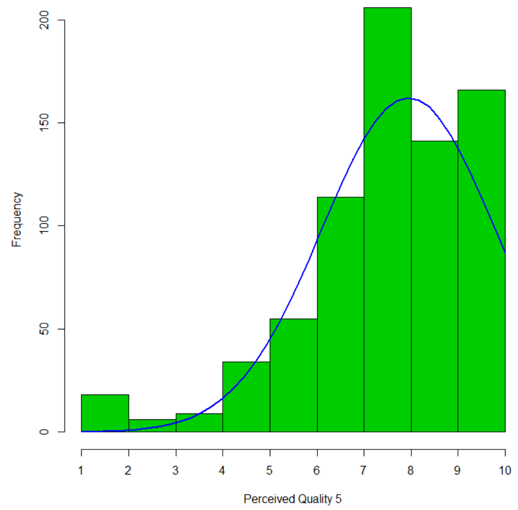


Figure A.5.13: Density Plot: Billing and payment services' reliability and quality (Perceived Quality 5)

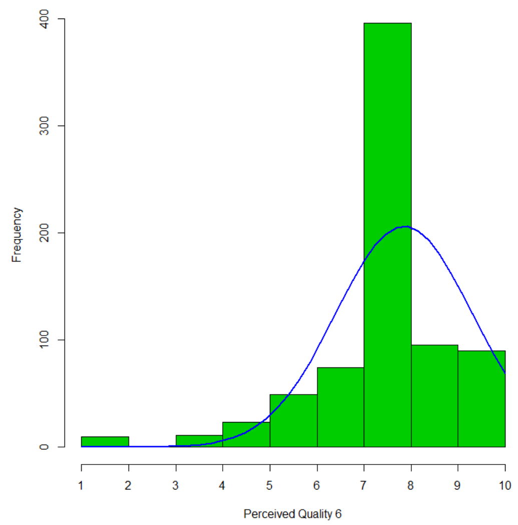


Figure A.5.14: Density Plot: Accessibility via digital channels to the provided services (Perceived Quality 6)

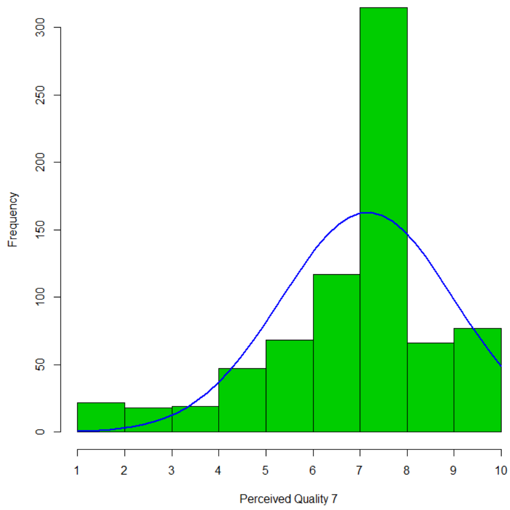


Figure A.5.15: Density Plot: Stores and agents accessibility and availability (Perceived Quality 7)

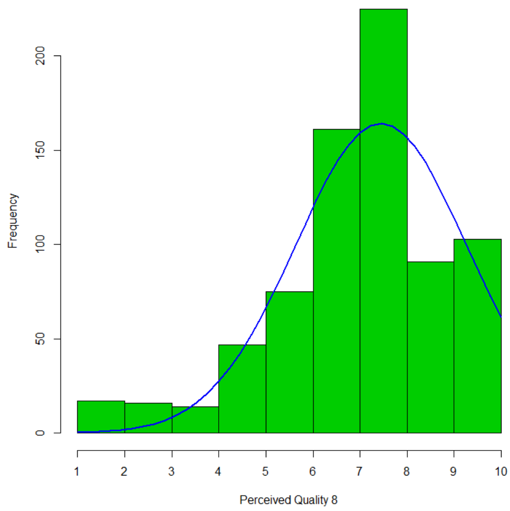


Figure A.5.16: Density Plot: Clarity and transparency in the information provided on contracting, billing and payment, complaints and commercial information (Perceived Quality 8)

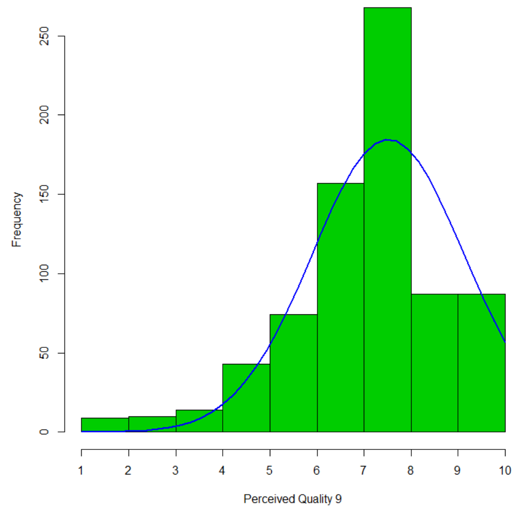


Figure A.5.17: Density Plot: Products and services' diversification (Perceived Quality 9)

