Beyond linearity - smooth weighting: a new Partial Least Squares - Path Modelling (PLS-PM) inner weighting scheme for detecting and approximating nonlinear structural relationships in Structural Equation Models*

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Abstract

A new inner weighting scheme for Partial Least Squares - Path Modelling (PLS-PM) is proposed to detect and approximate nonlinear structural relationships in Structural Equation Models (SEM). PLS-PM is an iterative method used for the estimation of Structural Equation Models (SEM), a widely used analytical tool for assessing causal relationships between latent variables. However, PLS-PM struggles to address the structural nonlinear relationships. To address this limitation, a new PLS-PM inner weighting scheme, *smooth weighting*, is proposed as an additional option to the traditional *centroid*, *factor*, and *path weighting* schemes. A real marketing dataset is used to demonstrate the usefulness of the method for finding evidence of nonlinearity, and a simulated dataset is used to assess its ability to approximate underlying (unknown) nonlinear structural relationships. The results show that the proposed scheme can recover several nonlinear functional forms, outperforming existing inner weighting schemes for commonly used sample sizes (larger than 75 units), regardless of the level of error contamination in the observed manifest variables.

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Contents

1 Introduction

Partial Least Squares - Path Modelling (PLS-PM) is one of the approaches used for estimation (Hair, Ringle, & Sarstedt, 2011) of Structural Equation Models (SEM) (Bollen, 1989; Hayduk, 1987), a widely used analytical tool for assessing plausible causal relationships between latent variables in many disciplines, including psychology, biology, management, economics, marketing, and medicine (Beran & Violato, 2010; Igolkina & Samsonova, 2018; Martínez-López, Gázquez-Abad, & Sousa, 2013; Reiss & Wolak, 2007; Wang & Rhemtulla, 2021; Williams, Vandenberg, & Edwards, 2009). However, PLS-PM, a iterative estimation method, struggles to address structural nonlinear relationships in its inner approximation stage. This study introduces and assesses a new PLS-PM inner weighting scheme to detect and approximate nonlinear structural relationships in structural equation relationships.

A SEM consists of two models: a measurement model (outer model) and a structural model (inner model). While the former groups manifest variables (observable variables or indicators) into corresponding latent variables (or constructs), the latter comprises a set of regression equations assessing the effects of explanatory latent variables on the dependent latent variable. Over the past 20 years, SEM, also referred to as a second-generation multivariate technique, has gained popularity (Elangovan & Rajendran, 2015; Hair et al., 2021; Igolkina & Samsonova, 2018).

Two approaches exist for estimating relationships in structural equation modelling: the covariance-based SEM (CB-SEM), mainly used for theory confirmation, and the variance-based SEM, also known as PLS-PM, commonly used for predicting causal relationships or confirming measurement (outer) models. Unlike CB-SEM, which uses the maximum likelihood (ML) estimation procedure, PLS-PM is based on ordinary least squares (OLS) and uses observable data (manifest variables) to estimate the structural relationships in the model, minimising the error terms (residual variance) of the endogenous latent variables. In other words, PLS-PM estimates the coefficients of path model relationships by maximising the R^2 values of the target endogenous latent variables.

Wold (1966) originally developed the PLS-PM technique through research devoted to nonlinear iterative least squares, which is the underlying idea of PLS-PM, in which structural equations are specified in linear parametric forms.

In the application framework of SEM and PLS-PM, it is common to find relationships between latent variables that are nonlinear in nature (see Tuu & Olsen (2010), for an extensive review of the relationships between satisfaction and loyalty used in the marketing literature).

Nevertheless, the nonlinear approaches to SEM are almost exclusively developed in the context of CB-SEM or Bayesian approaches. The former approaches include, for example, the work of Kenny & Judd (1984), who describe a procedure to estimate the nonlinear and interactive effects of latent variables in structural equation models, given that the latent variables are normally distributed. Pek, Sterba, Kok, & Bauer (2009) overview a semiparametric approach to modelling nonlinear relationships among latent variables using mixtures of linear structural equations. Marsh, Wen, & Hau (2004) propose an unconstrained approach to estimate interactions between latent variables through product indicators. A. Klein & Moosbrugger (2000) introduce a general interaction model with multiple latent interaction effects estimated by maximum likelihood via adaptation of an EM algorithm (latent moderated structural equations - LMS). A. G. Klein & Muthén (2007) introduce a nonlinear structural equation model where estimation is accomplished via a proposed quasi-maximum likelihood method for simultaneous estimation and testing of multiple nonlinear effects (quasi-maximum likelihood - QML). Kelava et al. (2011) compare the LMS (A. Klein & Moosbrugger, 2000) and QML (A. G. Klein & Muthén, 2007) estimators with product indicator approaches. Kelava, Nagengast, & Brandt (2014) extend previous work to the description of a nonlinear structural equation mixture approach that integrates the strength of parametric approaches (specification of the nonlinear functional relationship) and the flexibility of semiparametric structural equation mixture approaches to approximate the nonnormality of latent predictor variables. Nevertheless, all these approaches are limited to the consideration of interactions and quadratic effects. More recently, using a Bayesian approach, attention has been directed to the use of smoothers and additive models as a means to approximate nonlinear relationships between latent variables. Indeed, Song and Lu (2010) and Song, Lu, Cai, & Ip (2013) developed semiparametric models where the relationships between latent variables are described by an additive structural equation formulated by a series of unspecified smooth functions (Bayesian P-splines).

With the exception of the work by Henseler, Fassott, Dijkstra, & Wilson (2012), where four different PLS-PM approaches to estimate quadratic effects are compared, and the work of Bauer, Baldasaro, & Gottfredson (2012), which uses an adhoc two-stage methodology to diagnose the functional form of the structural relationships using latent variable scores estimated by the PLS-PM algorithm, no attempt has been made to endow the traditional PLS-PM algorithm with the ability to approximate nonlinear relationships in inner model estimation.

Although it has been suggested that PLS-PM can model nonlinear relationships between structural latent variables (Wold, 1982), the functional forms of the nonlinear relationships between latent variables have to be specified prior to data analysis (Henseler et al., 2012), or the nonlinear nature of the relationship is simply a result of interaction effects (Chin, Marcolin, & Newsted, 2003). Moreover, strict parametric forms are likely to miss subtle patterns. Customer satisfaction, for instance, could rapidly increase with an initial increase in perceived quality of service but then taper off with a further increase in perceived quality (Song et al., 2013).

To the best of author's knowledge, previous work on addressing non-linear relationships have been limited to interaction or quadratic effects. Also, with the exception of Henseler et al. (2012) work where four different PLS-SEM approaches to estimation of quadratics effects are compared and the work of Bauer et al. (2012) which uses an adhoc two stage methodology to diagnosis the functional form of the structural relationships using latent variable scores estimated by PLS-SEM traditional algorithm, no attempt has been made to endow traditional PLS-SEM algorithm with the ability to approximate non-linear relationships in inner model estimation.

With advances in statistical methods and computational technology, semiparametric and non-parametric modelling methods based on different smoothing techniques have become more accessible. These methods include smoothing splines and penalised splines (Wood, 2017). Smoothing offers a valuable alternative to traditional regression techniques. By emphasising patterns and trends in the data rather than fitting complex models, smoothing provides simplicity and interpretability. It excels in capturing the underlying structure of noisy or irregular data, making it particularly useful for exploratory data analysis and visualisation. Smoothing techniques, such as spline smoothing, offer flexibility to adapt to different data shapes and can effectively handle outliers. Moreover, they often require fewer assumptions than regression, reducing the risk of overfitting. Smoothing's ability to unveil hidden patterns and relationships in data makes it a powerful tool for gaining insight and simplifying complex datasets.

In this paper, we extend the traditional non-parametric PLS-PM algorithm to approximate nonlinear relationships between latent variables by proposing a new weighting scheme for inner approximation. The approximation of the structural relationships of any shape is enabled by the incorporation of additive models (Wood, 2017). Furthermore, the proposed framework, when used as an exploratory tool, enables researchers to visually examine and interpret the functional relationship between latent variables of interest. Indeed, based on a plot of the smooth fitted functions, a researcher can determine whether the relationship is sufficiently smooth and linear to be captured by a simple linear functional form. More importantly, the proposed framework is compared with PLS-PM using the quality measures that are widely applied by researchers in this field. This assessment is performed with both real and simulated data in a Monte Carlo simulation study.

To the best of our knowledge, no existing work has jointly addressed all the aforementioned issues and proposed a general framework to assess and estimate nonlinear structural relationships in PLS-PM.

The remainder of this paper is organised as follows. Section 2.1 describes the traditional PLS-PM approach and its consistent extension. Section 2.1 presents the new inner weighting scheme to incorporate the estimation of nonlinearities in the structural model, the so-called *smooth weighting* scheme. Section 2.2 describes the data used in the three examples. The actual dataset used in the first example is detailed in Section 2.2.1, and the details of the dataset resulting from a Monte Carlo simulation, including different nonlinear relationships in which the second example is based, are described in Section 2.2.2. Details of the software implementation of this algorithm are presented in Section 2.3. The results obtained in the first example and its comparison with those produced by the benchmark software are reported in Section 3.1. In Section 3.2, the performance of the proposed methodology is assessed against the traditional PLS-PM algorithm, and the results of the bias and root mean square error are detailed. The article ends with a discussion of the main results in Section 4.

2 Material and methods

2.1 A new PLS-PM inner weighting scheme: *smooth weighting*

The PLS-PM algorithm was originally developed by Wold (1966) in 1966 and later extended by Lohmöller (1989). This algorithm estimates the path coefficients of the structural model, and the weights and loadings of the manifest variables to maximise the explained variance of the endogenous latent variables. Tenenhaus, Vinzi, Chatelin, & Lauro (2005) and Hair et al. (2021) provide detailed descriptions of the stages of the PLS-PM algorithm. For illustration, we describe the algorithm as presented by Henseler, Ringle, & Sinkovics (2009) and Henseler et al. (2012) and rely also on Schamberger, Schuberth, Henseler, & Dijkstra (2020). Although this description is well-known, we reproduce it to establish a basis for the presentation of the novel *smooth weighting* scheme. The transcribed text is in italics, except for parts added by the authors.

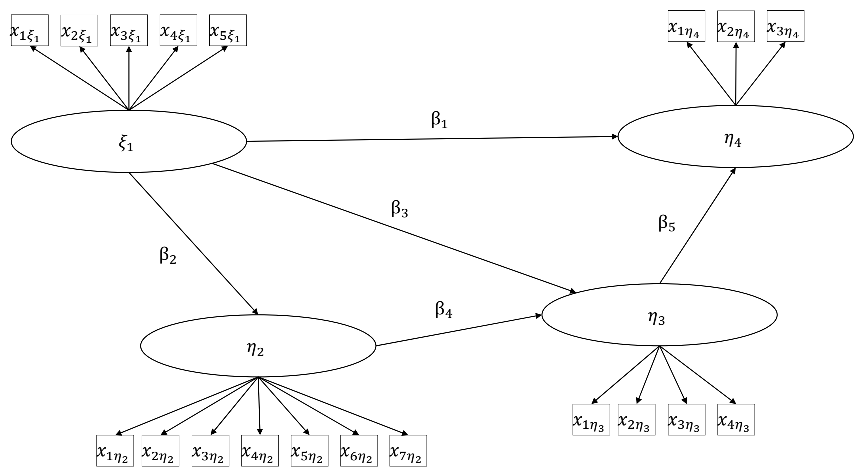

Figure 1: Example of a simple structural equation model with four latent variables and nineteen indicators

The PLS-PM algorithm is essentially a sequence of regressions in terms of weight vectors. [...] The basic PLS-PM algorithm, as suggested by Lohmöller (1989), includes the following three stages:

Stage 1: Iterative estimation of latent variables scores, consisting of a four-step iterative procedure that is repeated until convergence is obtained: (1) outer approximation of the latent variable scores, (2) estimation of the inner weights, (3) inner approximation of the latent *variable scores,and (4) estimation of the outer weights.*

Stage 2: Estimation of outer weights/loadings and path coefficients.

Stage 3: Estimation of location parameters.

[. . .]

These four steps are repeated until the change in outer weights between two iterations drops below a predefined limit. The algorithm terminates after step 1, delivering latent variable scores for all latent variables. Loadings and inner regression coefficients are then calculated in a straight forward way, given the constructed indices. In order to determine the path coefficients, for each endogenous latent variable a (multiple) linear regression is conducted.

Foreseeing its utility to illustrate our proposed novel approach, the notation used to depict the algorithm steps is established here. The model depicted in Figure 1 is used as a role model.

The structural model depicted in Figure 1 corresponds to the following set of structural equations:

$$
\begin{aligned}
\xi_1 &= \xi_1 + 0 \\
\eta_2 &= \beta_2 \xi_1 + \epsilon_1 \\
\eta_3 &= \beta_3 \xi_1 + \beta_4 \eta_2 + \epsilon_2 \\
\eta_4 &= \beta_1 \xi_1 + \beta_5 \eta_3 + \epsilon_3
\end{aligned}
\tag{2.1}
$$

We distinguish between exogenous latent variables, not explained by the model and therefore having no arrows ending on them (having no *predecessors*), and represented by ($\xi_{(\bullet)}$), and endogenous latent variables, explained by the model and having arrows ending or leaving them (can have *predecessors* or *successors*), and represented by ($\eta_{(\bullet)}$).

A model adjacency matrix, $\mathbf{D}$ is defined to represent the structural model. The entries of $\mathbf{D}$ are either 0 or 1. If entry $d_{ij} = 1$, latent variable i is a predecessor of latent variable j, and 0 otherwise. The matrix $\mathbf{D}$ is structured as an upper triangular matrix. *Exogenous* latent variables do not have *predecessors* in the structural model and correspond to variables where the *diagonal element is not zero.*

The structural model in Figure 1, for example, has only one exogenous latent variable, (ξ_1). The remaining variables, η_2, η_3, and η_4 are endogenous.

The structural model adjacency matrix $\mathbf{D}$ representing the model of Figure 1 is:

$$\mathbf{D} = \begin{array}{c} \\ \xi_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{array} \begin{array}{c} \begin{array}{cccc} \xi_1 & \eta_2 & \eta_3 & \eta_4 \end{array} \\ \begin{pmatrix} 1 & 1 & 1 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \end{pmatrix} \end{array} \tag{2.2}$$

Let us generically denote by $\boldsymbol{\mathcal{V}}' = (\boldsymbol{\xi}', \boldsymbol{\eta}')$ the vector of model's exogenous and endogenous latent variables. Its cardinality, denoted by $\#(\boldsymbol{\mathcal{V}})$ is H, and $\mathcal{V}_h$, $h = 1, \dots, H$ is the h^{th} element of $\boldsymbol{\mathcal{V}}$. Denote by $\boldsymbol{\beta}$ the matrix containing the structural coefficients, $\beta_{(\bullet)}$, wherever the adjacency matrix $\mathbf{D}'$ has ones, and ones wherever the adjacency matrix $\mathbf{D}'$ has zeros (for exogenous latent variables), and zero elsewhere.

Regarding the model in Figure 1, $\boldsymbol{\mathcal{V}}' = (\xi, \eta_1, \eta_2, \eta_3)$, $H = \#(\boldsymbol{\mathcal{V}}) = 19$ and $\boldsymbol{\beta}$ is:

$$\boldsymbol{\beta} = \begin{array}{c} \\ \xi_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{array} \begin{array}{c} \begin{array}{cccc} \xi_1 & \eta_2 & \eta_3 & \eta_4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ \beta_2 & 0 & 0 & 0 \\ \beta_3 & \beta_4 & 0 & 0 \\ \beta_1 & 0 & \beta_5 & 0 \end{pmatrix} \end{array} \tag{2.3}$$

Furthermore, let us denote by $\boldsymbol{\varepsilon}'$ the vector of measurement errors of structural equations.

In the case of the model represented in Figure 1, described by the system of equations (2.1), $\boldsymbol{\varepsilon}' = (0, \epsilon_2, \epsilon_3, \epsilon_4)$, and the structural model equations can be defined in matrix format as:

$$\boldsymbol{\mathcal{V}} = \boldsymbol{\mathcal{V}}\boldsymbol{\beta} + \boldsymbol{\varepsilon}, \tag{2.4}$$

where $\boldsymbol{\varepsilon}$ are assumed to be centred, i.e., $\mathrm{E}(\boldsymbol{\varepsilon}) = \mathbf{0}$.

Any exogenous latent variable, such as $\xi_{(\bullet)}$, and any endogenous latent variable, $\eta_{(\bullet)}$ are unobservable variables (or constructs) indirectly described by a block of *manifest variables* $\mathbf{x}_{(\bullet)}$, frequently also called *indicators*.

There are three ways to relate the manifest variables to their latent variables, respectively, called the **reflective** way, the **formative** one, and the **MIMIC** way. The changes in the PLS-PM method we propose in this work concern only the inner model approximation of the latent variable scores and the final estimation of structural relationships. Therefore, we do not detail here none of them as the reader can find a very detailed description in Tenenhaus et al. (2005).

Let x_{ph}, $p = 1, \dots, P_h$ and $h = 1, \dots, H$, be a set of P_h manifest variables or indicators related to latent variable $\mathcal{V}_h$, whatever the way (reflective, formative or MIMIC).

Additionally, let $\mathbf{w}_h$, $h = 1, \ldots, H$, be a column vector of length P_h. The $((P_1 + P_2 + \cdots + P_H) \times H)$ matrix of the outer weights $\mathbf{W}$, referred to in Stage 1 of the PLS-PM algorithm is composed of H blocks, corresponding the indicator vectors $\mathbf{x}'_h = (x_{1h}, \ldots, x_{ph})$, $p = 1, \ldots, P_h$ and $h = 1, \ldots, H$:

$$\mathbf{W} = \begin{array}{c} \\ \xi_1 \\ \cdots \\ \xi_h \\ \eta_{h+1} \\ \vdots \\ \eta_H \end{array} \begin{array}{c} \begin{array}{cccccc} \xi_1 & \cdots & \xi_h & \eta_{h+1} & \cdots & \eta_H \end{array} \\ \begin{pmatrix} \mathbf{w}_1 & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \ddots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{w}_h & \mathbf{0} & \cdots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{w}_{h+1} & \cdots & \vdots \\ \vdots & \ddots & \ddots & \ddots & \ddots & \mathbf{0} \\ \mathbf{0} & \cdots & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{w}_H \end{pmatrix} \end{array} \tag{2.5}$$

Regarding model depicted in Figure 1, $\mathbf{W}$ is:

$$\mathbf{W} = \begin{array}{c} \xi_1 \\ \eta_2 \\ \eta_3 \\ \eta_4 \end{array} \begin{array}{c} \begin{array}{cccc} \xi_1 & \eta_2 & \eta_3 & \eta_4 \end{array} \\ \begin{pmatrix} w_{11} & 0 & 0 & 0 \\ w_{21} & 0 & 0 & 0 \\ w_{31} & 0 & 0 & 0 \\ w_{41} & 0 & 0 & 0 \\ w_{51} & 0 & 0 & 0 \\ 0 & w_{12} & 0 & 0 \\ 0 & w_{22} & 0 & 0 \\ 0 & w_{32} & 0 & 0 \\ 0 & w_{42} & 0 & 0 \\ 0 & w_{52} & 0 & 0 \\ 0 & w_{62} & 0 & 0 \\ 0 & w_{72} & 0 & 0 \\ 0 & 0 & w_{13} & 0 \\ 0 & 0 & w_{23} & 0 \\ 0 & 0 & w_{33} & 0 \\ 0 & 0 & w_{43} & 0 \\ 0 & 0 & 0 & w_{14} \\ 0 & 0 & 0 & w_{24} \\ 0 & 0 & 0 & w_{34} \end{pmatrix} \end{array} \tag{2.6}$$

The adjacency matrix of the measurement model, $\mathbf{M}$, has the same structure as the matrix of outer weights $\mathbf{W}$ and it is used for the initialisation, as we will see, when the PLS-PM algorithm is described further ahead. If the entry $m_{ph} = 1$, the manifest variable x_{ph} is one of indicators of latent variable $\mathcal{V}_h$, $p = 1, \ldots, P_h$, $h = 1, \ldots, H$. The matrix $\mathbf{M}$ includes no information about the direction. So it does not tell us anything about the measurement mode of the blocks.