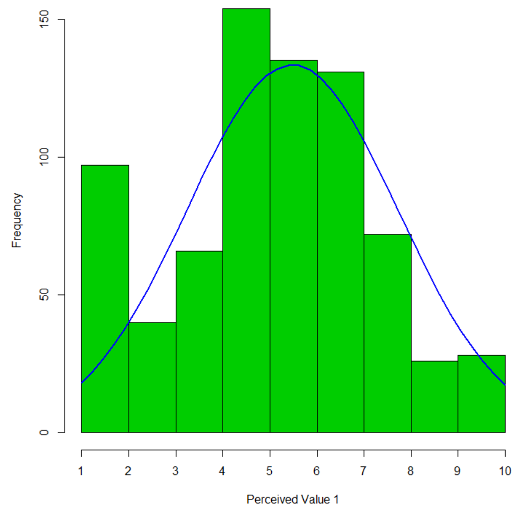


Figure A.5.18: Density Plot: Evaluation of the price paid, given the quality of products and services (Perceived Value 1)

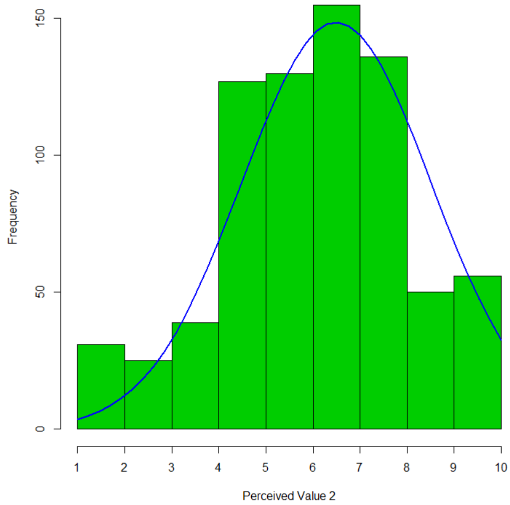


Figure A.5.19: Density Plot: Evaluation of the quality of products and services, given the price paid (Perceived Value 2)

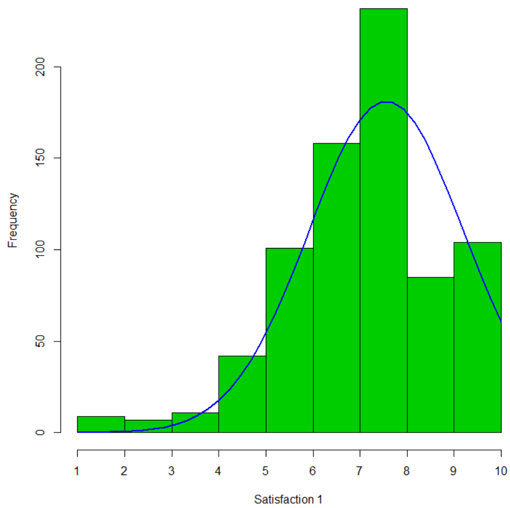


Figure A.5.20: Density Plot: Overall satisfaction with the company (Satisfaction 1)

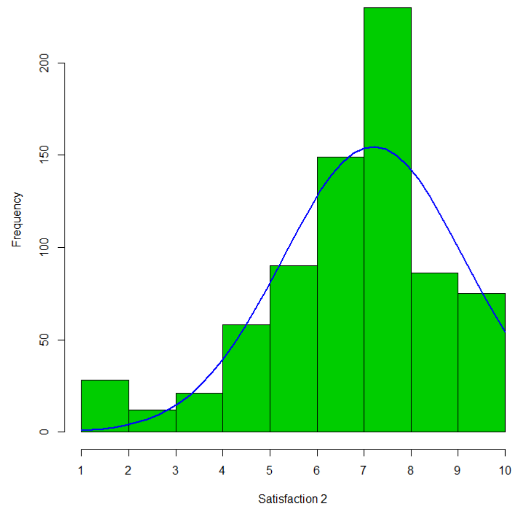


Figure A.5.21: Density Plot: Satisfaction compared to expectations (realization of expectations) (Satisfaction 2)

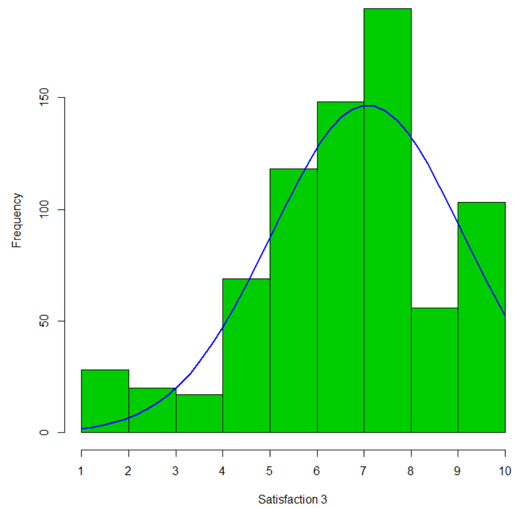


Figure A.5.22: Density Plot: Distance to the ideal electricity company (Satisfaction 3)

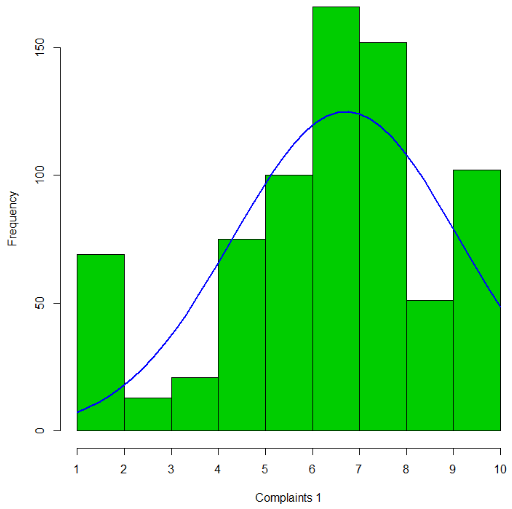


Figure A.5.23: Density Plot: Evaluation or Perceived evaluation of a complaint (Complaints 1)

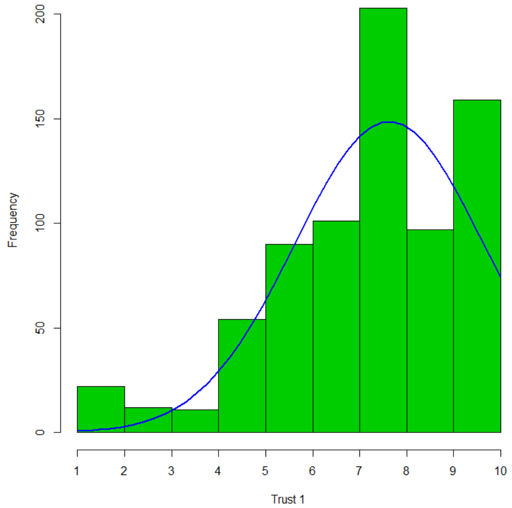


Figure A.5.24: Density Plot: Overall trust (Trust 1)

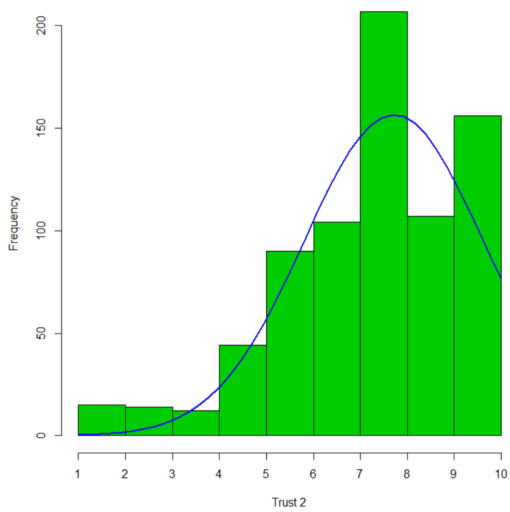


Figure A.5.25: Density Plot: Confidence in Company's performance (Trust 2)

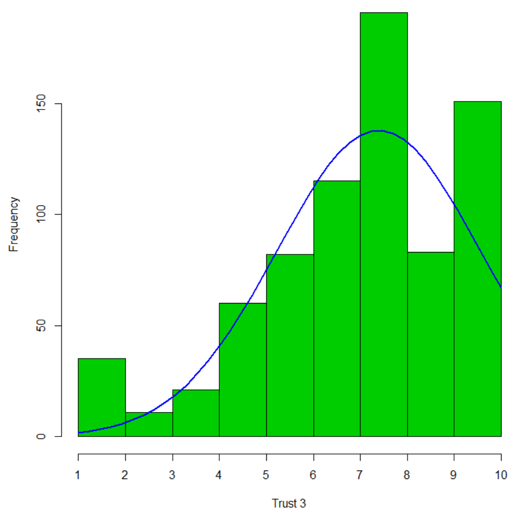


Figure A.5.26: Density Plot: Honesty in service providing (Trust 3)

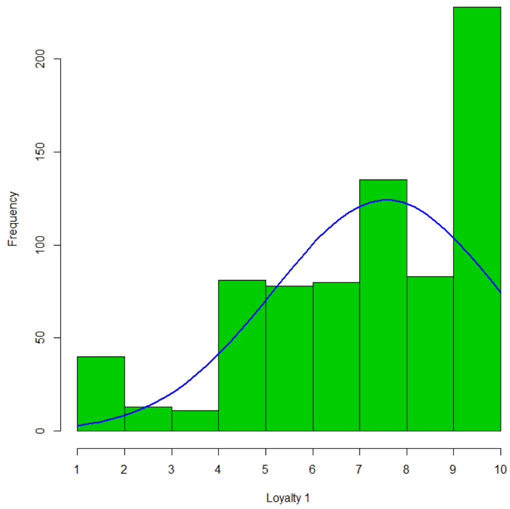


Figure A.5.27: Density Plot: Intention to remain as a customer (Loyalty 1)