In the model represented in Figure 1, for instance, the manifest variables $x_{1_\xi}, x_{2_\xi}, x_{3_\xi}, x_{4_\xi}, x_{5_\xi}$, are indicators of the latent variable ξ_1. Therefore, the adjacency matrix of the measurement model represented in Figure 1 is:

$$\mathbf{M} = \begin{array}{c} \\ x_{1_{\xi_1}} \\ x_{2_{\xi_1}} \\ x_{3_{\xi_1}} \\ x_{4_{\xi_1}} \\ x_{5_{\xi_1}} \\ x_{1_{\eta_2}} \\ x_{2_{\eta_2}} \\ x_{3_{\eta_2}} \\ x_{4_{\eta_2}} \\ x_{5_{\eta_2}} \\ x_{6_{\eta_2}} \\ x_{7_{\eta_2}} \\ x_{1_{\eta_3}} \\ x_{2_{\eta_3}} \\ x_{3_{\eta_3}} \\ x_{4_{\eta_3}} \\ x_{1_{\eta_4}} \\ x_{2_{\eta_4}} \\ x_{3_{\eta_4}} \end{array} \begin{array}{c} \begin{array}{cccc} \xi_1 & \eta_2 & \eta_3 & \eta_4 \end{array} \\ \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 1 \end{pmatrix} \end{array} \tag{2.7}$$

On the other hand, let $\mathbf{X}$ be the manifest variables matrix, having n rows, the sample size, and $(P_1 + \cdots + P_H)$ columns, the number of manifest variables.

The description of the PLS-PM algorithm and the incorporation of the nonlinearities estimation in inner approximation of the structural model results in a new inner weighting scheme named *smooth weighting* follows. Indeed, as Wold observed, PLS-PM can incorporate nonlinearities in the structural model through the hybrid approach (Wold, 1982) by including internal proxies for each nonlinear term during the iterative PLS-PM algorithm runtime. Based on this concept, we propose a **smoothing-based hybrid approach**.

Splines belong to to the broad class of regression models that are used to estimate a smooth function that represents the underlying trend of a set of data points. They are particularly useful when dealing with noisy data or when the relationship between variables is not well defined. Splines strike a balance between fitting the data closely and ensuring that the estimated curve remains smooth, making them a valuable tool in various scientific disciplines including statistics (Wahba, 2011), economics (Akhrif, Delgado-Márquez, Kouibia, & Pasadas, 2022), biology (Irizarry, 2004; Mullah, Hanley, & Benedetti, 2021), and engineering (Early & Sykulski, 2020; Utreras, 1990) projects. Smoothing splines can be used as a flexible tool for nonlinear regression, in which the relationship between the response and predictor variables is not linear. They are particularly useful when the functional form of the relationship is unknown.

Regression splines are constructed by selecting a basis and specifying the set of functions for which the function b is an element. This involves selecting basis functions, which are treated as known quantities; for example, if $b_j(x)$ is the j^{th} basis function, then f is represented as follows:

$$f(x; \boldsymbol{\alpha}, \mathbf{b}) = \sum_{j=1}^{K} \alpha_j b_j(x) \tag{2.8}$$

for some values of the unknown parameters, α_j, $j = 1, \ldots, K$. The model in (2.8) is linear in the parameters and penalised least squares may be employed to estimate the parameters α_j, $j = 1, \ldots, K$ with an appropriate degree of smoothing.

Here the choice of basis functions relies on the cubic regression splines (Wood, 2017). They are penalised by the conventional integrated square second derivative cubic spline penalty (Wood, 2017). Cubic regression splines are a very flexible class of smoothing functions and they might be combined additively when the dependent variable, y, is a function of several regressors. They result in a piecewise continuous linear additive model as follows:

$$y_i = f_1(x_{1i}; \boldsymbol{\alpha}_1, \mathbf{b}_1, K_1) + \cdots + f_L(x_{Li}; \boldsymbol{\alpha}_L, \mathbf{b}_L, K_L) + \epsilon_i \tag{2.9}$$

where $x_1, \ldots, x_L$, are regressor variables, f_l, $l = 1, \ldots, L$, are univariate cubic regression splines (Wood, 2017, p. 198), $\mathbf{b}_l' = (b_{l,1}(x), \ldots, b_{l,K_l}(x))$ is the vector of the K_l basis functions f_L is composed of and $\boldsymbol{\alpha}_l' = (\alpha_{l,1}, \ldots, \alpha_{l,K_l})$, is the vector of associated coefficients, and the ϵ_i are independent and identically distributed random variables such that $\mathrm{E}(\epsilon_i) = 0$. The cubic regression spline basis of $f_l(x_l)$ is defined by a set of K_l knots, $l = 1, \ldots, L$ spread evenly through the regressor variables domain. Thus, the nonlinear regression problem is split into several small linear regression problems using a set of transformations of the input variable(s), allowing the data to decide which transformations are important. Any identifiability constraints are imposed on the model before fitting ($f_1, \ldots, f_L$ are each only estimable to within an additive constant), and the additive model can be estimated by penalised least squares in the same way as used in the simple univariate model. The details of the penalised least squares estimation can be found in Wood (2017).

We assume **any structural relationship** is either approximated by an additive model of cubic regression splines, $f_{(\bullet)}(\mathcal{V}_l; \boldsymbol{\alpha}_{hl}, \mathbf{b}_{hl}, K_{hl})$, where $\boldsymbol{\alpha}_{hl}' = (\alpha_{h,l,1}, \ldots, \alpha_{h,l,K_{hl}-1})$ is the vector of coefficients associated to the piecewise basis functions $\mathbf{b}_{hl} = (b_{l1}(\mathcal{V}_h), \ldots, b_{l,K_{hl}-1}(\mathcal{V}_h))$, a linear relationship or a combination of the two:

$$\mathcal{V}_h = \sum_{l \in \mathcal{V}_h^{pred}} f_l(\mathcal{V}_l; \boldsymbol{\alpha}_{hl}, \mathbf{b}_{hl}, K_{hl}) + \epsilon_h, \tag{2.10}$$

or

$$\mathcal{V}_h = \sum_{l \in \mathcal{V}_h^{pred}} \beta_{hl} \mathcal{V}_l + \epsilon_h, \tag{2.11}$$

or

$$\mathcal{V}_h = \sum_{l \in \mathcal{V}_h^{pred_1}} \beta_{hl} \mathcal{V}_l + \sum_{l \in \mathcal{V}_h^{pred_2}} f_l(\mathcal{V}_l; \boldsymbol{\alpha}_{hl}, \mathbf{b}_{hl}, K_{hl}) + \epsilon_h, \tag{2.12}$$

where $h = \{\mathcal{V}_h : h \in \text{model's endogenous latent variables}\}$ and $\mathcal{V}_h^{pred}$ is the set of all latent variable h's predecessor latent variables defined in (2.20), $\mathcal{V}_h^{pred_1}$ is the set of all latent variable h's predecessor latent variables whose partial relationship with $\mathcal{V}_h$ is assumed to be linear (turning $f_l(\mathcal{V}_l; \bullet)$ in the identity function), $f_l(\mathcal{V}_l; \bullet) = \mathcal{V}_l$), $\mathcal{V}_h^{pred_2}$ is the set of all latent variable h's predecessor latent variables whose partial relationship with $\mathcal{V}_h$ is assumed to be nonlinear, $f_l(\bullet; \bullet)$ is defined above and ϵ_h are error terms such that $\mathrm{E}(\epsilon_h) = 0$. Thus, any endogenous latent variable is a linear combination of its predecessor latent variables or its piecewise transformations as determined by f, a cubic regression spline, or a combination of the two.

Step 1: Outer approximation of the latent variables scores: Outer proxies of the latent variables, $\hat{\xi}^{outer}$, are calculated as linear combinations of their respective indicators. These outer proxies are standardised; i.e. they have a mean of 0 and a standard deviation of 1.The weights of the linear combinations result from step 4 of the previous iteration. When the algorithm is initialised, and no weights are available yet, any arbitrary non trivial linear combination of indicators can serve as an outer proxy of a latent variable (Henseler et al., 2009).

Calculating outer proxies of latent variable scores: Outer proxies of the latent variables, ξ_j^0, are calculated as linear combinations of their respective indicators. The weights of the linear combinations result from step 4 of the previous iteration or are manually initialised. For each nonlinear term, a new proxy is created as the element-wise transformation of the respective outer estimates (Henseler et al., 2012).

The latent variable outer proxies are estimated as a weighted sum of their respective indicators:

$$\widehat{\boldsymbol{\mathcal{V}}}^{outer} = \mathbf{X}\widehat{\mathbf{W}} \tag{2.13}$$

To kick-off the algorithm, the outer proxies of the latent variable scores are initialised from (2.13) by setting the $\widehat{\mathbf{W}} = \mathbf{M}$.

To ensure the identification of the weights they need to be normalised. This normalisation is typically can be done using two different methods. The first is ensuring that after computing the outer proxies, $\widehat{\boldsymbol{\mathcal{V}}}^{outer}$ in (2.13), the weights of the indicators associated to each latent variable h, $h = 1, \ldots, H$, sum to 1, $\sum_{p=1}^{P_h} w_{ph} = 1$. The second fixes the variance of each proxy to one, i.e., $\mathbf{w}_h' \mathbf{R}_h \mathbf{w}_h = 1$, where $\mathbf{R}_h$ is the empirical correlation matrix of these manifest variables or indicators of the block h (assuming all the manifest variables are scale to zero mean and unit variance).

Assuming all the manifest variables, x_{ph}, $p = 1, \ldots, P_h$, $h = 1, \ldots, H$, are scaled ($\mathrm{E}(x_{ph}) = 0$ and $\mathrm{Var}(x_{ph}) = 1$), the latent variables are also centred (at 0), but must be scaled to have unit variance:

$$\hat{\mathcal{V}}_h^{outer} = \frac{\hat{\mathcal{V}}_h^{outer}}{\sqrt{\mathrm{Var}(\hat{\mathcal{V}}_h^{outer})}}, h = 1, \ldots, H, \tag{2.14}$$

where $\mathrm{Var}(\hat{\mathcal{V}}_h^{outer})$ is the empirical variance of the outer proxy h, $h = 1, \ldots, H$. Thus, the matrix of outer proxies is obtained $\widehat{\boldsymbol{\mathcal{V}}}^{outer} = (\hat{\boldsymbol{\xi}}_1^{outer}, \ldots, \hat{\boldsymbol{\xi}}_h^{outer}, \hat{\boldsymbol{\eta}}_{h+1}^{outer}, \ldots, \hat{\boldsymbol{\eta}}_H^{outer})$.

The $n \times H$ matrix $\widehat{\boldsymbol{\mathcal{V}}}^{outer}$ of outer approximation of latent variable proxies resulting from step 1 ((2.13) and (2.14)) is augmented to a new matrix $\widehat{\boldsymbol{\mathcal{V}}}_{Aug}^{outer}$ whose number of columns depends upon the specification of the structural model relationships.

The matrix $\widehat{\boldsymbol{\mathcal{V}}}_{Aug}^{outer}$, in (2.13), has H columns given by

$$\hat{\boldsymbol{\mathcal{V}}}_h^{outer\prime} = (\hat{\mathcal{V}}_{1h}^{outer}, \ldots, \hat{\mathcal{V}}_{nh}^{outer}), h = 1, \ldots, H,$$

where $\widehat{\mathcal{V}}_{ih}^{outer}$ is the estimated outer proxy of i^{th} observation resulting from step 1, as usual, but it is expanded to accommodate as many columns as necessary to account for the nonlinear relationships that are assumed to be nonlinear. Thus, for each partial nonlinear relationship approximated by a cubic regression spline with K_h knots, the matrix $\widehat{\boldsymbol{\mathcal{V}}}^{outer}$ contains $K_h - 1$ additional columns,

$$\begin{array}{rcl}
\mathbf{b}_1(\hat{\boldsymbol{\mathcal{V}}}_h^{outer})' & = & (b_1(\hat{\mathcal{V}}_{1h}^{outer}), \ldots, b_1(\hat{\mathcal{V}}_{nh}^{outer})), \\
\mathbf{b}_2(\hat{\boldsymbol{\mathcal{V}}}_h^{outer})' & = & (b_2(\hat{\mathcal{V}}_{2h}^{outer}), \ldots, b_2(\hat{\mathcal{V}}_{nh}^{outer})), \\
\ldots & = & \ldots \\
\mathbf{b}_{K_h-1}(\hat{\boldsymbol{\mathcal{V}}}_h^{outer})' & = & (b_{K_h-1}(\hat{\mathcal{V}}_{1h}^{outer}), \ldots, b_{K_h-1}(\hat{\mathcal{V}}_{nh}^{outer})), h = 1, \ldots, H,
\end{array}$$

where $b_k(\widehat{\mathcal{V}}_{ih}^{outer})$ denotes the basis of piecewise linear transformations of the estimated outer proxies, $\widehat{\mathcal{V}}_{ih}^{outer}$, $i = 1, \ldots, n$, $h = 1, \ldots, H$ resulting as usual from step 1. The piecewise linear transformations are determined entirely by the locations at which the linear pieces join up, and the knots $\{\mathcal{V}_{hk}^* : h = 1, \ldots, H,\ k = 1, \ldots, K_h\}$, assuming $\mathcal{V}_{h,k}^* > \mathcal{V}_{h,(k-1)}^*$.

The columns of matrix $\widehat{\boldsymbol{\mathcal{V}}}_{Aug}^{outer}$ should be scaled to a mean of zero and unit variance, as in (2.14). The identifiability restriction mentioned at the end of the previous section plays a role here. Indeed, K_h must be chosen up to a maximum, such that $(\max(K_h) - 1) \times H < n$,

$h = 1, \ldots, H$, where n is the effective sample size.

It is worth mentioning that the level of smoothness for the model, determined by the basis dimension K_h, may be subjective. In fact, as Wood (2017) points out, the basis dimension can be set slightly larger than what is believed to be necessary, as the model's smoothness is regulated by adding a penalty to the least squares fitting objective function.

The implementation referred to in Section 2.3 allows the user to set the value of K_h. If the user does not have a clue about the dimension of the basis to be used, we recommend to use the value $K_h = 10$, the default value used by `mgcv` package or adjust it to the maximum possible value (fewer than 10) if the sample size does not allow such dimension. The author's software implementation contains a diagnosis function that allows the user to adjust K_h in a interactive fashion. It even allows the user to downscale a structural partial relationship initially approximated by a smoothing function with a dimension of the basis $K_h \geq 3$ to a linear form. More details on the cubic regression spline piecewise basis functions, $b_k(\hat{\mathcal{V}}_{ih})$, $k = 1, \ldots, K_h - 1$, $i = 1, \ldots, n$, $h = 1, \ldots, H$ are given in Wood (2017).

For the sake of a comprehensive understanding of this novel inner weighting scheme, an illustration using the structural model of Figure 1 follows. Let us assume the structural model depicted in Figure 1 is described by the following set of structural equations:

$$\begin{aligned}
\xi_1 &= \xi_1 + 0 \\
\eta_2 &= \beta_2 \xi_1 + \epsilon_1 \\
\eta_3 &= f(\xi_1; \boldsymbol{\alpha}_{\xi_1}, \mathbf{b}_{\xi_1}; K_{\xi_1}) + \beta_4 \eta_2 + \epsilon_2 \\
\eta_4 &= \beta_1 \xi_1 + f(\eta_3; \boldsymbol{\alpha}_{\eta_3}, \mathbf{b}_{\eta_3}; K_{\eta_3}) + \epsilon_3.
\end{aligned} \tag{2.15}$$

We are assuming η_2 is a linear function of ξ_1, η_3 is a function of two partial relationships, one is a smooth function of ξ_1 (a cubic regression spline with a dimension of the basis given by K_{ξ_1}) and the other is a linear function of η_2, and η_4 is another function of two partial relationships, one is a linear function of ξ_1 and the other is a smooth function of η_3 (a cubic regression spline with a dimension of the basis given by K_{ξ_1}).

The $(n \times (4 + (K_{\xi_1} - 1) + (K_{\eta_3} - 1)))$ outer proxies augmented matrix $\widehat{\boldsymbol{\mathcal{V}}}^{outer}_{Aug}$ is given by

$$\begin{pmatrix}
\hat{\xi}_{11} & \hat{\eta}_{12} & \hat{\eta}_{13} & \hat{\eta}_{14} & b_1(\hat{\xi}_{11}) & \cdots & b_{K_{\xi_1}-1}(\hat{\xi}_{111}) & b_1(\hat{\eta}_{13}) & \cdots & b_{K_{\eta_3}-1}(\hat{\eta}_{13}) \\
\hat{\xi}_{21} & \hat{\eta}_{22} & \hat{\eta}_{23} & \hat{\eta}_{24} & b_1(\hat{\xi}_{21}) & \cdots & b_{K_{\xi_1}-1}(\hat{\xi}_{121}) & b_1(\hat{\eta}_{23}) & \cdots & b_{K_{\eta_3}-1}(\hat{\eta}_{23}) \\
\vdots & \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\
\hat{\xi}_{n1} & \hat{\eta}_{n2} & \hat{\eta}_{n3} & \hat{\eta}_{n4} & b_1(\hat{\xi}_{n1}) & \cdots & b_{K_{\xi_1}-1}(\hat{\xi}_{1n1}) & b_1(\hat{\eta}_{n3}) & \cdots & b_{K_{\eta_3}-1}(\hat{\eta}_{n3})
\end{pmatrix} \tag{2.16}$$

Step 2: Estimation of the inner weights: Inner weights are calculated for each latent variable in order to reflect how strongly the other latent variables are connected to it. There are three schemes available for determining the inner weights. Wold (1982) originally proposed the *centroid scheme. Later, Lohmöller (1989) developed the factor weighting and path weighting schemes. The centroid scheme uses the sign of the correlations between a latent variable or, more precisely, the outer proxy and its adjacent latent variables; the factor weighting scheme uses the correlations. The path weighting scheme pays tribute to the arrow orientations in the path model. The weights of those latent variables that explain the focal latent variable are set to the regression coefficients stemming from a regression of the focal latent variable (regressant) on its latent regressor variables. The weights of those latent variables, which are explained by the focal latent variable, are determined in a similar manner as in the factor weighting scheme. Regardless of the weighting scheme, a weight of zero is assigned to all non-adjacent latent variables* (Henseler et al., 2009).