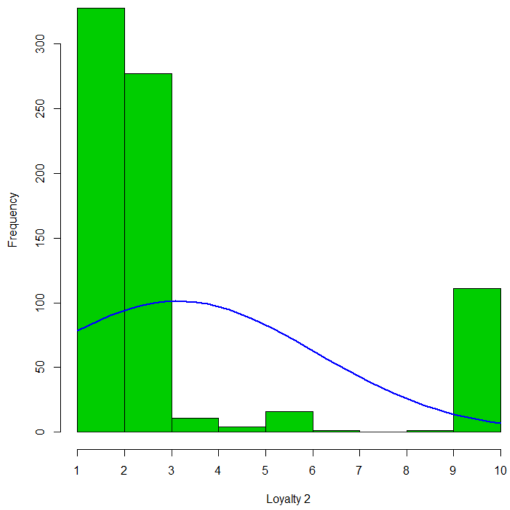


Figure A.5.28: Density Plot: Price sensitivity (Loyalty 2)

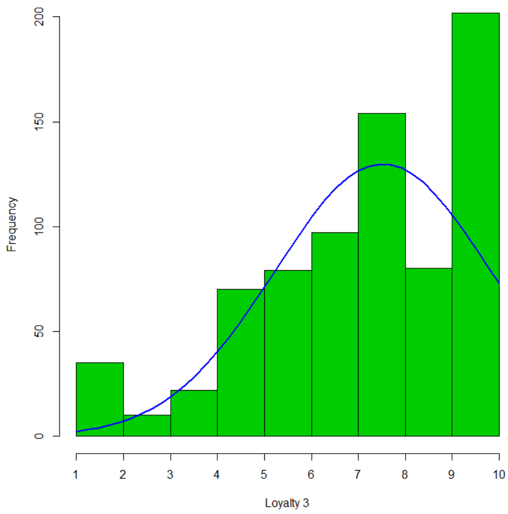


Figure A.5.29: Density Plot: Intention to recommend the company to colleagues and friends (Loyalty 3)

A.6 Application Outer Model Summary: Cross-Loadings

Manifest Variable	Image	Expectation	Perceived Quality	Perceived Value	Satisfaction	Complaints	Trust	Loyalty
Image 1	**0.87**	0.65	0.72	0.51	0.73	0.52	0.74	0.60
Image 2	**0.68**	0.49	0.50	0.30	0.43	0.31	0.41	0.38
Image 3	**0.84**	0.58	0.61	0.47	0.60	0.41	0.57	0.48
Image 4	**0.87**	0.60	0.72	0.54	0.73	0.55	0.70	0.58
Image 5	**0.82**	0.58	0.66	0.50	0.64	0.45	0.60	0.56
Expectation 1	0.66	**0.91**	0.65	0.50	0.64	0.45	0.61	0.51
Expectation 2	0.65	**0.93**	0.68	0.50	0.63	0.44	0.62	0.52
Expectation 3	0.61	**0.88**	0.64	0.48	0.61	0.42	0.58	0.49
Perceived Quality 1	0.79	0.73	**0.83**	0.59	0.82	0.60	0.79	0.67
Perceived Quality 2	0.47	0.53	**0.61**	0.46	0.49	0.34	0.48	0.42
Perceived Quality 3	0.63	0.57	**0.79**	0.51	0.62	0.46	0.63	0.51
Perceived Quality 4	0.66	0.57	**0.82**	0.52	0.69	0.54	0.69	0.60
Perceived Quality 5	0.59	0.53	**0.77**	0.47	0.61	0.44	0.61	0.54
Perceived Quality 6	0.50	0.46	**0.71**	0.43	0.52	0.42	0.54	0.45
Perceived Quality 7	0.47	0.45	**0.69**	0.46	0.51	0.42	0.48	0.39
Perceived Quality 8	0.66	0.57	**0.85**	0.54	0.71	0.55	0.69	0.58
Perceived Quality 9	0.61	0.57	**0.78**	0.56	0.63	0.50	0.61	0.53
Perceived Value 1	0.49	0.47	0.56	**0.92**	0.60	0.44	0.55	0.49
Perceived Value 2	0.57	0.53	0.66	**0.93**	0.69	0.50	0.64	0.61
Satisfaction 1	0.72	0.62	0.69	0.53	**0.84**	0.51	0.67	0.61
Satisfaction 2	0.66	0.60	0.75	0.67	**0.90**	0.60	0.74	0.68
Satisfaction 3	0.68	0.60	0.72	0.63	**0.89**	0.62	0.82	0.74
Complaints 1	0.56	0.48	0.63	0.51	0.66	**1.00**	0.70	0.63
Trust 1	0.71	0.63	0.76	0.59	0.81	0.66	**0.95**	0.74
Trust 2	0.71	0.65	0.75	0.62	0.80	0.63	**0.95**	0.72
Trust 3	0.70	0.61	0.78	0.60	0.78	0.68	**0.93**	0.70
Loyalty 1	0.58	0.54	0.66	0.60	0.73	0.57	0.71	**0.91**
Loyalty 2	0.25	0.19	0.23	0.20	0.28	0.22	0.27	**0.60**
Loyalty 3	0.67	0.57	0.70	0.58	0.79	0.67	0.80	**0.90**

Table 3: Outer Model Summary: Cross-Loadings

A.7 Application: Inner Model Summary

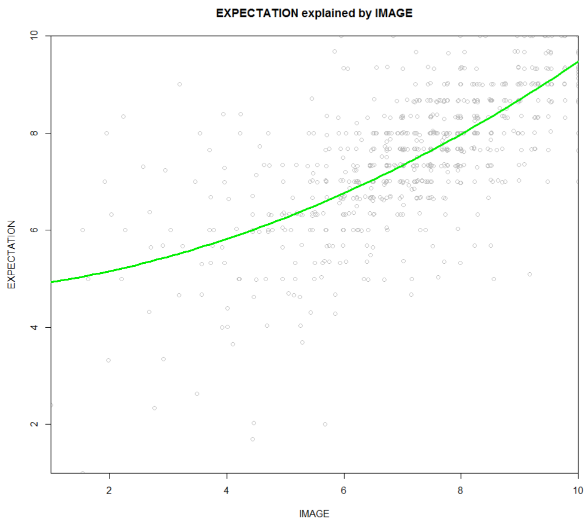


Figure A.7.1: Inner Model Summary: Expectation explained by Image

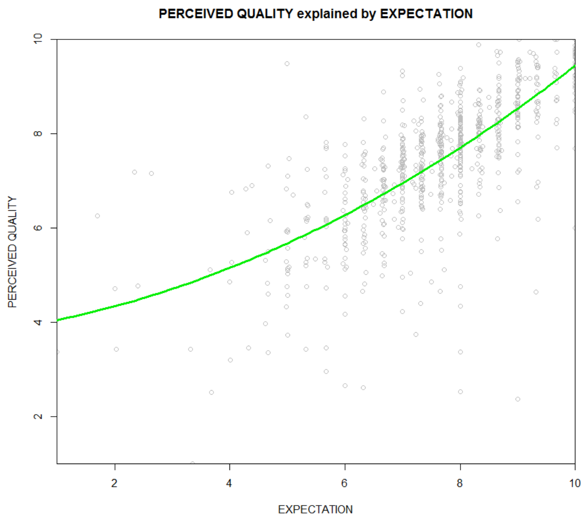


Figure A.7.2: Inner Model Summary: Perceived Quality explained by Expectation

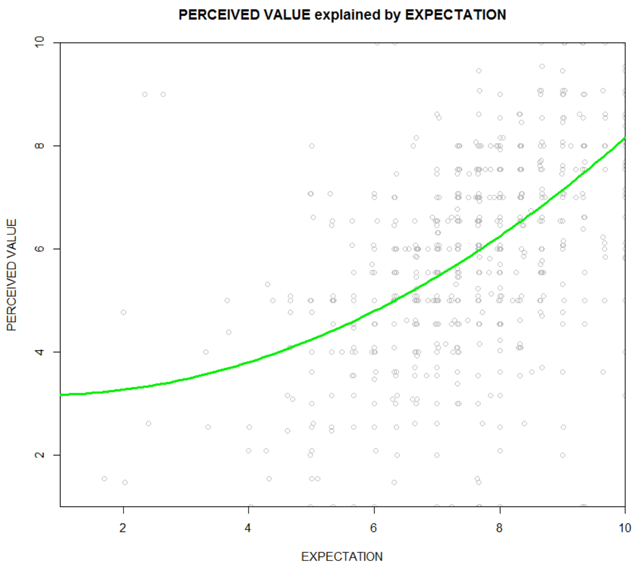


Figure A.7.3: Inner Model Summary: Perceived Value explained by Expectation

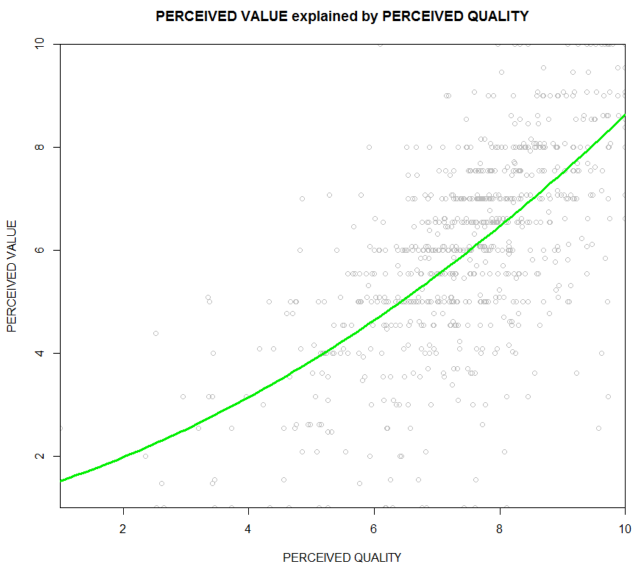


Figure A.7.4: Inner Model Summary: Perceived Value explained by Perceived Quality