Estimating inner weights: For each outer proxy, inner weights are calculated to reflect how strongly the proxies of the other latent variables are connected to it. Several inner weighting schemes are available. Wold (1982) originally proposed that the sign should be used of the correlations between a latent variable and its adjacent latent variables (which is the so-called centroid scheme). Alternatives are the factor weighting scheme and the path weighting scheme (Lohmöller, 1989). *Regardless of the weighting scheme, a weight of zero is assigned to all non-adjacent latent variables.* (Henseler et al., 2012).

For any the structural model, the adjacency matrix (2.2), $\mathbf{D}$ (referring to model in Figure 1) accounts for the directionality. For every $d_{ij} = 1$, there is an link between from node i and node j. We could also say, the columns indicate the *successors*, whereas the rows indicate the *predecessors*. As we will see, the adjacency matrix $\mathbf{D}$ facilitates the calculation of the inner weights. For all the weighting schemes, each latent variable is constructed as a weighted sum of the latent variables it is related with. The weighting schemes differ in the way the relation is defined. Furthermore, let us denote $\hat{\mathbf{R}} = \mathrm{Cor}(\hat{\boldsymbol{\mathcal{V}}}^{outer})$, the empirical correlation matrix for the latent variables proxies resulting from the outer estimation, $r_{ij} = \mathrm{Cor}(\hat{\mathcal{V}}_i^{outer}, \hat{\mathcal{V}}_j^{outer})$, $i, j = 1, ...H$, and $\mathbf{C} = \mathbf{D} + \mathbf{D}'$ a symmetrical matrix indicating whether two latent variables are neighbours, $c_{ij} = 1$, and $c_{ij} = 0$ otherwise, $i, j = 1, \ldots, H$.

If the *centroid weighting* scheme is used, the elements of the inner weights matrix, $\mathbf{E}$, are given by

$$e_{ij} = \begin{cases} sign(r_{ij}), & \text{for } c_{ij} = 1, \\ 0, & \text{otherwise} \end{cases}, \; i, j = 1, \ldots, H. \tag{2.17}$$

If the *factorial weighting* scheme is used, the elements of the inner weights matrix, $\mathbf{E}$, are given by

$$e_{ij} = \begin{cases} r_{ij}, & \text{for } c_{ij} = 1, \\ 0, & \text{otherwise} \end{cases}, \; i, j = 1, \ldots, H. \tag{2.18}$$

For the *path weighting* scheme the predecessors and successors of a latent variable play a different role in the relation. Let us define the successor set of a node h as the set of latent variables variable h impacts on, represented by the vector

$$\boldsymbol{\mathcal{V}}_h^{succ'} = \{\mathcal{V}_l : l \in \text{successors of } \mathcal{V}_h\}. \tag{2.19}$$

Likewise, a predecessor set of a node h is the set of latent variables impacting on h, denoted by the vector

$$\boldsymbol{\mathcal{V}}_h^{pred'} = \{\mathcal{V}_l : l \in \text{predecessors of } \mathcal{V}_h\}. \tag{2.20}$$

.

The relation for one specific latent variable $\mathcal{V}_h$ with its successors is determined by their correlation, $\mathrm{Cor}(\hat{\mathcal{V}}_h, \widehat{\boldsymbol{\mathcal{V}}}_h^{succ})$. For the predecessors it is determined by a multiple regression

$$\hat{\mathcal{V}}_h = \widehat{\boldsymbol{\mathcal{V}}}_h^{pred\prime} \boldsymbol{\gamma}_h + \zeta_h,\ \mathrm{E}(\zeta_h) = 0,\ h = 1, \ldots, H. \tag{2.21}$$

Therefore, the elements of matrix $\mathbf{E}$ are:

$$e_{ij} = \begin{cases} \hat{\gamma}_h, & \text{for } j \in \mathcal{V}_h^{pred}, \\ \mathrm{Cor}(\hat{\mathcal{V}}_h, \widehat{\boldsymbol{\mathcal{V}}}_h^{succ}), & \text{for } j \in \mathcal{V}_h^{succ},\ i, j = 1, \ldots, H \\ 0, & \text{otherwise} \end{cases} . \tag{2.22}$$

It is noteworthy to mention that, according to Noonan & Wold (1982), all of three described schemes yield similar results.

For the hybrid approach, in *smooth weighting* scheme, the inner weights were also determined for each piecewise linear term described in (2.16) connected to a latent variable. As in *path weighting* scheme, the endogenous and exogenous latent variables have different treatments.

The inner weights matrix, $\mathbf{E}^{Aug}$, will also be augmented. It will contain as many rows as columns of $\widehat{\boldsymbol{\mathcal{V}}}_{Aug}^{outer}$ and H columns, the number of latent variables.

Every endogenous latent variable is given by one of the models in (2.10), (2.11) or (2.12).

Every exogenous latent variable has a set other latent variables it impacts on, its successors defined in (2.19). The impact on its successors may be through it own direct impact and/or through a set of piecewise linear terms as determined in (2.10), (2.11) or (2.12).

The elements of the columns of $\mathbf{E}^{Aug}$ regarding exogenous latent variables ($\boldsymbol{\xi}_h$) are given as follows:

1. $\mathrm{Cor}(\hat{\xi}_h, \hat{\mathcal{V}}_l)$, if ξ_h is exogenous and impacts directly on $\mathcal{V}_l \in \boldsymbol{\xi}_h^{succ}$;
2. $\mathrm{Cor}(\hat{\xi}_h, \mathbf{b}_{l,1}(\hat{\mathcal{V}}_l)), ..., \mathrm{Cor}(\hat{\xi}_h, \mathbf{b}_{l,K_h-1}(\hat{\mathcal{V}}_l))$ if ξ_h is exogenous and impacts on $\mathcal{V}_l \in \boldsymbol{\xi}_h^{succ}$ through its piecewise linear transformations;
3. 0, otherwise,

where $\mathrm{Cor}(\hat{\xi}_h, b_{l,1}(\hat{\mathcal{V}}_l)), ..., \mathrm{Cor}(\hat{\xi}_h, b_{l,K_h-1}(\hat{\mathcal{V}}_l)$ are the empirical correlations between $\hat{\xi}_h$ and the piecewise transformations of $\mathcal{V}_l$ as defined in (2.10) or (2.12) and $\mathrm{Cor}(\hat{\xi}_h, \hat{\mathcal{V}}_l)$ is the empirical correlation between $\hat{\xi}_h$ and $\hat{\mathcal{V}}_l$.

The elements of the columns of $\mathbf{E}^{Aug}$ regarding endogenous latent variables ($\boldsymbol{\eta}_h$) are given as follows:

1. β_l if $\mathcal{V}_l \in \boldsymbol{\eta}_h^{pred}$ and $\mathcal{V}_l$ impacts directly on η_h;
2. $\alpha_{l,1}, \ldots, \alpha_{l,(K_l-1)}$ if $\mathcal{V}_l \in \boldsymbol{\eta}_h^{pred}$ and $\mathcal{V}_l$ impacts on η_h through its piecewise linear transformations;
3. 0, otherwise,

where β_l is the coefficient of the regression as defined in (2.11) and $\alpha_{l,1}, \ldots, \alpha_{l,(K_l-1)}$ are the regression coefficients associated to piecewise transformations of $\mathcal{V}_l$, $b_{l,1}(\hat{\mathcal{V}}_l), \ldots, b_{l,K_h-1}(\hat{\mathcal{V}}_l)$ as defined in (2.10) or (2.12).

Again, let us assume the structural model depicted in Figure 1 is described by the set of structural equations in (2.15). An illustration of $\widehat{\mathbf{E}}_{Aug}$ using the structural model of Figure 1 follows. The $(4 + (K_{\xi_1} - 1) + (K_{\eta_3} - 1)) \times 4$ matrix of augmented inner weights of the structural model depicted in Figure 1 is:

$$
\widehat{\mathbf{E}}_{Aug} =
\begin{array}{c|cccc}
\text{Columns of } \widehat{\boldsymbol{\mathcal{V}}}_{Aug}^{outer} & \xi_1 & \eta_2 & \eta_3 & \eta_4 \\
\hline
\xi_1 & 0 & \beta_2 & 0 & \beta_1 \\
\eta_2 & \mathrm{Cor}(\hat{\xi}_1, \hat{\eta}_2) & 0 & \beta_4 & 0 \\
\eta_3 & 0 & 0 & 0 & 0 \\
\eta_4 & 0 & 0 & 0 & 0 \\
\hline
b_1(\hat{\xi}_1) & 0 & 0 & \alpha_{\xi_1,1} & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
b_{K_{\xi_1}-1}(\xi_1) & 0 & 0 & \alpha_{\xi_1,K_{\xi_1}-1} & 0 \\
\hline
b_1(\eta_3) & \mathrm{Cor}(\hat{\xi}_1, b_1(\hat{\eta}_3)) & 0 & 0 & \alpha_{\eta_3,1} \\
\vdots & \vdots & \vdots & \vdots & \vdots \\
b_{K_{\eta_3}-1}(\eta_3) & \mathrm{Cor}(\hat{\xi}_1, b_{K_{\eta_3}-1}(\hat{\eta}_3)) & 0 & 0 & \alpha_{\eta_3,K_{\xi_1}-1}
\end{array}
$$

Indeed, η_2 is a linear function of ξ_1, η_3 is a linear function of piecewise transformations of ξ_1 and a linear function of η_2, and η_4 is a linear function ξ_1 and a linear function of piecewise transformations of η_3, and ξ_1 is exogenous and its direct successors are η_2, and it impacts on η_3 and the piecewise transformations of η_3.

Step 3: Inner approximation of the latent variable scores: Inner proxies of the latent variables, ξ_j^{inner}, are calculated as linear combinations of the outer proxies of their respective adjacent latent variables, using the afore-determined inner weights (Henseler et al., 2009).

Calculating inner proxies of latent variable scores: Inner proxies of the latent variables, ξ_j^0, are calculated as linear combinations of their respective adjacent latent variables' outer proxies, *using the previously determined inner weights* (Henseler et al., 2012).

In the inner approximation, we estimate each latent variable as a weighted sum of its neighbouring latent variables. The weighting depends on the used scheme described above:

$$\widehat{\boldsymbol{\mathcal{V}}}^{inner} = \widehat{\boldsymbol{\mathcal{V}}}^{outer}\widehat{\mathbf{E}}. \tag{2.23}$$

The estimated inner proxies $\widehat{\boldsymbol{\mathcal{V}}}^{inner} = (\hat{\xi}_1^{inner}, \ldots, \hat{\xi}_h^{inner}, \hat{\eta}_{h+1}^{inner}, \cdots, \hat{\eta}_H^{inner})$ are obtained by scaling the recomputed latent variables proxies to have unit variance:

$$\hat{\mathcal{V}}_h^{inner} = \frac{\hat{\mathcal{V}}_h^{inner}}{\sqrt{\mathrm{Var}(\hat{\mathcal{V}}_h^{inner})}}, h = 1, \ldots, H, \tag{2.24}$$

where $\mathrm{Var}(\hat{\mathcal{V}}_h^{inner})$ is the empirical variance of the outer proxy h, $h = 1, \ldots, H$.

In the **smoothing-based hybrid approach**, the piecewise basis linear functions of the latent variable outer scores in (2.16), $b_k(\hat{\xi}_{ih})$, $k = 1, \ldots, K_h$, $i = 1, \ldots, n$ and $h = 1, \ldots, H$ are also used to estimate endogenous latent variables' inner proxies.

In the inner approximation we estimate each latent variable as a weighted sum of its neighbouring latent variables,

$$\widehat{\boldsymbol{\mathcal{V}}}_{Aug}^{inner} = \widehat{\boldsymbol{\mathcal{V}}}_{Aug}^{outer}\widehat{\mathbf{E}}^{Aug}. \tag{2.25}$$

The inner proxies are scaled to have unit variance:

$$\hat{\mathcal{V}}_h^{inner} = \frac{\hat{\mathcal{V}}_h^{inner}}{\sqrt{\mathrm{Var}(\hat{\mathcal{V}}_h^{inner})}}, \; h = 1, \ldots, H, \tag{2.26}$$

Step 4: Estimation of the outer weights: The outer weights are calculated either as the covariances between the inner proxy of each latent variable and its indicators (in Mode A), or as the regression weights resulting from the ordinary least squares regression of the inner proxy of each latent variable on its indicators (in Mode B) (Henseler et al., 2009).

Mode A: A multivariate regression coefficient with the block of manifest variables as response and the latent variable as the regressor:

$$\hat{\mathbf{w}}'_h = (\hat{\mathcal{V}}_h^{inner\prime}\hat{\mathcal{V}}_h^{inner})^{-1}\hat{\mathcal{V}}_h^{inner\prime}\mathbf{X}_h \tag{2.27}$$

$$= \mathrm{Cor}(\hat{\mathcal{V}}_h^{inner}, \mathbf{X}_h), h = 1, \ldots, H. \tag{2.28}$$

Mode B: A multiple regression coefficient with the latent variable as response and its block of manifest variables as regressors:

$$\hat{\mathbf{w}}_h' = (\mathbf{X}_h'\mathbf{X}_h)^{-1}\mathbf{X}_h\hat{\mathcal{V}}_h^{inner} \tag{2.29}$$

$$= \mathrm{Var}(\mathbf{X}_h)^{-1}\mathrm{Cor}(\mathbf{X}_h, \hat{\mathcal{V}}_h^{inner}), h = 1, \ldots, H. \tag{2.30}$$

These steps are iterated until the change in outer weights between two consecutive iterations falls below a predefined relative tolerance,

$$\max\left(\frac{w_{ph}^{(i)} - w_{ph}^{(i+1)}}{w_{ph}^{(i+1)}}\right) < T_r,\ p = 1, \ldots, P_h;\ h = 1, \ldots, H, \tag{2.31}$$

or absolute tolerance,

$$\max\sqrt{\left(w_{ph}^{(i)} - w_{ph}^{(i+1)}\right)^2} < T_a,\ p = 1, \ldots, P_h;\ h = 1, \ldots, H, \tag{2.32}$$

where i denotes the iteration. The default tolerance used in the authors' software implementation relative tolerance, T_r, is fixed at a very tiny level, 1×10^{-7}, whereas the absolute tolerance, T_a is fixed at 0.001.

Once again, to ensure the identification of the weights they need to be normalised which is done as before, that is, ensuring that after computing the inner weights of the indicators associated to each latent variable h, $h = 1, \ldots, H$, sum to 1, $\sum_{p=1}^{P_h} w_{ph} = 1$, or by fixing the variance of each proxy to one, i.e., $\mathbf{w}_h'\mathbf{R}_h\mathbf{w}_h = 1$, where $\mathbf{R}_h$ is the empirical correlation matrix of these manifest variables or indicators of the block h (assuming all the manifest variables are scale to zero mean and unit variance).

In the **smoothing-based hybrid approach** no additional procedure is required in this step 4 because the piecewise linear terms do not have any assigned manifest variables, as determined by the hybrid approach.

Once convergence has been achieved, the latent variable scores are the outer proxies resulting from the last iteration, which are to estimate the path coefficients. Although other methods may be used, the path coefficients can be estimated by ordinary least squares (OLS), according to the structural model (1). For each latent variable $\mathcal{V}_h$, $h = 1, \ldots, H$, the path coefficient is the regression coefficient on its predecessor set $\boldsymbol{\mathcal{V}}_h^{pred}$:

$$\boldsymbol{\beta}_h = (\widehat{\boldsymbol{\mathcal{V}}}_h^{pred'}\widehat{\boldsymbol{\mathcal{V}}}_h^{pred})^{-1}\widehat{\boldsymbol{\mathcal{V}}}_h^{pred'}\hat{\mathcal{V}}_h \tag{2.33}$$

$$= \mathrm{Cor}(\widehat{\boldsymbol{\mathcal{V}}}_h^{pred}, \widehat{\boldsymbol{\mathcal{V}}}_h^{pred})^{-1}\mathrm{Cor}(\widehat{\boldsymbol{\mathcal{V}}}_h^{pred}, \hat{\mathcal{V}}_h). \tag{2.34}$$

As has been described, the PLS-PM algorithm is closely related to OLS estimation techniques. It focuses on predicting a specific set of hypothesised linear relationships that maximise the explained variance in the dependent variables (endogenous latent variables), similar to OLS regression models. This feature makes PLS-PM a suitable technique for prediction, although its potential for explanation should not be overlooked (Hair et al. (2011)). Nevertheless, PLS-PM does not aim to optimise a global scalar function. The focus of PLS-PM is the discrepancy between the observed (in the case of manifest variables) or approximated (in the case of latent variables) values of the dependent variables and the values predicted by the model (Hair et al., 2021). Consequently, researchers using PLS-PM usually rely on quality indices, such as R^2, cross-validated communality, or redundancy, to judge the quality of the model.

However, it is worth considering whether the traditional assumption of linear relationships between latent variables and observed indicators is sufficient to capture all relationships in every case. This is especially true, given that some theories suggest that nonlinear relationships may exist in some situations (for example, Tuu & Olsen (2010)). If the answer to this question is no, it is unclear what alternative methods could be used to account for measurement errors in manifest variables while avoiding contamination of latent variable scores and ultimately affecting structural path coefficients (Dijkstra & Henseler, 2015a; Dijkstra & Henseler, 2015b).

In the **smoothing-based hybrid approach**, the structural relationships in (2.10), (2.11) and (2.12) are estimated using the factor scores. Estimation is conducted using penalised least squares for all the structural relationships involving at least one regression cubic spline.

This **smoothing-based hybrid approach** comprising the novel inner *smooth weighting* scheme, the changes in steps 1, 2 and 3, and the new approach to estimate structural relationships is hereafter denoted by **PLSs-PM**.