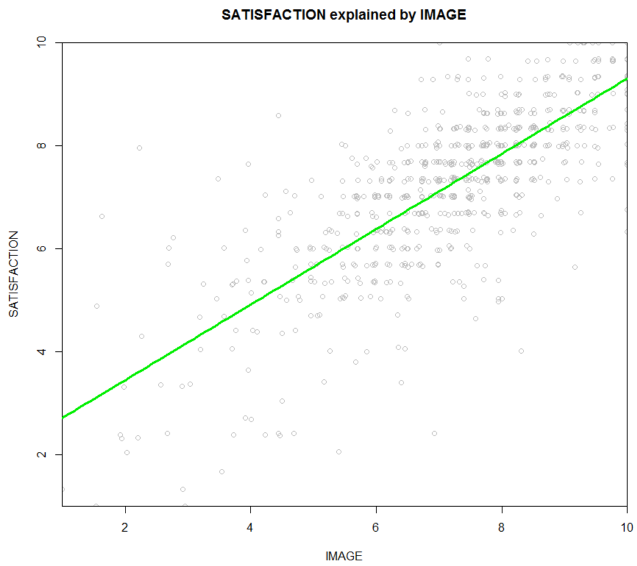


Figure A.7.5: Inner Model Summary: Satisfaction explained by Image

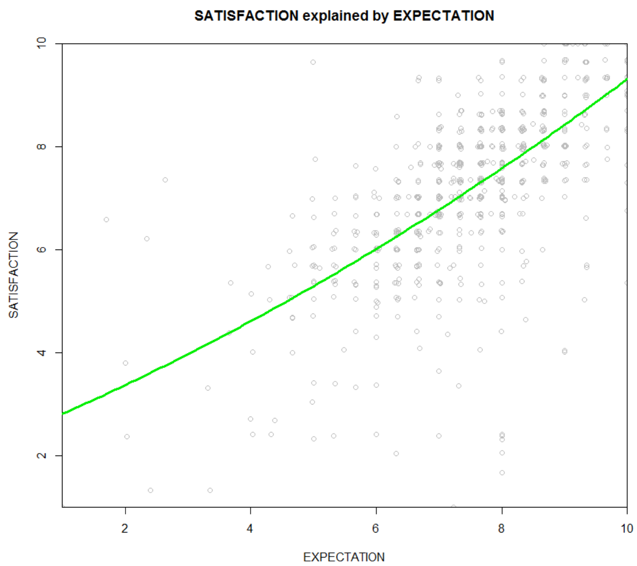


Figure A.7.6: Inner Model Summary: Satisfaction explained by Expectation

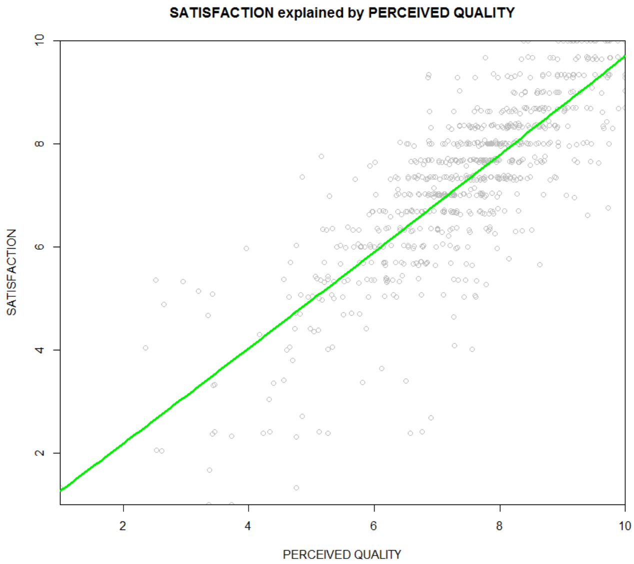


Figure A.7.7: Inner Model Summary: Satisfaction explained by Perceived Quality

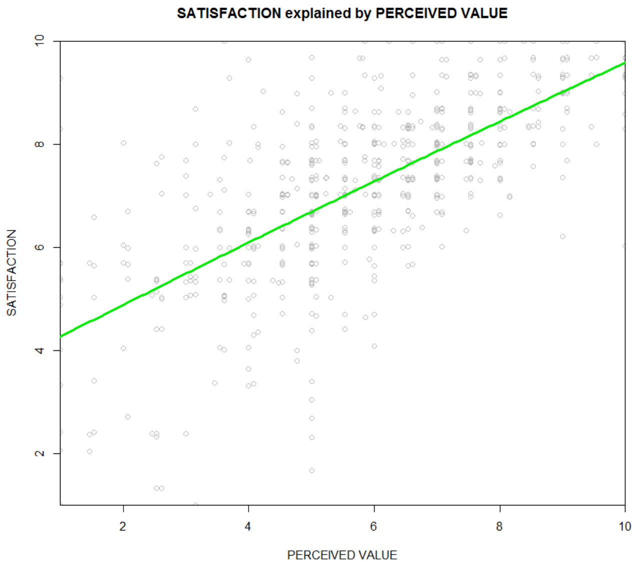


Figure A.7.8: Inner Model Summary: Satisfaction explained by Perceived Value

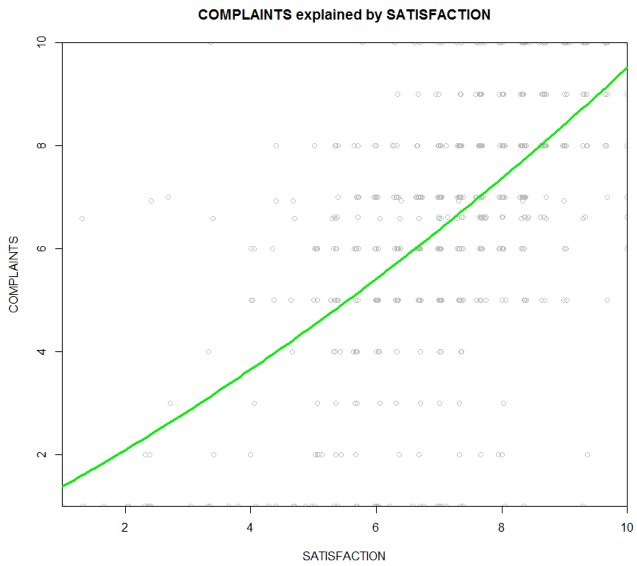


Figure A.7.9: Inner Model Summary: Complaints explained by Satisfaction

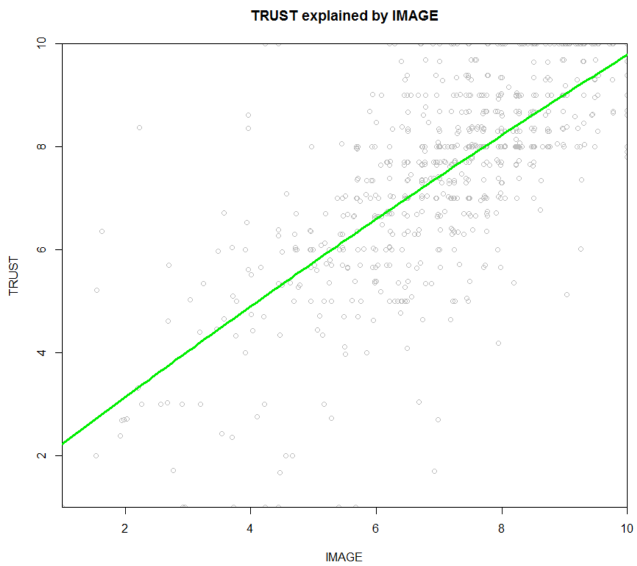


Figure A.7.10: Inner Model Summary: Trust explained by Image

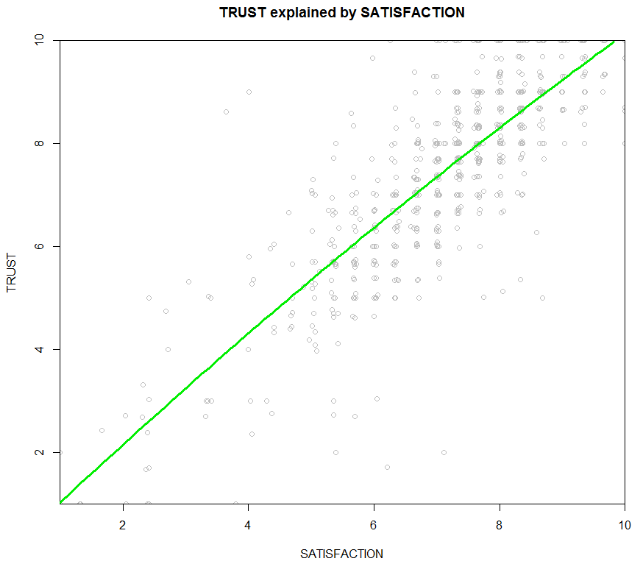


Figure A.7.11: Inner Model Summary: Trust explained by Satisfaction

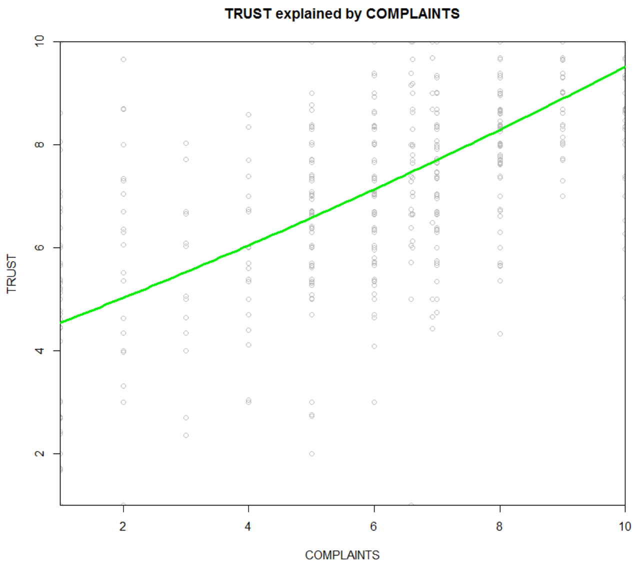


Figure A.7.12: Inner Model Summary: Trust explained by Complaints