Let $\hat{\boldsymbol{\beta}}$ be the estimator of $\boldsymbol{\beta}$, the transition matrix for the structural model:

$$\hat{\beta}_{hj} = \begin{cases} \beta_{hj}, & j \in \boldsymbol{\mathcal{V}}_h^{pred} \\ 0, & \text{otherwise} \end{cases} \quad h = 1, \ldots, H. \tag{2.35}$$

The impact of all model latent variables on a single latent variable is given by the matrix of total effects $\hat{\boldsymbol{\tau}}$. It can be obtained as the sum of the 1 to H step transition matrices:

$$\hat{\boldsymbol{\tau}} = \sum_{h=1}^{H} \hat{\boldsymbol{\beta}}^h = \underbrace{\hat{\boldsymbol{\beta}} \times \hat{\boldsymbol{\beta}} \times \cdots \times \hat{\boldsymbol{\beta}}}_{h \text{ times}}. \tag{2.36}$$

For example $\hat{\boldsymbol{\beta}}^2$ contains all the indirect effects mediated by only one latent variable. The cross and outer loadings are estimated as:

$$\hat{\mathbf{\Lambda}}^{cross} = \mathrm{Cor}(\mathbf{X}, \boldsymbol{\mathcal{V}}^{\hat{outer}}), \tag{2.37}$$

$$\hat{\lambda}_{ph}^{outer} = \begin{cases} \hat{\lambda}_{ph}^{cross}, & m_{ph} = 1 \\ 0 & \text{otherwise}, \end{cases} \tag{2.38}$$

where m_{ph}, $p = 1, \ldots, P_h$, $h = 1, \ldots, H$ are the element of the adjacency matrix of the outer model $\mathbf{M}$. In the particular case of the model depicted in Figure 1, $\mathbf{M}$ is given in (2.7).

In 2015, to address the bias in structural regression parameter estimates caused by the inclusion of measurement errors in composites, Dijkstra & Henseler (2015a) and Dijkstra & Henseler (2015b) developed the consistent PLS-PM (PLSc). This was done by utilising PLS-PM indicator weights for mode A weighting and reflective indicators to establish a consistent estimate of the reliability of a composite variable:

$$\rho_A(\hat{\mathcal{V}}_h) = (\hat{\mathbf{w}}_h'\hat{\mathbf{w}}_h)^2 \frac{\hat{\mathbf{w}}_h'(\mathbf{S}_h - \mathrm{diag}(\mathbf{S}_h))\hat{\mathbf{w}}_h}{\hat{\mathbf{w}}_h'(\hat{\mathbf{w}}_h\hat{\mathbf{w}}_h' - \mathrm{diag}(\hat{\mathbf{w}}_h\hat{\mathbf{w}}_h'))\hat{\mathbf{w}}_h}, \tag{2.39}$$

where $\hat{\mathbf{w}}_h$ is the vector of estimated outer weights of $\mathcal{V}_h$ indicators' block obtained in Step 3 and $\mathbf{S}_h$ is its empirical correlation matrix, h, $h = 1, \ldots, H$.

In the first step, the traditional PLS-PM algorithm is applied. This computes the outer latent variable proxies, $\hat{\mathcal{V}}_h^{outer}$, and outer weight vectors, $\hat{\mathbf{w}}_h$ for each latent variable proxy, $h = 1, \ldots, H$. The biased estimate of the latent variable correlation between latent variables $\hat{\mathcal{V}}_h$ and $\hat{\mathcal{V}}_{h'}$ is then corrected using the well-known correction for attenuation introduced by Spearman (1904):

$$\mathrm{Cor}(\hat{\mathcal{V}}_i, \hat{\mathcal{V}}_j) = \frac{\mathrm{Cor}^*(\hat{\mathcal{V}}_i, \hat{\mathcal{V}}_j)}{\sqrt{\rho_A(\hat{\mathcal{V}}_i)\rho_A(\hat{\mathcal{V}}_j)}},\ i, h = 1, \ldots, H, \tag{2.40}$$

where $\mathrm{Cor}^*(\hat{\mathcal{V}}_i, \hat{\mathcal{V}}_j)$ is the empirical correlation matrix between $\hat{\mathcal{V}}_i^{outer}$'s and $\hat{\mathcal{V}}_j^{outer}$'s outer proxies.

Finally, consistent estimates of loadings can be derived using $\rho_A(\hat{\mathcal{V}}_h)$ and $\hat{\mathbf{w}}_h$.

Dijkstra & Henseler (2015a) conducted initial simulation studies that showed that the estimates provided by PLSc were close to that of the maximum likelihood (ML) estimator, with little bias and comparable precision for structural parameters but less precision for item loadings. This was later confirmed by a comparison using a real dataset, where PLSc estimates were found to be close to those obtained through covariance-based estimates (Henseler, 2017). However, not all studies have found similar encouraging results. Huang (2013) and Rönkkö, McIntosh, Antonakis, & Edwards (2016) found that PLSc loading estimates were less precise and also more biased than traditional maximum likelihood estimates. They also showed that PLSc tends to overestimate small correlations and underestimate large correlations, which may be due to the capitalisation on chance and overestimation of reliability (Aguirre-Urreta, Rönkkö, & McIntosh, 2019). Additionally, PLSc produces more inaccurate results, and most recently, Yuan, Y. Wen, & Tang (2020) (pp. 334) argue that there is no clear advantage of PLSc over using unweighted scales and disattenuating with a coefficient of (Cronbach's alpha). Dijkstra & Henseler (2015b) (pp. 309) noted that, *among the consistent techniques, PLSc typically had the lowest statistical power.*

2.2 Data

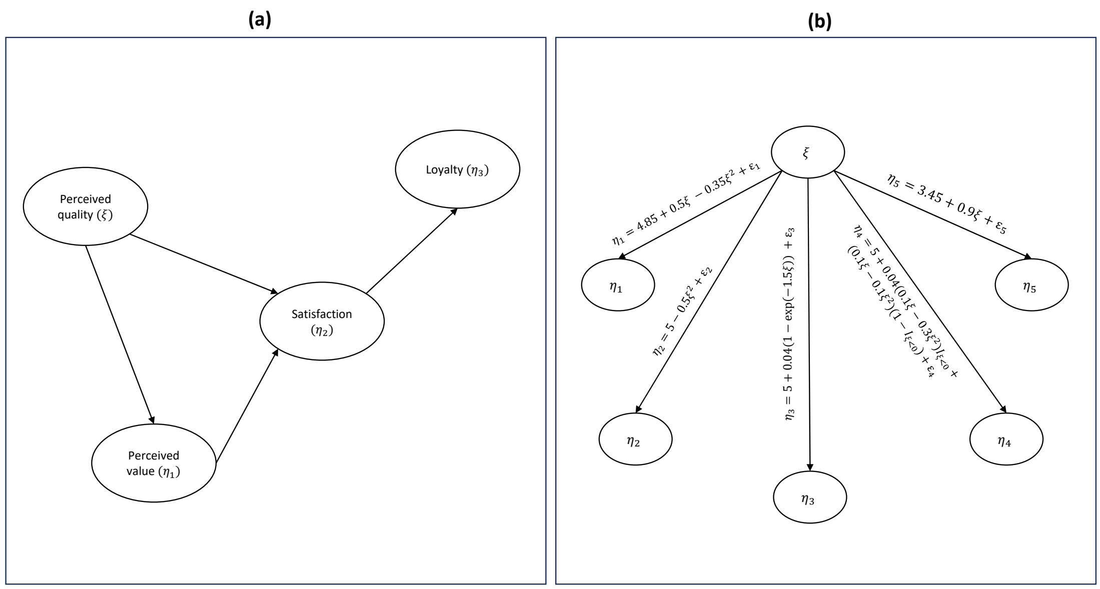

Figure 2: Structural equation models used in examples 1 and 2. (a) Structural equation model representing the causes and consequences of customer satisfaction (reduced version of the European Customer Satisfaction Index (ECSI) model). (b) Structural model implemented in the Monte Carlo simulation study.

Assessing the performance of PLS-PM (using the *centroid weighting* scheme) and PLSs-PM algorithms is a critical step. In this context, utilising both an actual dataset and a simulated dataset can provide valuable insights into the efficacy of the two inner weighting approaches.

The PLS-PM algorithm has been widely used for decades to analyse latent variable relationships in structural equation models. However, it may struggle to capture the complex nonlinear relationships that exist in real-world scenarios. To address this limitation, a novel inner weighting scheme, that was specifically designed to accommodate nonlinear relationships among latent variables is proposed.

By applying PLS-PM and PLSs-PM on an actual dataset, we can evaluate their ability to uncover meaningful relationships and assess the model fit. In addition, the use of a simulated dataset allows for controlled experimentation, enabling a direct comparison of the performance of the two schemes under various conditions.

Key performance metrics can be compared between the traditional and new algorithms. This empirical assessment will provide valuable insights into the strengths and weaknesses of each approach and guide researchers in selecting the most appropriate inner weighting scheme for their specific modelling needs. Moreover, leveraging both actual and simulated datasets to evaluate both schemes offers a comprehensive approach to assess their performance and enhances our understanding of their capabilities in handling complex structural equation models, particularly when nonlinear relationships are at play.

The datasets used in this work are available in Supplementary Material.

2.2.1 Example I: European Customer Satisfaction Index (ECSI) data

The European Customer Satisfaction Index (ECSI) is a tool that measures and evaluates customer satisfaction levels across various industries and sectors throughout Europe. Developed to provide a comprehensive understanding of customer experiences, the ECSI plays a pivotal role in helping businesses and policy-makers make informed decisions to improve products and services.

The ECSI assesses customer satisfaction by gathering feedback on various aspects, including product quality, pricing, customer service, and overall experience. This data is then compiled and analysed to generate a satisfaction score for each participating company or organization. These scores enable businesses to benchmark their performance against industry competitors, identify areas for improvement, and devise strategies to enhance customer satisfaction.

The ECSI actual dataset draws in Vilares, Almeida, & Coelho (2010). We used a ECSI banking sector dataset to illustrate the performance of the suggested methodology as it might contain potential nonlinear relationships, particularly with respect to the link between the satisfaction and loyalty latent variables.

The data are assumed to be generated by the reduced ECSI model depicted in Figure 2(a). The model comprises one formative (Perceived Quality) and three reflective latent variables (Perceived Value, Satisfaction and Loyalty) for the banking sector. Table A1 describes their indicators along with the unidimensionality measures, Cronbach's alpha (α) and Dillon-Goldstein's rho (ρ), for the reflective blocks of manifest variables.

2.2.2 Example II: a simulated dataset

The second example dataset results from a Monte Carlo procedure in three steps. First, we define the true underlying model. Second, we generated random data from the defined model.

Third, given random data, we used the PLS-PM and PLSs-PM algorithms to estimate the model. Finally, the performance of the two algorithms is compared using the absolute bias (B) and the Root Mean Square Error (RMSE). These results were further analysed in terms of algorithmic performance as number of iterations necessary to converge, depending on the level of communality and sample size, and their capability of avoiding negative outer weights for some indicators. Indeed, when a variable possess a very limited number of links to other variables and/or when those links are not of linear nature, the information available by the linear-based inner weighting schemes (e.g. the *centroid* scheme) in the inner approximation is scarce or deviates significantly from the true relationship. This situation may generate negative weights in the outer approximation, especially when the level of shared variance between the latent variable and its indicators (communality) is low.

We define a model consisting of four endogenous latent variables, each of which has a different nonlinear relationship with a exogenous latent variable. The selected functional forms were those used in Bauer et al. (2012). For completeness, we decided to add a true linear relationship to assess the extent to which the PLSs-PM can capture these relationships, as a particular case. The equations representing the relationships between latent variables are as follows:

$$\xi_1 = \mathrm{N}(0,1) \tag{2.41}$$

$$g_1(\xi) = \eta_1 = 4.85 + 0.5\xi - 0.35\xi^2 + \epsilon_1 \tag{2.42}$$

$$g_2(\xi) = \eta_2 = 5 - 0.5\xi^2 + \epsilon_2 \tag{2.43}$$

$$g_3(\xi) = \eta_3 = 5 + 0.04(1 - \exp(-1.5\xi)) + \epsilon_3 \tag{2.44}$$

$$g_4(\xi) = \eta_4 = 5 + (0.1\xi - 0.3\xi^2)I_{\xi<0} + (0.1\xi - 0.1\xi^2)(1 - I_{\xi<0}) + \epsilon_4 \tag{2.45}$$

$$g_5(\xi) = \eta_5 = 3.45 + 0.9\xi + \epsilon_5 \tag{2.46}$$

where $I_{\xi<0}$ is the indicator function, taking the value 1 if $\xi < 0$, and 0 otherwise, and the vector of disturbances, $\boldsymbol{\epsilon}' = c(\epsilon_1, \epsilon_2, \epsilon_3, \epsilon_4, \epsilon_5)$ is sampled from a 5-variate normal distribution $\mathrm{N}_5(\mathbf{0}, \boldsymbol{\Sigma}_\eta)$ where the covariance matrix is

$$\boldsymbol{\Sigma}_\xi = \begin{pmatrix} 0.5 & 0 & 0 & 0 & 0 \\ 0 & 0.5 & 0 & 0 & 0 \\ 0 & 0 & 0.5 & 0 & 0 \\ 0 & 0 & 0 & 0.5 & 0 \\ 0 & 0 & 0 & 0 & 0.5 \end{pmatrix}$$

The five functions are visually compared in Figure 3.

To guaranty the conditions for the Partila Least Squares consistency, the measurement model

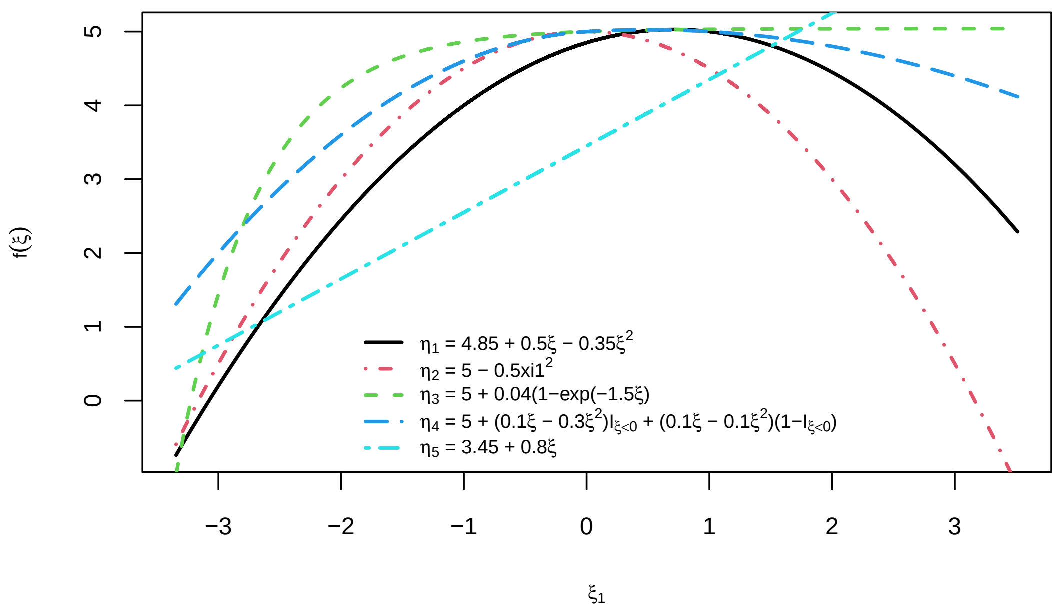

Figure 3: Structural model functional form of the relationships implemented in the Monte Carlo simulation study.

has a minimum and fixed number of five indicators per latent variable and unit loadings:

$$x_{l_\xi} = \xi + \delta_\xi,\ l = 1, 2, 3, 4, 5, \tag{2.47}$$

$$x_{l_{\eta_h}} = \eta_h + \delta_{\eta_h},\ h = 1, \ldots, 5;\ l = 1, 2, 3, 4, 5, \tag{2.48}$$

where the residual variances, $\delta_{(\bullet)}$, follows a 5-variate normal distribution $\mathrm{N}_5(\mathbf{0}, \mathbf{\Sigma}_\delta)$ where $\mathbf{\Sigma}_\delta$ is a diagonal matrix where the residual variance is held constant across indicators and three distinct levels of variance, 3, 1, and 1/3, corresponding to communalities of 25%, 50%, 75%, respectively.

Because the implementation of additive models through regressions splines to approximate nonlinear functional relationships may consume a large number of degrees of freedom, we decided to implement the experiment with different sample sizes ranging from 75 to 900 observations (i.e. 75, 100, 150, 250, 300, 500, 750, and 900). The minimum sample size used, $n = 75$, was imposed such that all models could be estimated using a smoothing spline with $K = 10$ (see the restriction mentioned in Section 2.1 in step 1 of the *smooth weighting* scheme).

Following the described methodology, three populations of 10,000 units were generated (corresponding to the three levels of residual variance). Then, $M = 1,000$ random samples

Table 1: Population means and standard deviations of simulated latent variables of example 2 and sample counterparts based on the 10 000 generated observations).

Latent variable	μ	$\bar{x}$	σ	s
η_1	4.50	4.49	1.00	0.99
η_2	4.50	4.50	1.00	0.98
η_3	4.92	4.93	0.79	0.77
η_4	4.80	4.80	0.78	0.81
η_5	3.45	3.45	1.14	1.14

of size $n = 75, 100, 150, 250, 300, 500, 750, 900$ were randomly drawn from the three levels of communality.

A full factorial design (1,000 samples $\times$ eight sample sizes $\times$ three levels of residual variance) was implemented to capture the eventual interactions at different levels of association between manifest and latent variables and different sample sizes.

Denoting the indices $s = 1, 2, 3, 4, 5, 6, 7, 8$ and $m = 1, 2, 3$ represent the eight different sample sizes and three levels of residual variance, respectively, the absolute bias (B) is defined as:

$$\mathrm{B}_{sm} \approx \frac{1}{300} \sum_{i=1}^{300} |\bar{g}_h(\xi_i) - g_h(\xi_i)|, \; h = 1, \ldots, 5, \tag{2.49}$$

and root mean square error (RMSE) is given by:

$$\mathrm{RMSE}_{sm} \approx \sqrt{\frac{1}{M} \sum_{j=1}^{M} \left(\frac{1}{300} \sum_{i=1}^{300} (\hat{g}_h(\xi_i) - g_h(\xi_i)) \right)}, \; h = 1, \ldots, 5, \tag{2.50}$$

where M is the number of Monte Carlo samples, and

$$\bar{g}_h(\xi) = \frac{1}{M} \sum_{i=1}^{M} \hat{g}_h(\xi_i), \; h = 2, \ldots, 6$$

is the mean estimated functional relationship between ξ and η_h, $h = 1, \ldots, 5$, evaluated at a fixed and evenly distributed grid of $i = 1, \ldots, 300$ points throughout the range of ξ, and $g_h(\xi)$ are the known functional relationships given by (2.42) to (2.46). All the calculations and figures were done using the estimated final standardised outer proxies (as explained in Section 2.1) transformed to the original scale using the *theoretical means* (μ) and *theoretical standard deviations* (σ). Table 1 presents the the empirical means and standard deviation (calculated using the 10 000 generated observations) and the theoretical ones obtained as described in Supplementary Material A.2.