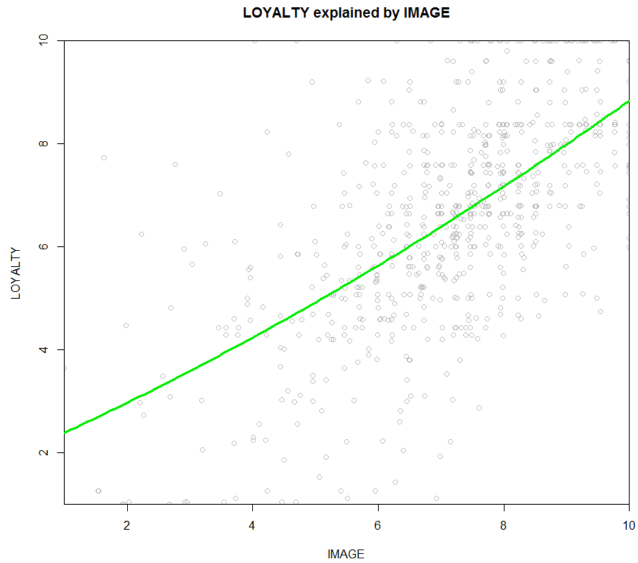


Figure A.7.13: Inner Model Summary: Loyalty explained by Image

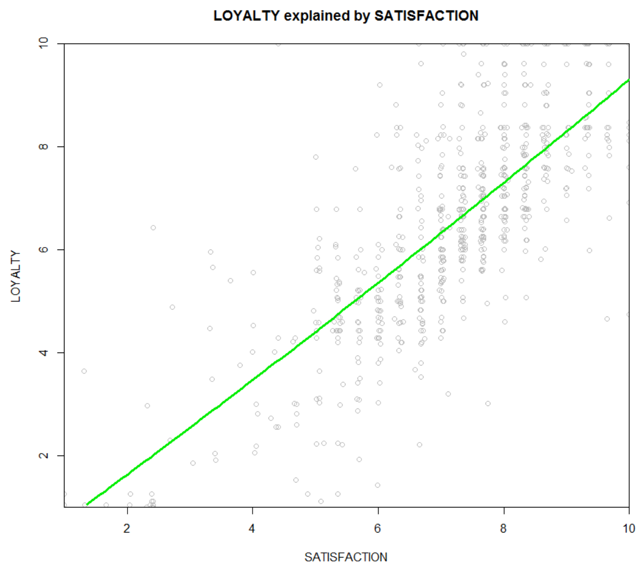


Figure A.7.14: Inner Model Summary: Loyalty explained by Satisfaction

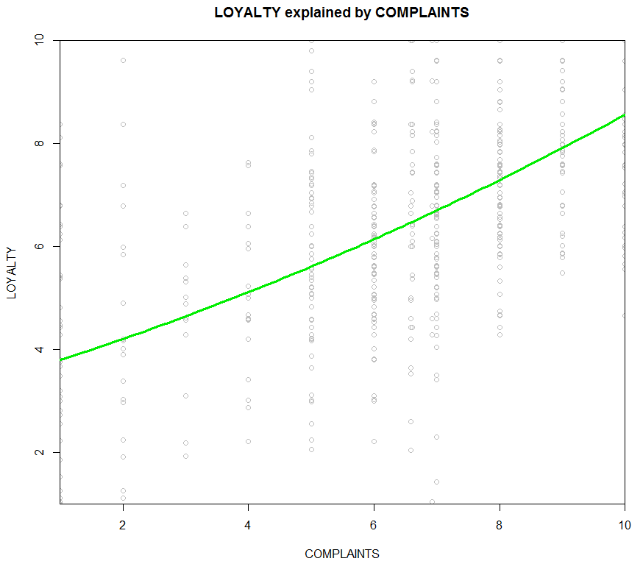


Figure A.7.15: Inner Model Summary: Loyalty explained by Complaints

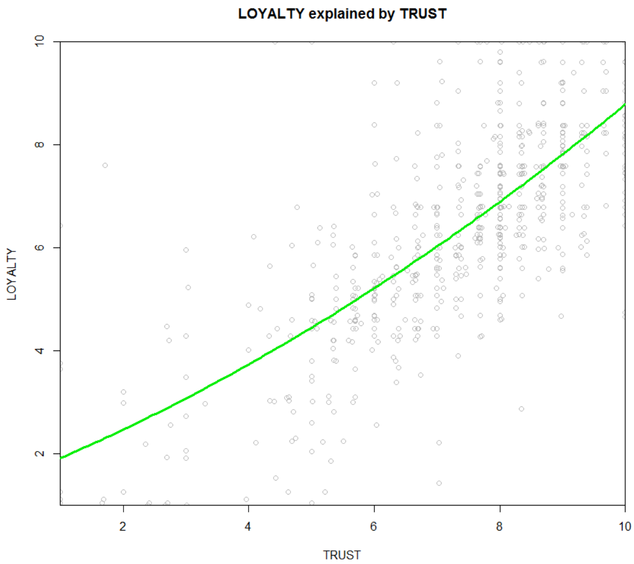


Figure A.7.16: Inner Model Summary: Loyalty explained by Trust