2.3 Software implementation

To implement the proposed approach and compare it in terms of performance, it was necessary to implement the PLS-PM algorithm (with the three usual inner weighting schemes (as described in Section 2.1) and extend it to include the *smooth weighting* scheme as described in Section 2.1, using features of package `mgcv` [Wood (2003);Wood (2004);Wood (2011); Wood, N., Pya, & Säfken (2016);Wood (2017)). Building on version 1.0-10 (2013) of `semPLS` package (Monecke & Leisch, 2012), authors changed the code including the *smooth weighting* scheme as an additional option and the estimation of the structural relationships involving cubic regression splines. The resulting set of functions was named `semEXTplspm`. We used `R` software, version 4.0.5 (Team, 2021). The `semEXTplspm` `R` code can be found GITHUB REPOSITORY along with a user manual, that is also reproduced in the Supplementary Material A.3.

The correctness of the PLS-PM code was verified by comparing the results obtained with the author's implementation (using the *centroid weighting* scheme) with the results of the packages `plspm` (Sanchez, Trinchera, & Russolillo, 2023) and `SeminR` (Ray, Danks, & Calero Valdez, 2022) on the dataset used in Example 1. The results were identical, except for some negligible differences owing to rounding inaccuracies. More details can be found in Supplementary Material A.1.

3 Results

3.1 Example I: European Customer Satisfaction Index (ECSI) data

The model described in Section 2.2.1 and represented in Figure 2(a) was used to illustrate the PLSs-PM algorithm, test the author's PLS-PM algorithm implementation and highlight the potential of the `plsExtpm` software.

Table 2: R^2 values of the centroid weighting and smooth weighting schemes. R^2 values are based on correlations between estimated and predicted factor scores

Latent variable	PLS-PM	PLSs-PM	
	All linear	All nonlinear	Loyalty -Satisfaction nonlinear
Value	60.9	62.1	60.2
Satisfaction	91.3	91.6	91.2
Loyalty	72.2	82.3	82.3

Table 2 presents the R-squared values of the endogenous latent variables for the PLS-PM and PLSs-PM algorithms (Section 2.1) (in the case of the latter with (1) all nonlinear relationships with basis dimension $K = 10$ and (2) all linear relationships, except the relationship between Satisfaction and Loyalty that is considered to be nonlinear with basis dimension $K = 10$).

The PLSs-PM algorithm tends to produce larger R-squared values than the PLS-PM algorithm, when all structural relationships are considered to be nonlinear. The differences were more pronounced when the comparison was performed for satisfaction and loyalty, which are factors that have more conspicuous nonlinear relationships with their predictors. These results are consistent with the hypothesis that, by better representing the nonlinear nature of some effects, the PLSs-PM algorithm may offer greater explanatory power than the traditional approaches.

Figure 4 illustrates the estimated partial structural relationships assuming they are all nonlinear and approximated by a cubic regression spline ($K = 10$) (see A.3 for references on how to plot the partial structural relationships). The `plsExtpm` contains a function to plot the estimated partial impacts of the structural model and to assess the appropriateness of the used dimension of the basis. Furthermore, taking advantage of the features of package `mgcv`, a function was specifically developed to check the choice of the basis dimension of the penalised regression smoothers (see Supplementary Material
refsec:AppC).

The shape pf the estimated factor scores in Figure 4 shows the estimated direct relationship between Perceived Quality and Perceived Value may be described by a linear relationship. The estimated relationship seems to be affected by the leverage effect of some scores on

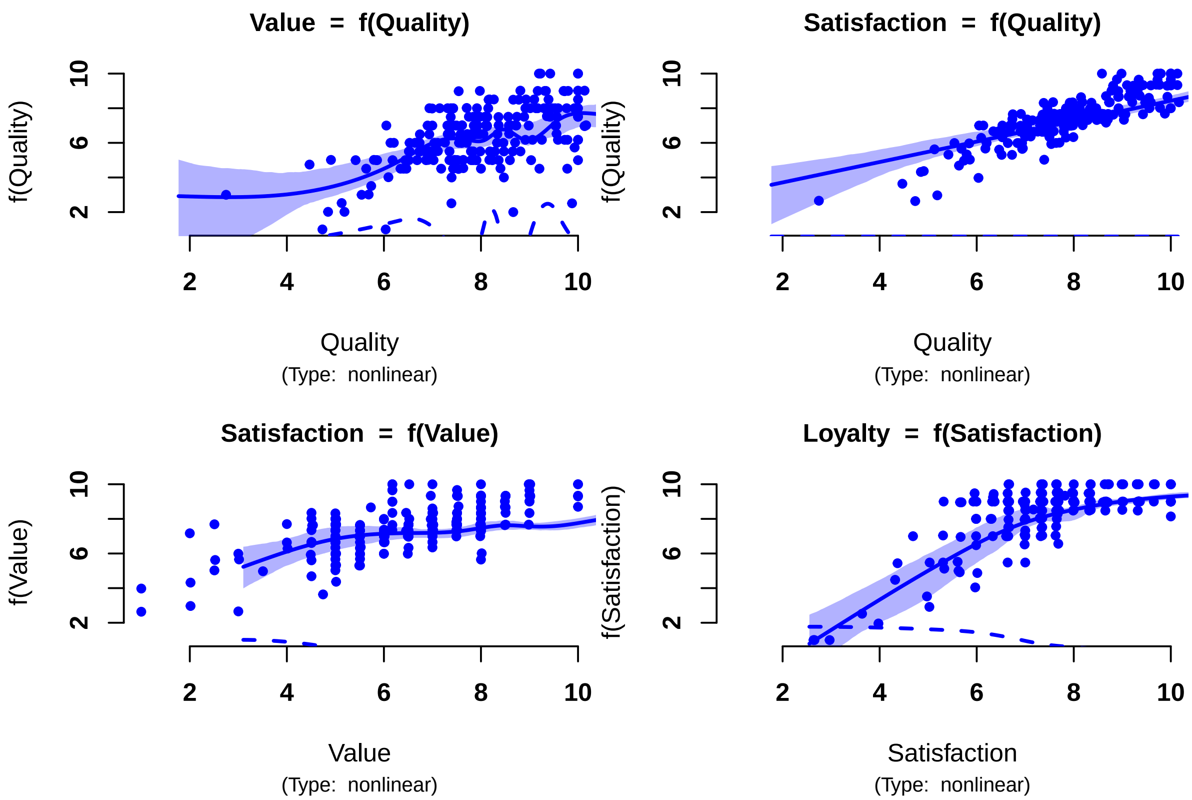

Figure 4: Estimated partial relationships of the reduced ECSI model of Example I, assuming they are all nonlinear and approximated by a cubic regression spline with dimension of the basis $K = 10$. The smooth weighting scheme estimated factor scores are represented as •. The solid blue line corresponds to the estimated relationship, and the area in light blue the corresponding 95% bootstrap credible intervals based on 500 replicates. The first derivative of the partial relationship is represented by the dashed blue line.

the left side of the plot. Moreover, the partial relationships of Customer Satisfaction (with Perceived Quality and Perceived Value), exhibit also a linear pattern. The figure suggests that the PLSs-PM might generalise to other relationship shapes when a linear relationship exists. Indeed, the analysis of these plots are an crucial tool for the practitioner change the nature of some relationships in the structural model.

Figure 4 also illustrates the estimated direct relationship between Customer Satisfaction Customer Loyalty. The ability to capture nonlinear relationships is particularly noteworthy. Indeed, the PLS-PM algorithm estimates the loyalty vector of scores, as a linear function of the satisfaction scores whereas its PLSs-PM counterpart estimates the loyalty scores as a piecewise linear combination of piecewise basis functions of the satisfaction scores. The additive nature of this model results in a nonlinear relationship, as shown in Figure 4. The gain in the R-squared is significant as Table 2 shows. Furthermore, the manner in which the scores appear in the plot from left to right shows an initial increasing relationship between

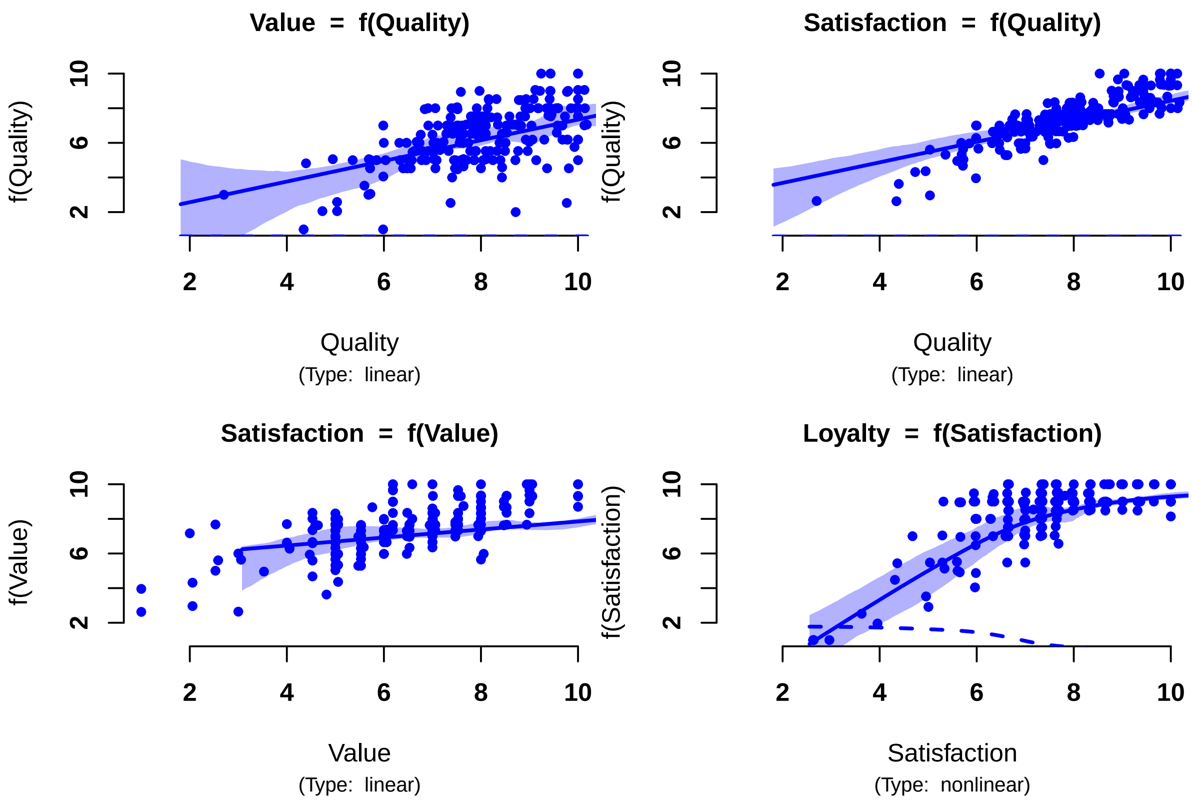

Figure 5: Estimated partial relationships of the reduced ECSI model of Example I, assuming only the relationship between Customer Satisfaction and Customer Loyalty is nonlinear and approximated by a cubic regression spline with dimension of the basis $K = 10$. The smooth weighting scheme estimated factor scores are represented as •. The solid blue line corresponds to the estimated relationship, and the area in light blue the corresponding 95% bootstrap credible intervals based on 500 replicates. The first derivative of the partial relationship is represented by the dashed blue line.

satisfaction and loyalty. However, their concentration in the top-right corner of the plot hardly suggests a linear relationship over the satisfaction level domain. Indeed, it suggests a decreasing growth rate of the loyalty levels, as first relationship derivative represented by the dashed blue line clearly shows, which is in line with literature mentioned in Section 1 (Song et al., 2013).

Bearing in mind these conclusion we decided to change the nature of three relationships in the structural model. Changing to linear the first three relationships mentioned in the previous paragraph a second attempt was made. The results are shown in Figure 5. The simplification of the model is the first three relationships does not bring significant losses. Indeed, Table 2 shows the values of the R-Squared are similar to the previous solution, keeping the gain in the explanation of the variance of the Customer Loyalty. Furthermore, one can test whether the basis dimension for a (partial) relationship is adequate as is described in Wood (2017)

(Section 5.9). More details can be found in Section @A.3. The results of the test indicate the used dimension of the basis, $K = 10$ is not to low. Werther it is to high is not a real problem as long as the sample size is large enough. Indeed, as discussed in Section @ref{sec:pls} about the trade-off between dimension of the basis and penalisation term shows that even if the dimension increases it is compensated by the penalisation parameter of the penalised least squares method.

In this example, where real data were used, performance was judged by visual inspection of plots describing the relationships and the R-Square values. Indeed, as true population relationships are unknown, it is impossible to assess the estimation accuracy. Consequently, the results of the second illustration comprising the model depicted in Figure 2(b) and the data generated through the Monte Carlo study described in Section 2.2.2 are presented in Section 3.2, which assesses the performance with respect to the recovery of the functional forms of the relationships, as measured by the absolute bias and root mean square error of the estimators.

3.2 Example II: a simulated dataset

The second experiment aimed to measure the performance of the PLSs-PM algorithm in detecting and approximating the nonlinear relationships between latent variables. As stated earlier, the novel PLSs-PM algorithm does not produce estimates of the parameters of the closed-form structural linear relationships. Instead, it smooths the structural relationships by estimating the coefficients associated with each piecewise linear model in (2.8). Hence, a direct comparison between the existing and the novel weighting scheme should be accomplished by evaluating their ability to recover structural relationships. Therefore, performance was evaluated with respect to the recovery of the regression function as a whole, as measured by the absolute bias and root mean squared error (RMSE), as described in Section 2.2.2.

The absolute bias (B) and root mean square error (RMSE) of the five relationships for the 24 possible combinations of sample size and residual variance, as described in Section 2.2.2, are presented in Appendix A.2.

Figure 6 represents a summary of the convergence results. The more computationally demanding nature of PLSs-PM algorithm anticipates it would be convergent less frequently than the PLS-PM. Indeed, it is what Figure 6 illustrates. However, both approaches is exhibit similar performance when the communality level reaches a level of 75% and sample size are larger or equal to 300 units. Both of these levels are commonly achieved is real-world studies. Furthermore, it is noteworthy to mention we are using cubic regression splines with $K = 10$ knots. As the number of knots gets fewer, it would be expected to achieve these levels of agreement between the two approaches with smaller samples sizes.

Figure 7 confirmed this result. Indeed, although for the lower levels of communality (25% and 50%) the average number of iterations PLSs-PM needs to reach convergence is higher

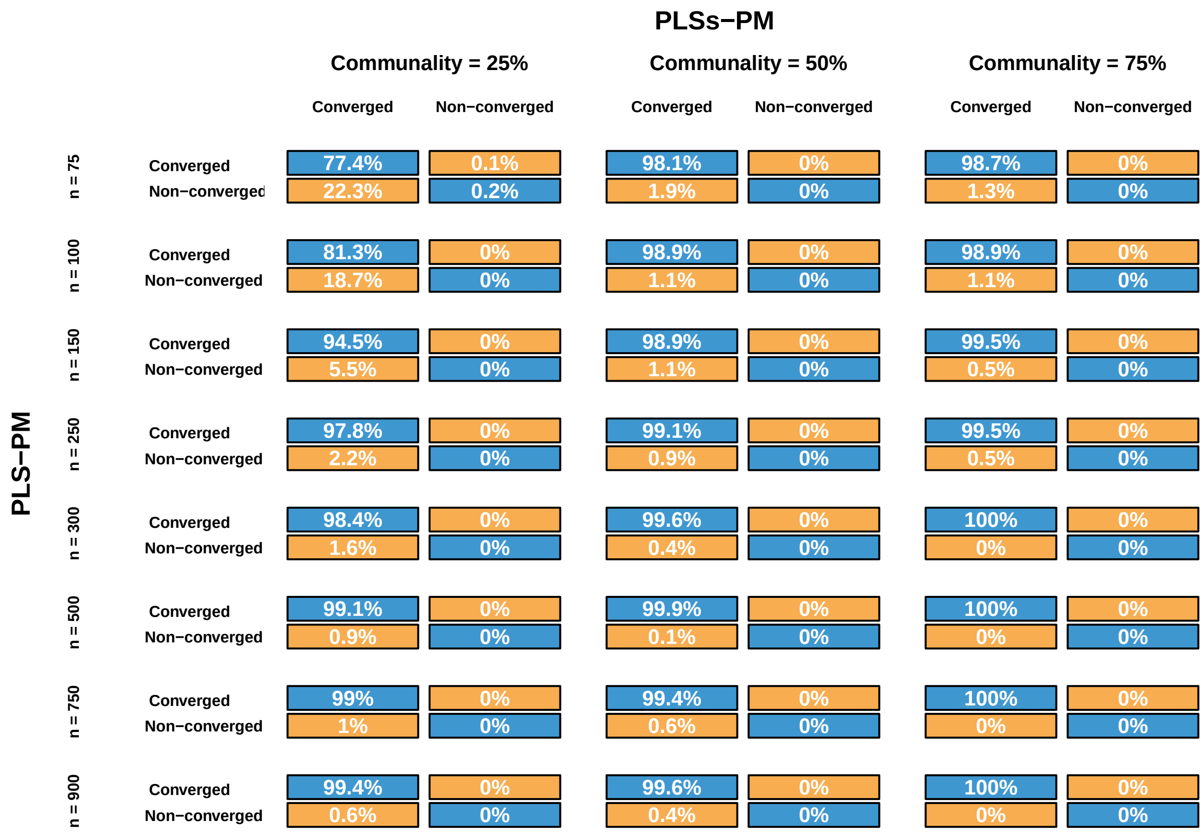

Figure 6: Assessment of the PLS-PM and PLSs-PM algorithms convergence. Each matrix depicts the confusion matrix of *Converged* and *Non-converged* iterations, for the same sample, by level of communality and sample size.

than PLS-PM, when the level of communality reaches 75%, the former outperforms the latter when the sample size exceeds 300 units.

In Section 2.2.2, the outer approximation of the PLS-PM algorithm may generate negative outer weights for some indicators when a latent variable presents a very limited number of links to other variables and/or when those links are not linear. One believes that this happens because either the information generated in the inner approximation might be scarce or deviates significantly from the true nature of the structural relationships. Figure 8 illustrates the performance achieved by PLS-PM and PLSs-PM algorithms in what regards to this matter. Although this problem cannot be completely avoided by the PLSs-PM, it consistently outweighs the PLS-PM.

Figures 9 and 10 compare the accuracy of the PLS-PM and PLSs-PM algorithms on absolute bias and root mean square error regards, respectively.

Table A7 presents the absolute bias and root mean square error of the PLSs-PM scheme as an index of the PLS-PM (base 100).

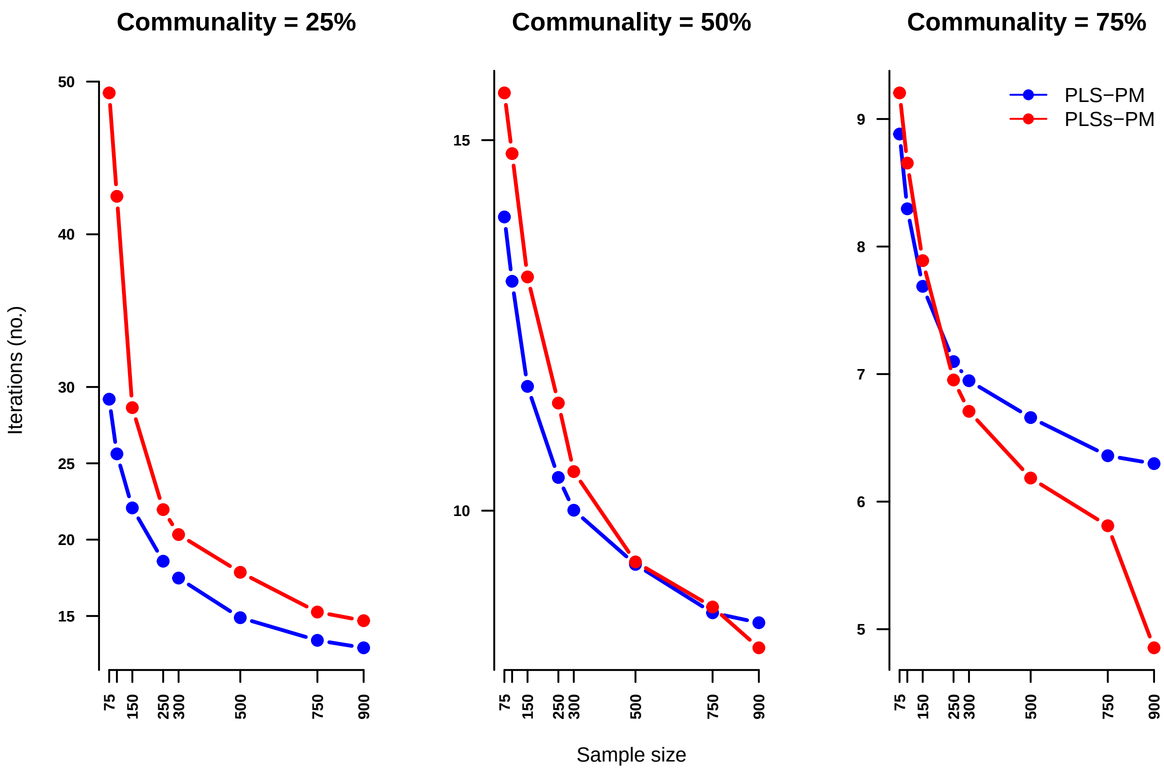

Figure 7: Mean number of iterations to obtain convergence (out of the converged ones), by sample size and communality level. The points in the plots mark, respectively sample sizes of 75, 100, 150, 250, 300, 500, 750 and 900 units. Althought PLS-PM using the *centroid* scheme outperforms PLSs-PM when the level of comunality is very low (25%), when the communality is 50% the latter outperforms the former when sample size is greater or equal than 500 units. And when the communality reaches 75% (which is not in general an hard assumption) it performs better when sample size is gretar or equal than 250 units.

The absolute bias and mean square error were consistently lower for PLSs-PM than PLS-PM, except in the case of a linear relationship (η_5). Indeed, regarding absolute bias, PLSs-PM algorithm was consistently superior to PLS-PM for the four tested nonlinear forms for sample sizes larger than 75. For the linear relationship η_5, PLSs-PM exhibits similar levels of absolute bias (see Figure 9 and Table A7). This is not a surprising result after looking at the results of Example I, where _smooth weighting showed its ability to accommodate linear relationships, but simultaneously it can be generalised to other shapes.

The RMSE of PLSs-PM tended to decrease with increasing sample size, leading to progressively increasing precision over PLS-PM. Specifically, PLSs-PM outperformed PLS-PM for nonlinear relationships. An exception occurred in the linear relationship. In this case, its accuracy only gets closer to PLS-PM's when the sample size increases, even though it happens quickly as the communality levels diminish (see Figure 10 and Table A7).

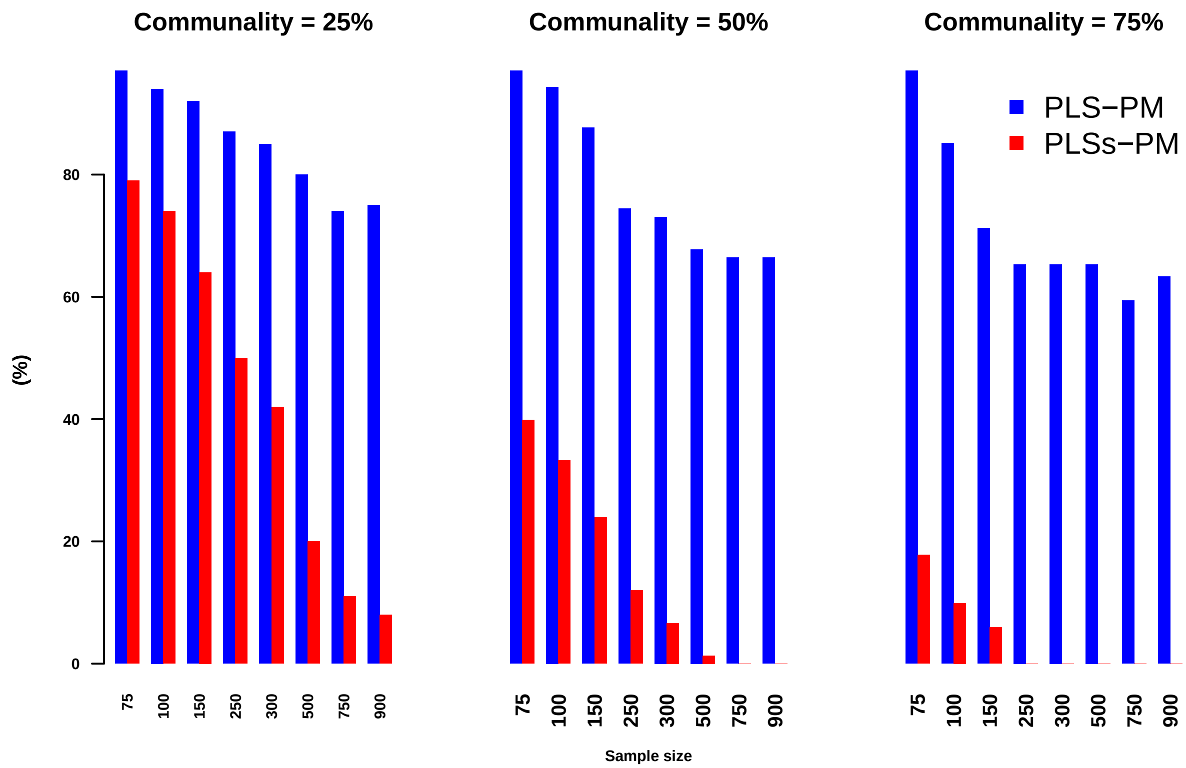

Figure 8: Percentage of samples (out of the converged ones) with with at least one negative outer weight, by sample size and communality level. The percentage of generated outer weights decreases as both the samples size and the communality increase. However, PLSs-PM scheme outperforms PLS-PM in all cases, and it even generates zero negative outer weigths when the communality is 75% and samples size is greater or equal than 300 units.

For illustration purposes, Figure 11 represents the true (population) relationships and the estimated ones by PLS-PM and PLSs-PM; in the latter case, the 95% credibility bands between ξ and η_1, a quadratic relationship, and ξ and η_5, the linear relationship. Figure 11(a) illustrates, among other things, the results of Table A7, in particular, the excellent performance of PLSs-PM in terms of absolute bias and mean square error. Figure 11(b) shows that the results of PLS-PM and PLSs-PM are almost visually identical when the structural relationships are linear, although Table A7 demonstrates that, in this case, PLS-PM consistently outperforms the PLSs-PM algorithm.

An analysis of variance using the method (PLS-PM and PLSs-PM), communality ($h = 25$), and sample size ($n = 75, 100, 150, 250, 300, 500, 750, 900$), and interactions between the method and communality and between the method and sample size as factors was performed to test whether each level of the factors or interactions among them used in the assessment exhibited significant statistical differences for both the absolute bias and root mean square error. The results are presented in Tables A7 and A7 of Appendix A.2.

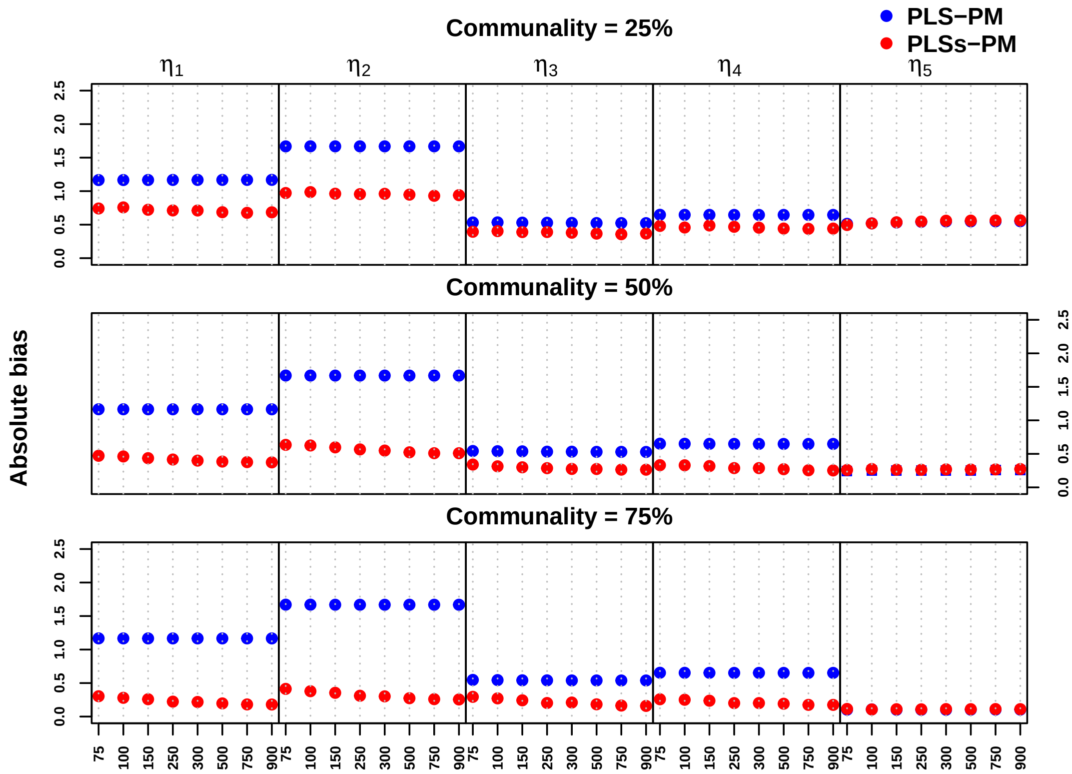

Figure 9: Absolute bias comparison of the five endogenous variables ($\eta_1, \ldots, \eta_5$) for the eight different sample sizes ($n = 75, \ldots, 900$) and three levels of communality (25%, 50% and 75%).

Regarding the absolute bias, almost all factors/levels considered are not statistically significant, except in the case of η_5. Indeed, the sample size is not significant. Indeed, the method, communality level, and interaction between method and communality are not statistically significant, except in the case of η_5 (linear relationship). However, when associated with PLSs-PM, the sample size was significant for all tested functional forms for sample sizes larger than 100, confirming an absolute bias improvement of PLSs-PM as the sample size increased. Communality shows differences between levels only in linear functional form.

Regarding the RMSE, the method is generally statistically significant. The sample size was not significant. Communality is statistically significant, except in the case of η_1 and η_2 for the two highest levels of communality (50% and 70%). The interaction between the method and communality is not statistically significant, and its interaction with sample size is statistically insignificant in the case of η_5 when it comes to the interaction with sample sizes of 100 and 500 units.

These results confirm that PLSs-PM consistently produces better levels of absolute bias and mean square error for nonlinear relationships. Indeed, PLSs-PM tends to produce a smaller absolute bias for nonlinear relationships whose functional forms are of the type of equations tested. This is generally true for all levels of communality, although the differences between

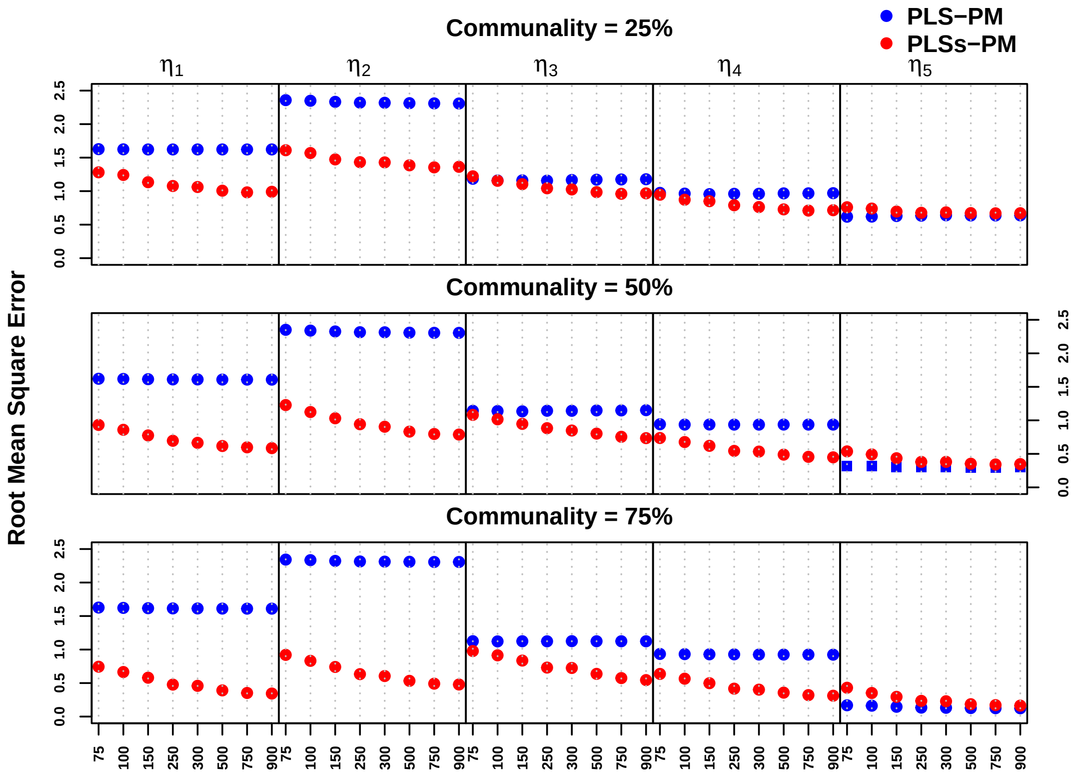

Figure 10: Root mean square error comparison of the five endogenous variables ($\eta_1, \ldots, \eta_5$) for the eight different sample sizes ($n = 75, \ldots, 900$) and three levels of communality (25%, 50% and 75%).

the two methods increase as the level of communality and the sample size increase.

4 Discussion

This study proposed and tested a new inner weighting scheme and structural relationships estimation method in PLS-PM algorithm. We compared the traditional PLS-PM and the proposed PLSs-PM approaches for the inner approximation of latent variable proxies and structural relationships in the context of Partial Least Squares. A method using additive models based on cubic regression splines was embedded in the PLS-PM algorithm using the Wold's hybrid approach, *smooth weighting*. The novel inner weighting scheme was introduced and used to estimate two structural equation models using both real and simulated data. Regarding the real data case, although it was not possible to compare numeric measures of accuracy for the real dataset, visual inspection of the estimated structural relationships, as well as the determinantion coefficients, indicated that PLSs-PM can capture nonlinear structural relationships.

The two methods were compared using a simulated dataset that mimicked four nonlinear structural relationships and a linear relationship as case controls. Several scenarios were

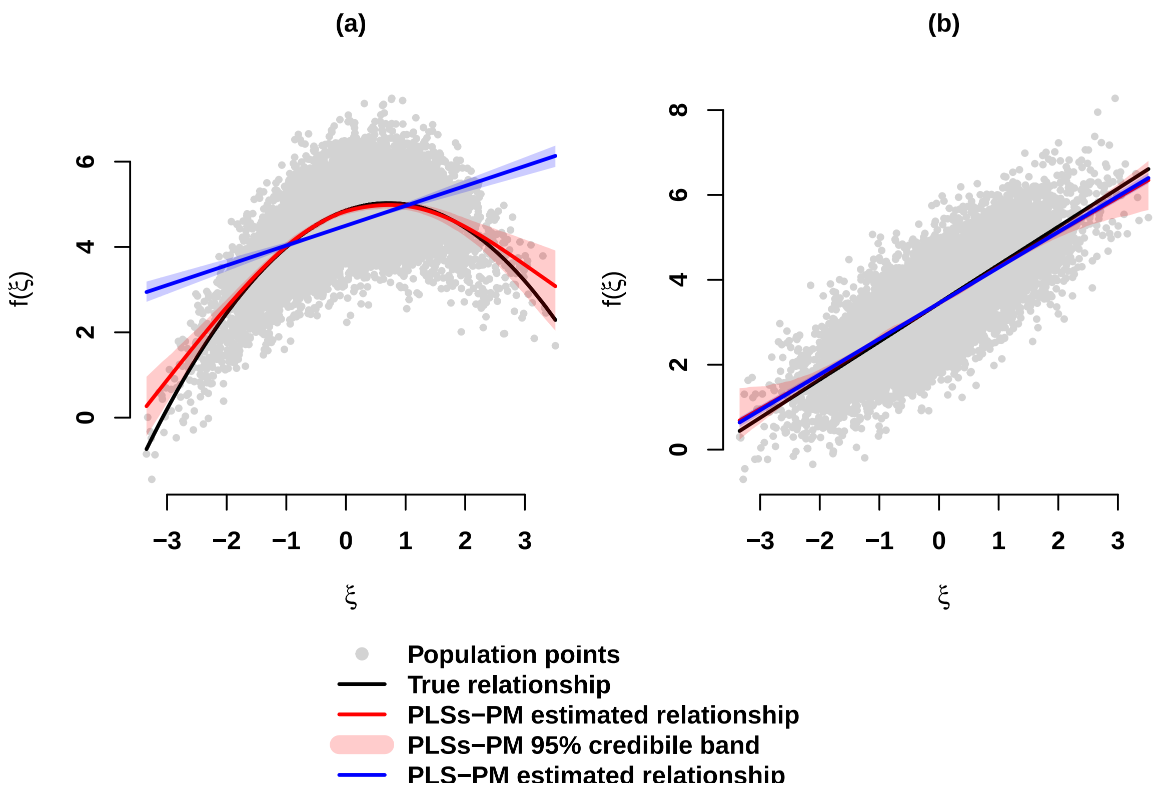

Figure 11: Estimated relationships between ξ and η_4 and η_5 of the simulated data set of example II. The population factor scores are represented as dots in light gray. The solid black line corresponds to the true relationship. The solid blue line corresponds to the relationship as estimated by PLS-PM algorithm. The solid red line and the light red shaded area corresponds to the relationship as estimated by PLSs-PM algorithm and the corresponding 95% credibility intervals.

tested for different levels of communality between the latent variables, observed indicators, and eight different sample sizes. The methods were compared based on the absolute bias and root mean square error. PLSs-PM performed globally better than PLS-PM, except for linear relationships, although the differences between the two were less obvious for very small sample sizes. This result is in line with expectations as the estimation of nonlinear functions demanding in terms of factor determination (i.e., the informativeness of the observed data). Another important observation is the observed ability of PLSs-PM to adjust to linear relationships, as the bias diminishes consistently with the sample size. Nevertheless, for exact linear relationships, the PLSs-PM's RMSE tends to be larger than that of PLS-PM. This is a result of the increased variance in the estimation of PLSs-PM, as it is more demanding in the number of parameters to estimate.

Although PLSs-PM does not account for PLS-PM inconsistency, it succeeds in it main aim: maximise the explained variance of the endogenous latent variables due to its ability of approximating structural relationships whose functional form is not known and cannot be *a priori* specified as linear. Nevertheless, the fact that the approximation relies on linear combinations of piecewise functions of the predecessor latent variables, it suggests future possible adaptations to produce consistent estimates of structural relationships.

Structural equation models are commonly used in many scientific areas, including social, behavioural, health, and management sciences, to evaluate relationships among latent variables that cannot be observed directly or without noise. Without any empirical or theoretical verification, it is generally assumed that the latent variables are linearly related. As discussed by Bauer et al. (2012), this is an exception, suggesting that scatter plots between observed variables should be inspected for potential nonlinear trends. Nevertheless, it is admited that the contamination of manifest variables by measurement errors might mask the underlying nonlinear relationships and suggest detection procedures at the level of the structural model.

Extensive attention has been paid to modelling nonlinear trends using quadratic or product-interaction terms, without considering that one rarely has prior knowledge of the nature of the relationships, and that frequently they present patterns that can not be adequately represented by these specific structures. The notable absence of research on methods for estimating nonlinear relationships in structural equation modelling contrasts with the extensive use of (general) additive models for observed (non-latent) variables.

There is little reason to believe that nonlinear effects are less common for latent variables than observed variables. If anything, the nonlinear effects might be harder to visualise and detect with observed variables owing to contamination by measurement error. Therefore, the absence of discussion on techniques for detecting and estimating nonlinear effects in latent variable models is likely related to the fact that few techniques have been proposed or evaluated for this purpose. Because the main consequences of using traditional linear PLS-PM in the presence of structural nonlinear relationships might be a lack of ability to understand the true nature of the relationships between constructs, potential underestimation or overestimation of the relative importance of the drivers of endogenous latent constructs and the fact that estimates of model parameters (loadings, regression coefficients) are biased or suboptimal, it was our goal to propose a new technique and compare its performance with traditional linear PLS-PM.

Future work should be performed to test the performance of these two methods under different conditions, namely when other types of smoothers and/or other types of knot definitions are considered. Improvements on the edges of the relationships are particularly needed, and natural cubic splines are limited to linear relationships beyond the lowest and highest generated proxy values. Moreover, it is important to test whether the performance of the PLSs-PM method is different in the case formative constructs. It is even more important to provide PLSs-PM with automatic mechanisms to detect the presence of nonlinearity and automatically choose a linear or nonlinear estimation procedure. Statistical tests of the additive components of the smoothers can maintain the algorithm on the correct path.

This new methodology may be useful for modelling nonlinear relationships between latent variables and indicators as well as for formative or reflective measurement models.

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A Suplementary material

A.1 Suplementary results of Example I

A.1.1 Latent variables and their indicators

Table A1: Measurement model for reduced European Satisfaction Satisfaction Index (ECSI) - banking sector. All indicators are measured in a 10-point scale, from 1 to 10, where 1 expresses a very negative opinion and 10 a very positive opinion. The values α and ρ represent Cronbach's α and Dillon-Goldstein's ρ.

Reliability	Indicator
Perceived quality	
	(a) Overall perceived quality (QUAL1)
	(b) Quality of products and services (QUAL2)
	(c) Customer service and personal advice (QUAL3)
	(d) Availability of contact channels (QUAL4)
	(e) Reliability of products and services (QUAL5)
	(f) Diversity of products and services (QUAL6)
	(g) Clarity and transparency of information provided (QUAL7)
	(h) Accessibility (QUAL8)
	(i) Quality of physical facilities (QUAL9)
Perceived value	
$\alpha = 0.9$	(a) Evaluation of price given quality (VALU1)
$\rho = 0.95$	(b) Evaluation of quality given price (VALU2)
Customer satisfaction	
$\alpha = 0.84$	(a) Overall satisfaction (SATI1)
$\rho = 0.91$	(b) Fulfilment of expectations (SATI2)
	(c) Distance to ideal bank (SATI3)
Customer loyalty	
$\alpha = 0.82$	(a) Intention to remain as a customer (LOYA1)
$\rho = 0.92$	(b) Recommendation to friends and colleagues (LOYA2)

A.1.2 Comparison of results obtained with the ECSI dataset of Example I in *plspm*, *SeminR* and authors' implementation

Table A2: Outer model weights

Indicator	plspm	SeminR	Authors' implementation
Quality			
QUAL1	0.40	0.40	0.40
QUAL2	0.24	0.24	0.24
QUAL3	-0.11	-0.11	-0.11
QUAL4	0.10	0.10	0.10
QUAL5	0.01	0.01	0.00
QUAL6	0.40	0.40	0.40
QUAL7	0.06	0.06	0.07
QUAL8	0.11	0.11	0.09
QUAL9	-0.03	-0.03	-0.02
Value			
VALU1	0.50	0.50	0.50
VALU2	0.55	0.55	0.55
Satisfaction			
SATI1	0.35	0.35	0.35
SATI2	0.40	0.40	0.40
SATI3	0.39	0.39	0.39
Loyalty			
LOYA1	0.52	0.52	0.52
LOYA2	0.57	0.57	0.57

Table A3: Outer model loadings

Indicator	plspm	SeminR	Authors' implementation
Value			
VALU1	0.95	0.95	0.95
VALU2	0.96	0.96	0.96
Satisfaction			
SATI1	0.86	0.86	0.86
SATI2	0.88	0.88	0.88
SATI3	0.88	0.88	0.88
Loyalty			
LOYA1	0.91	0.91	0.91
LOYA2	0.93	0.93	0.93

Table A4: Inner model: Dillon Goldsteins's ρ and R^2

	Value	Satisfaction	Loyalty
plspm			
Dillon Goldsteins's ρ	0.95	0.91	0.92
R^2 (%)	37.09	83.42	52.16
SeminR			
Dillon Goldsteins's ρ	0.91	0.95	0.92
R^2 (%)	36.95	83.6	52.17
Authors' implementation			
Dillon Goldsteins's ρ	0.95	0.91	0.92
R^2 (%)	60.9	91.34	72.22

Table A5: Inner model: path coefficients

	Value	Satisfaction	Loyalty
plspm			
Quality	0.61	0.74	
Value		0.25	
Satisfaction			0.72
SeminR			
Quality	0.61	0.74	
Value		0.25	
Satisfaction			0.72
Author's implementation			
Quality	0.61	0.74	
Value		0.25	
Satisfaction			0.72

Table A6: Inner model: total effects

	Satisfaction	Value	Loyalty
plspm			
Quality	0.89	0.61	0.64
Satisfaction			0.72
Value	0.25		0.18
Loyalty			
SeminR			
Quality	0.89	0.61	0.64
Satisfaction			0.72
Value	0.25		0.18
Loyalty			
Author's implementation			
Quality	0.89	0.61	0.64
Satisfaction			0.72
Value	0.25		0.18
Loyalty			

A.2 Supplementary results of Example II

A.2.1 Population values of endogenous variables used in factor scores scaling

The following paragraphs present the calculations to find the population expected values and variances of the five endogenous variables of the structural model of Example III. These population value were used to scale the PLS-PM and PLSs-PM factor scores computed in the last iteration of the algorithms. These scaled scores allow direct comparison with functional relationships described in Figure 3, in Section 2.2.2 and presented in Figure 11, as well as the computation of Absolute Bias and Root Mean Square Error reported in Figures 9, 10, in Section 3.2, and Tables A7, A8 and A9 of the current Appendix A.2.

The latent variable η_1 is a function of ξ and ϵ_1, both following standard normal distribution. It is described by $\eta_1 = g(\xi, \epsilon_1) = 4.85 + 0.5\xi - 0.35\xi^2 + \epsilon_1$. We can use the properties of mathematical expectation and variance.

The exogenous random variable follows a standard normal distribution, $\xi \sim N(0, 1)$. The perturbances $\epsilon_i \sim N(0, 0.5)$, $i = 1, 2, 3, 4, 5$, and are independent of each other and of ξ.

Hence, the expected value of η_1 is given by:

$$\begin{aligned}
\mathrm{E}(\eta_1) &= \mathrm{E}(4.85 + 0.5\xi - 0.35\xi^2 + \epsilon_1) \Leftrightarrow \\
&= \mathrm{E}(4.85) + 0.5\mathrm{E}(\xi) - 0.35\mathrm{E}(\xi^2) + \mathrm{E}(\epsilon_1) \Leftrightarrow \\
&= 4.85 - 0.35 \times 1 + 0 = 4.5.
\end{aligned}$$

Assuming that ϵ_1 is independent from ξ, variance of ξ is given by:

$$\begin{aligned}
\mathrm{Var}(\eta_1) &= \mathrm{Var}(4.85 + 0.5\xi - 0.35\xi^2 + \epsilon_2) \Leftrightarrow \\
&= \mathrm{Var}(4.85) + 0.5^2\mathrm{Var}(\xi) + 0.35^2\mathrm{Var}(\xi^2) + \mathrm{Var}(\epsilon_1).
\end{aligned}$$

As $\mathrm{Var}(\xi) = 1$ and ξ^2 follows a χ^2 distribution with 1 degree of freedom, which implies that $\mathrm{Var}(\xi^2) = 2$, and $\mathrm{Var}(\epsilon_1) = 0.5$;

$$\mathrm{Var}(\eta_1) = 0.25 \cdot 1 + 0.35^2 \cdot 2 + 0.5 = 0.995.$$

The latent variable η_2 is a function of ξ described by $\eta_2 = g(\xi) = 5 - 0.5\xi^2 + \epsilon_2$. Its expected value is given by:

$$\begin{aligned}
\mathrm{E}(\eta_2) &= \mathrm{E}(5 - 0.5\xi^2 + \epsilon_{\eta_2}) \Leftrightarrow \\
&= 5 - 0.5\mathrm{E}(\xi^2) + \mathrm{E}(\epsilon_{\eta_2}) \Leftrightarrow \\
&= 5 - 0.5 \times 1 + 0 = 4.5.
\end{aligned}$$

Its variance, assuming η_2 is independent of ϵ_{η_2} and taking into account the same properties of ξ^2 mentioned above, is given by:

$$\begin{aligned}
\mathrm{Var}(\eta_2) &= \mathrm{Var}(5 - 0.5\xi^2 + \epsilon_{\eta_2}) \Leftrightarrow \\
&= 0.5^2\mathrm{Var}(\xi^2) + \mathrm{Var}(\epsilon_{\eta_2}) \Leftrightarrow \\
&= 0.25 \cdot 2 + \sigma^2_{\epsilon_{\eta_2}} \Leftrightarrow \\
&= 0.5 + 0.5 = 1.
\end{aligned}$$

The latent variable η_3 is a function of ξ described by $\eta_3 = g(\xi) = 5 + 0.04(1 - e^{-1.5\xi}) + \epsilon_{\eta_3}$.

Assuming ϵ_4 is independent of ξ and it determines η_3 additively, we use the change of variable technique to find the distribution of $\eta_3^* = h(\xi) = 5 + 0.04(1 - e^{-1.5\xi})$ in first place.

The transformation of a random variable ξ through a deterministic function is a straightforward application of probability theory. To find the density function of ξ, we can use the probability density function transformation method.

Let $\eta_3^* = h(\xi) = 5 + 0.04(1 - e^{-1.5\xi})$.

The probability density function of η_4 is given by $f_{\eta_3}(\eta_3) = f_\xi(h^{-1}(\eta_3^*))|(h^{-1})'(\eta_3^*)|$, where $(h^{-1})'(\eta_3)$ is the derivative of $h^{-1}(\eta_3^*)$ and f_ξ is the probability density function of the standard normal variable.

Solving $h(\xi)$ for η_3^* we obtain:

$$\begin{aligned}
\eta_3^* &= 5 + 0.04(1 - e^{-1.5\xi}) \Leftrightarrow \\
\eta_3^* - 5 &= 0.04(1 - e^{-1.5\xi}) \Leftrightarrow \\
\frac{\eta_3^* - 5}{0.04} &= 1 - e^{-1.5\xi} \Leftrightarrow \\
1 - \frac{\eta_3^* - 5}{0.04} &= e^{-1.5\xi} \Leftrightarrow \\
\log\left(1 - \frac{\eta_3^* - 5}{0.04}\right) &= -1.5\xi \Leftrightarrow \\
\xi &= -\frac{1}{1.5}\log\left(\frac{0.04 - \eta_3^* + 5}{0.04}\right).
\end{aligned}$$

The derivative of $(h^{-1})'(\eta_3^*)$ is:

$$
\begin{aligned}
(h^{-1})'(\eta_3^*) &= -\frac{1}{1.5}\log\left(\frac{0.04-\eta_3^*+5}{0.04}\right) \Leftrightarrow \\
&= -\frac{1}{1.5}\left[\log\left(\frac{0.04-\eta_3^*+5}{0.04}\right)\right]' \Leftrightarrow \\
&= -\frac{1}{1.5}\frac{1}{\left(\dfrac{0.04-\eta_3^*-5}{0.04}\right)}\left(\frac{0.04-\eta_3^*+5}{0.04}\right)' \Leftrightarrow \\
&= -\frac{1}{1.5}\frac{1}{\dfrac{0.04-\eta_3^*+5}{0.04}}\left(-\frac{1}{0.04}\right) \Leftrightarrow \\
&= \frac{25\cdot 0.04}{1.5(0.04-\eta_3^*+5)} \Leftrightarrow \\
&= \frac{1}{1.5(0.04-\eta_3^*+5)}.
\end{aligned}
$$

Now, substitute $h^{-1}(\eta_3^*)$ and $(h^{-1})'(\eta_3^*)$ into the density function formula

$$
\begin{aligned}
f_{\eta_3^*}(\eta_3^*) &= f_\xi\left(-\frac{1}{1.5}\log\left(\frac{0.04-\eta_3^*+5}{0.04}\right)\right)\left|\frac{1}{1.5(0.04-\eta_3^*+5)}\right| \Leftrightarrow \\
&= \frac{1}{\sqrt{2\pi}1.5(0.04-\eta_3^*+5)}e^{-\frac{1}{2}\left(\frac{1}{1.5}\log\left(\frac{0.04-\eta_3^*+5}{0.04}\right)\right)^2}.
\end{aligned}
$$

The support of η_3^* is given by

$$
\begin{aligned}
&-\infty \le \xi \le +\infty \Leftrightarrow \\
&-\infty \le -1.5\xi \le +\infty \Leftrightarrow \\
&-\infty \le -e^{-1.5\xi} \le 0 \Leftrightarrow \\
&-\infty \le 1-e^{-1.5\xi} \le 1 \Leftrightarrow \\
&-\infty \le 0.04(1-e^{-1.5\xi}) \le 0.04 \Leftrightarrow \\
&-\infty \le 5+0.04(1-e^{-1.5\xi}) \le 5.04. -\infty \qquad\qquad \le \eta_3^* \le 5.04.
\end{aligned}
$$

Therefore the expected value of η_3^* is given by

$$
\begin{aligned}
\mathrm{E}(\eta_3^*) &= \int_{-\infty}^{5.04}\eta_3^*\cdot\frac{1}{\sqrt{2\pi}1.5(0.04-\eta_3^*-5)}e^{-\frac{1}{2}\left(\frac{1}{1.5}\log\left(\frac{0.04-\eta_3^*+5}{0.04}\right)\right)^2}d\eta_3^* \Leftrightarrow \\
&= 4.9168.
\end{aligned}
$$

Consequently, the expected value of η_3 is:

$$\mathrm{E}(\eta_3) = \mathrm{E}(\eta_3^*) + \mathrm{E}(\epsilon_3) = 4.9168.$$

The variance of η_3^* can be obtained through the equation $\mathrm{Var}(\eta_3^*) = \mathrm{E}((\eta_3^*)^2) - \mathrm{E}(\eta_3^*)^2$. The first term of the right-hand side of theis equation is given by:

$$\begin{aligned}\mathrm{E}(\eta_3^2) = \int_{-\infty}^{5.04} \eta_3^2 \cdot \frac{1}{\sqrt{2\pi}1.5(0.04 - \eta_3 - 5)} e^{-\frac{1}{2}\left(\frac{1}{1.5}\log\left(\frac{0.04-\eta_3+5}{0.04}\right)\right)^2} d\eta_3 \Leftrightarrow \\ = 24.3037.\end{aligned}$$

Consequently, the variance of η_3^* is:

$$\begin{aligned}\mathrm{Var}(\eta_3^*) &= \mathrm{E}((\eta_3^*)^2) - \mathrm{E}(\eta_3^*)^2 \Leftrightarrow \\ &= 0.1288.\end{aligned}$$

Finally, the variance of η_3 is give by:

$$\begin{aligned}\mathrm{Var}(\eta_3) &= \mathrm{Var}(\eta_3^*) + \mathrm{Var}(\epsilon\eta_3) \Leftrightarrow \\ &= 0.1288 + 0.5 = 0.6288.\end{aligned}$$

The latent variable η_4 is a function of ξ described by the following expression:

$$\eta_4 = g(\xi) = \begin{cases} 5 + 0.1\xi - 0.3\xi^2 + \epsilon_4, & \xi < 0 \\ 5 + 0.1\xi - 0.1\xi^2 + \epsilon_4, & \xi > 0. \end{cases}$$

As $\xi \sim N(0,1)$, $\mathrm{P}(\xi < 0) = \mathrm{P}(\xi > 0) = 0.5$, thus

$$\eta_4 = g(\xi) = \begin{cases} 5 + 0.1\xi - 0.3\xi^2 + \epsilon_4, & \text{with probability } p = 0.5 \\ 5 + 0.1\xi - 0.1\xi^2 + \epsilon_4, & \text{with probability } p = 0.5. \end{cases}$$

Its expected value is given by:

$$\begin{aligned}\mathrm{E}(\eta_4) &= 0.5\left(\mathrm{E}(5 + 0.1\xi - 0.3\xi^2 + \epsilon_4\right) + 0.5\left(\mathrm{E}(5 + 0.1\xi - 0.1\xi^2\epsilon_{\eta_2} + \epsilon_4)\right) \Leftrightarrow \\ &= 0.5\left(5 + 0.1\mathrm{E}(\xi) - 0.3\mathrm{E}(\xi^2) + \mathrm{E}(\epsilon_4^2)\right) + 0.5\left(5 + 0.1\mathrm{E}(\xi) - 0.1\mathrm{E}(\xi^2) + \mathrm{E}(\epsilon_4^2)\right) \Leftrightarrow \\ &= 0.5(5 - 0.3 \cdot 1) + 0.5(5 - 0.1 \cdot 1) = 4.5\end{aligned}$$

Its variance, assuming η_4 is independent of ϵ_{η_4} by:

$$\begin{aligned}
\mathrm{Var}(\eta_4) &= 0.5\left(\mathrm{Var}(5 + 0.1\xi - 0.3\xi^2 + \epsilon_4\right) + 0.5\left(\mathrm{Var}(5 + 0.1\xi - 0.1\xi^2\epsilon_{\eta_2} + \epsilon_4)\right) \Leftrightarrow \\
&= 0.5\left(0.1^2\mathrm{Var}(\xi) + 0.3^2\mathrm{Var}(\xi^2) + \mathrm{Var}(\epsilon_4^2)\right) + 0.5\left(0.1^2\mathrm{Var}(\xi) + 0.1^2\mathrm{Var}(\xi^2) + \mathrm{Var}(\epsilon_4^2)\right) \Leftrightarrow \\
&= 0.5(0.1^2 \cdot 1 + 0.3^2 \cdot 2 + 0.5) + 0.5(0.1^2 \cdot 1 + 0.1^2 \cdot 2 + 0.5) = 0.61
\end{aligned}$$

The latent variable η_5 is a function of ξ described by $\eta_5 = g(\xi) = 3.45 + 0.9\xi + \epsilon_5$. It is a linear transformation of ξ, therefore its expected value is given by:

$$\begin{aligned}
\mathrm{E}(\eta_5) &= \mathrm{E}(3.45 + 0.9\xi + \epsilon_5) \Leftrightarrow \\
&= \mathrm{E}(3.45) + 0.9\mathrm{E}(\xi) + \mathrm{E}(\epsilon_5) \Leftrightarrow \\
&= 3.45.
\end{aligned}$$

Its variance, assuming ξ is independent of ϵ_5, is given by:

$$\begin{aligned}
\mathrm{Var}(\eta_5) &= \mathrm{Var}(3.45 + 0.9\xi + \epsilon_5) \Leftrightarrow \\
&= 0.9^2\mathrm{Var}(\xi) + \mathrm{Var}(\epsilon_5) \Leftrightarrow \\
&= 0.81 + \sigma_{\epsilon_5}^2 \Leftrightarrow \\
&= 0.81 + 0.5 = 1.31.
\end{aligned}$$

A.2.2 Additional results on Absolute Bias and Root Mean Square Error

Table A7: PLSs-PM absolute bias and root mean square error as a index number of PLS-PM absolute bias and root mean square error (base 100).

	Bias					RMSE				
Sample size	η_1	η_2	η_3	η_4	η_5	η_1	η_2	η_3	η_4	η_5
Communality = 25%										
n100	65.00	59.08	75.52	70.72	99.85	76.45	66.79	99.59	90.48	119.33
n150	61.90	57.64	73.39	75.45	100.63	69.88	63.17	95.09	88.95	110.62
n250	61.00	57.27	73.77	72.47	101.00	66.38	61.74	90.10	82.22	106.80
n300	60.91	57.54	72.16	70.45	101.93	65.44	61.63	87.93	79.37	106.86
n500	58.72	56.78	69.89	68.45	102.18	62.06	59.90	84.15	75.29	105.52
n75	63.61	58.29	73.94	74.30	96.54	78.75	68.30	103.12	97.16	122.79
n750	57.91	55.77	68.27	67.88	102.32	60.53	58.66	81.73	73.37	105.07
n900	58.56	56.35	70.19	68.41	102.43	61.06	59.05	82.12	73.77	105.02
Communality = 50%										
n100	39.57	37.46	58.18	50.66	108.12	53.10	48.06	89.21	72.20	154.22
n150	37.40	35.78	55.73	48.94	105.93	48.01	44.31	83.51	66.08	142.03
n250	35.66	33.95	53.77	44.30	104.10	43.16	40.68	77.27	58.13	125.92
n300	34.26	32.91	51.66	44.30	105.59	41.26	39.09	74.24	57.02	125.69
n500	33.04	31.37	51.65	41.80	104.82	38.37	36.03	69.87	52.14	118.31
n75	40.44	38.02	62.74	50.80	106.17	57.48	52.24	94.70	78.21	168.92
n750	32.32	30.57	49.84	39.35	105.17	37.15	34.54	65.74	48.64	114.74
n900	31.98	30.56	49.89	38.99	106.26	36.41	34.19	63.78	47.84	115.72
Communality = 75%										
n100	24.01	22.66	49.88	38.42	98.93	41.00	35.62	81.45	60.69	216.65
n150	22.18	21.25	44.80	36.28	108.37	35.85	31.88	74.32	53.61	201.36
n250	19.13	18.63	37.50	30.85	106.97	29.56	27.36	65.07	44.88	175.36
n300	18.69	18.10	38.89	30.89	110.69	28.44	26.16	64.46	43.42	174.39
n500	16.86	16.41	33.95	29.40	107.42	24.25	23.08	56.69	38.61	145.39
n75	26.04	24.75	53.85	39.52	111.03	45.73	39.30	86.93	68.12	255.00
n750	15.55	15.57	30.52	26.82	108.42	21.88	21.28	51.10	34.67	137.24
n900	15.43	15.28	29.55	26.76	106.98	21.34	20.74	48.47	33.72	131.77

Table A8: ANOVA results. Dependent variable: absolute bias. p-values are indicated within brackets next to parameter estimates.

Factor | Level	η_1	η_2	η_3	η_4	η_5
Sample size					
$n = 100$	0.000 (0.997)	-0.001 (0.970)	-0.003 (0.771)	-0.001 (0.907)	0.001 (0.897)
$n = 150$	0.000 (0.968)	-0.001 (0.958)	-0.006 (0.616)	-0.002 (0.832)	0.005 (0.600)
$n = 250$	0.000 (0.953)	0.000 (0.970)	-0.007 (0.528)	-0.002 (0.831)	0.008 (0.409)
$n = 300$	0.000 (0.940)	0.000 (0.975)	-0.008 (0.456)	-0.002 (0.797)	0.008 (0.389)
$n = 500$	0.000 (0.996)	0.000 (0.997)	0.001 (0.913)	0.001 (0.913)	-0.007 (0.489)
$n = 750$	0.001 (0.938)	-0.001 (0.964)	-0.009 (0.429)	-0.002 (0.783)	0.009 (0.341)
$n = 900$	0.001 (0.926)	-0.001 (0.963)	-0.009 (0.400)	-0.002 (0.791)	0.011 (0.278)
Method					
PLSs-PM	-0.408 (0.000)	-0.662 (0.000)	-0.118 (0.000)	-0.163 (0.000)	0.002 (0.847)
Communality					
h=50%	-0.002 (0.623)	-0.001 (0.951)	0.007 (0.334)	0.003 (0.454)	-0.285 (0.000)
h=75%	-0.001 (0.898)	0.000 (0.960)	0.014 (0.054)	0.006 (0.147)	-0.435 (0.000)
Method | Communality					
PLSs-PM|h=50%	-0.295 (0.000)	-0.392 (0.000)	-0.098 (0.000)	-0.170 (0.000)	0.010 (0.251)
PLSs-PM|h=75%	-0.480 (0.000)	-0.639 (0.000)	-0.178 (0.000)	-0.254 (0.000)	0.003 (0.750)
Method | Sample size					
PLSs-PM|$n = 100$	-0.028 (0.005)	-0.025 (0.197)	-0.016 (0.311)	0.002 (0.828)	0.003 (0.843)
PLSs-PM|$n = 150$	-0.050 (0.000)	-0.052 (0.011)	-0.031 (0.056)	-0.026 (0.015)	0.001 (0.918)
PLSs-PM|$n = 250$	-0.057 (0.000)	-0.059 (0.004)	-0.035 (0.035)	-0.030 (0.006)	0.006 (0.678)
PLSs-PM|$n = 300$	-0.078 (0.000)	-0.081 (0.000)	-0.047 (0.005)	-0.043 (0.000)	0.004 (0.747)
PLSs-PM|$n = 500$	0.006 (0.529)	0.010 (0.591)	0.012 (0.448)	0.010 (0.323)	-0.003 (0.809)
PLSs-PM|$n = 750$	-0.089 (0.000)	-0.096 (0.000)	-0.059 (0.001)	-0.055 (0.000)	0.005 (0.696)
PLSs-PM|$n = 900$	-0.088 (0.000)	-0.094 (0.000)	-0.057 (0.001)	-0.055 (0.000)	0.006 (0.659)

Table A9: ANOVA results. Dependent variable: RMSE. p-values are indicated within brackets next to parameter estimates.

Factor | Level	η_1	η_2	η_3	η_4	η_5
Sample size					
$n = 100$	-0.003 (0.769)	-0.013 (0.574)	0.000 (0.995)	-0.003 (0.762)	-0.007 (0.731)
$n = 150$	-0.005 (0.632)	-0.024 (0.318)	0.001 (0.950)	-0.002 (0.827)	-0.011 (0.584)
$n = 250$	-0.006 (0.612)	-0.026 (0.281)	0.005 (0.802)	-0.003 (0.781)	-0.009 (0.632)
$n = 300$	-0.007 (0.537)	-0.030 (0.204)	0.008 (0.696)	-0.001 (0.926)	-0.013 (0.512)
$n = 500$	0.003 (0.761)	0.010 (0.673)	0.011 (0.586)	0.006 (0.562)	0.001 (0.953)
$n = 750$	-0.008 (0.500)	-0.033 (0.166)	0.009 (0.648)	-0.001 (0.934)	-0.014 (0.480)
$n = 900$	-0.008 (0.500)	-0.034 (0.156)	0.011 (0.575)	-0.001 (0.961)	-0.013 (0.513)
Method					
PLSs-PM	-0.380 (0.000)	-0.739 (0.000)	0.028 (0.215)	-0.064 (0.000)	0.130 (0.000)
Communality					
h=50%	-0.011 (0.131)	-0.005 (0.714)	-0.025 (0.043)	-0.027 (0.000)	-0.326 (0.000)
h=75%	-0.007 (0.297)	-0.007 (0.618)	-0.045 (0.001)	-0.037 (0.000)	-0.492 (0.000)
Method | Communality					
PLSs-PM|h=50%	-0.370 (0.000)	-0.491 (0.000)	-0.149 (0.000)	-0.206 (0.000)	0.038 (0.032)
PLSs-PM|h=75%	-0.588 (0.000)	-0.791 (0.000)	-0.270 (0.000)	-0.321 (0.000)	0.053 (0.004)
Method | Sample size					
PLSs-PM|$n = 100$	-0.089 (0.000)	-0.080 (0.022)	-0.066 (0.024)	-0.045 (0.005)	-0.046 (0.108)
PLSs-PM|$n = 150$	-0.167 (0.000)	-0.148 (0.000)	-0.144 (0.000)	-0.119 (0.000)	-0.087 (0.004)
PLSs-PM|$n = 250$	-0.188 (0.000)	-0.170 (0.000)	-0.166 (0.000)	-0.135 (0.000)	-0.088 (0.004)
PLSs-PM|$n = 300$	-0.243 (0.000)	-0.228 (0.000)	-0.227 (0.000)	-0.179 (0.000)	-0.112 (0.000)
PLSs-PM|$n = 500$	0.060 (0.001)	0.068 (0.048)	0.055 (0.056)	0.062 (0.000)	0.046 (0.106)
PLSs-PM|$n = 750$	-0.270 (0.000)	-0.261 (0.000)	-0.274 (0.000)	-0.208 (0.000)	-0.120 (0.000)
PLSs-PM|$n = 900$	-0.274 (0.000)	-0.264 (0.000)	-0.290 (0.000)	-0.212 (0.000)	-0.121 (0.000)

A.3 The `plsExtpm` software

The model described in Section 2.2.1 and represented in Figure 2(a) is used here to illustrate the `plsExtpm` software.

The `plsExtpm` main function is:

```
plsExtpm(data, strucmod, measuremod, maxit=200, tol=1e-7, scaled=TRUE,
imputed = FALSE, wscheme = 'centroid', sum1 = FALSE, ngrid = 300,verbose
= TRUE, convCrit=c('relative','absolute')
```

This function contains three mandatory arguments: the *data*, the *structural model* and the *measurement model*. The data should be a `data frame` containing the manifest variables used in the measurement model. By default, the function does not impute the missing data (`imputed = FALSE`; when `TRUE` missing data imputed using mean imputation), scales the manifest variables to zero mean and unit standard deviation (`scaled = TRUE`), and runs the algorithm for 200 iterations using by default a `relative` convergence criterion (`convCrit`) with a `tolerance` of 1×10^{-7}. The default inner weighting scheme is `wscheme = "centroid` (the other alternatives are `"factorial"`, `"pathWeigthing"`, and `"smoothWeighting"`). If the default method is provided or any other of the traditional schemes, *factorial* and *pathWeighting*, but any of the partial structural relationships is nonlinear, it is automatically changed to `smoothWeighting`. If `verbose = TRUE`, informative messages regarding data checks are printed out. Finally, the estimated partial structural relationships are predicted on a `grid` of 300 points evenly distributed between the minimum and the maximum of the independent latent variable estimated factor scores.

The structural model is a four-column data frame. The columns should be named `source`, `target`, `type` and `K`, respectively. Whether a partial relationship between the `source` and the `target` latent variables is linear (`ln`) or nonlinear (`nln`) is indicated in the column `type`. If the partial relationship is linear, the column `K` should me set to `NA`, otherwise the dimension of the basis of the cubic regression spline is indicated in column `K`. To achieve the objectives referred to above, we show how to model the data in incremental way. Therefore, we start with a structural model assuming all partial relationships are nonlinear and approximated by a cubic regression spline with $K = 10$ knots (see Section 2.1 about the trade-off between dimension of the basis and penalisation term). This structural model is represented as follows:

```
ECSIsm_all_nlinear
```

```
##           source       target type  K
## 4        Quality        Value  nln 10
## 7        Quality Satisfaction  nln 10
## 8          Value Satisfaction  nln 10
## 10 Satisfaction      Loyalty  nln 10
```

The measurement model is a two-column matrix. The columns should be named `source` and `target`, respectively. Whether a latent variable is measured in a reflective or formative fashion depends upon the order they are represented in the measurement model. A reflective variable appears in the column `source` and its indicators in the column `target`. The formative indicators are represented the other way around. The reduced ECSI model of Example I is composed of three reflective latent variables, *Perceived Value*, *Customer Satisfaction* and *Customer Loyalty* and one formative latent variable, *Perceived Quality*. The measurement model is represented as follows:

```
ECSImm
```

```
##       source         target
##  [1,] "QUAL1"        "Quality"
##  [2,] "QUAL2"        "Quality"
##  [3,] "QUAL3"        "Quality"
##  [4,] "QUAL4"        "Quality"
##  [5,] "QUAL5"        "Quality"
##  [6,] "QUAL6"        "Quality"
##  [7,] "QUAL7"        "Quality"
##  [8,] "QUAL8"        "Quality"
##  [9,] "QUAL9"        "Quality"
## [10,] "Value"        "VALU1"
```

```
## [11,] "Value"        "VALU2"
## [12,] "Satisfaction" "SATI1"
## [13,] "Satisfaction" "SATI2"
## [14,] "Satisfaction" "SATI3"
## [15,] "Loyalty"      "LOYA1"
## [16,] "Loyalty"      "LOYA3"
```

To plot the estimated partial impacts of the structural model and to assess the appropriateness of the used dimension of the basis `plsExtpm` contains the function:

```
plsExtplot(pls.object, boot.object = NULL,x.LV = NULL, y.LV = NULL, verbose
= TRUE)
```

This function has only one mandatory argument, `pls.object`. It is as object of class `plsExtpm` resulting from a `plsExtpm()` run. If no variables are indicated in arguments `x.LV` and `y.LV` the function plots all partial structural relationships, otherwise, it plots only the requested *valid* relationship. Information messages regarding data inputs checks are printed out if `verbose = TRUE`, the default. If the user runs the bootstrap procedure (using the function `plsExtboot` described below), prior to the `plsExtplot` call, the result object of class `plsExtboot` can be provided the partial structural relationships plots contain the bootstrapped credible intervals. This analysis allows the user to decides whether each partial relationship should remain as a nonlinear one or change to the linear form.

Furthermore, taking advantage of the features of package `mgcv`, a function was specifically developed to check the choice of the basis dimension of the penalised regression smoothers, `plsExtcheck()`:

```
plsExtcheck(pls.object)
```

This function has only one mandatory argument, `pls.object`. It is as object of class `plsExtpm` resulting from a `plsExtpm()` run. Recurring to the `mgcv` package function `gam.check`, it takes a fitted `pls.object` object produced by `plsExtpm()` and produces some diagnostic information about the fitting procedure and results. For more information about the diagnostic information and plot produced we refer to Wood (2017).

If the user runs the bootstrap procedure (using the function `plsExtboot` described below), prior to the `plsExtplot` call, the result object of class `plsExtboot` can be provided the partial structural relationships plots contain the bootstrapped credible intervals. This analysis allows the user to decides whether each partial relationship should remain as a nonlinear one or change to the linear form.

The bootstrap procedure runs through function

```
plsExtboot(pls.object, nboot=200, start=c("ones", "old"), conf.level = 0.95,
verbose=TRUE)
```

This function `plsExtboot()` only requires as input an object of class `plsExtpm`. It runs a bootstrap procedure for 200 replicates (the default), with *outer weights* initialised to 1 (`start = 'ones'`; the alternative, which speeds up the procedure, `start = 'old'`, uses the outer weights resulting from the last iteration of the PLS-PM algorithm). Using the default confidence level of 95% (`conf.level = 0.95`) the function computes upper and lower credible limits for the partial structural relationships that might be used in `plsExtplot`. By default, the function prints out important messages of the bootstrap procedure (`verbose = TRUE`).