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Developments in PLS-PM for the building of a System of Composite Indicators

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Developments in PLS-PM
for the building of a System of Composite Indicators

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Introduction

The real world is characterized by deep complexity. Many social, economic and psychological phenomena are manifold and therefore difficult to measure and to evaluate. A phenomenon is defined as complex when the relevant aspects of a particular problem cannot be captured by using a single perspective [43]. It is necessary to consider the concept formed by different dimensions, each representing different aspects of it, which interact with each other. For this reason, most of the time, the complexity implies also multidimensionality [25], and this affects the measuring process of phenomenon that we are analyzing. Nowadays, phenomena such as Development, Progress, Poverty, Social Inequality, Well-Being, and Quality of Life, etc., require, in order to be measured, that the 'combination' of different dimensions are considered together as the proxy of the phenomenon. This combination can be obtained by applying methodologies known as *Composite Indicator* [100]; [69].
According to Saisana et al. [138], a *Composite Indicator (CI)* is defined as *a mathematical combination of single indicators that represent different dimensions of a concept whose description is the objective of the analysis*. CIs are very useful in order to deal with those phenomena that can not be observed directly.

The existing literature offers different alternative approaches in order to obtain a CI: *Theory Based*, obtained through the synthesis of selected Elementary Indicators (EIs), and *Data Driven*, obtained through an optimal synthesis of a suitable set of EIs . *Theory Based CIs*, computed by aggregation methods, usually require strong knowledge or assumptions about the phenomena under study and consequently are constructed with a small number of variables. *Data Driven CIs* allow for the use of a large number of variables that usually are needed in representing the real world, but they have an normative aim. *Theory Based* and *Data Driven* approaches present several limitations: no explicit mention is made about the relationship between EIs and their own CIs (the reflective or formative measurement model); no predictive use of CIs is possible: their scope is essentially descriptive with, therefore, a restricted use in decision making processes; no systemic vision is considered in their building; no relationship with other CIs is taken into account; the CIs assume the same role, not distinguishing between input, output and outcome variables; and the EIs are based just on a numerical scale. To overcome these restrictions, a *Model Based CI* can take into account a-priori knowledge on the field of interest by: specifying the CI measurement model (reflective, formative or both (MIMIC)); including any kind of CI relationship (logical, hierarchical, temporal or spatial); contextualizing the CI with respect to other CIs according to a given path model in a systemic vision; defining the roles of the CIs in the model; and in addition making use of non numerical data (ordinal and nominal) which is possible by suitable internal quantification according to optimal scaling methods.

In order to compute a *Model Based CI*, taking into account all a-prior information, a relevant role is played by the *Structural Equation Modeling (SEM)* methodology. This is a statistical technique for testing and estimating causal relationships using a combination of statistical data and qualitative causal assumptions. SEM [84] is an extension of the general linear model that simultaneously estimates relationships between multiple independent, dependent and Latent Variables (LVs). According to this methodology, it is possible to define a CI as a multidimensional LV not measurable directly and related to its single indicators or Manifest Variables (MVs) by a reflective or formative relationship, or both (this defines the measurement or outer model). Each CI is related to the other CIs, in a systemic vision, by linear regression equations specifying the so-called Structural Model (or Inner Model). As a result a Systemic CI or a System of CIs is obtained, where the word "systemic" derives from the definition of system given by Ludwig von Bertalanffy [96], according to which "a system is a set of elements in interaction", not just an aggregation of EIs, but a set of indicators related to each other by mutual relationships, expressed through functional links and summarized in a specific model.

Two different approaches exist to estimate model parameters in SEMs: the *covariance-based* techniques [76];[77] and the *component-based* techniques [186];[187];[95]. The first approach is primarily used to confirm (or reject) theories (i.e. a set of systematic relationships between multiple variables that can be tested empirically). In contrast, in *component-based* techniques, LV (i.e CI) estimation plays a main role. As a matter of fact, the aim of *component-based* methods is to provide an estimate of the LVs in such a way that they are the most highly correlated with one another (according to the path diagram structure) and the most representative of each corresponding block of MVs.
Among the several methods that have been developed to estimate SEMs, we focus on the *component-based* techniques, in particular on the *PLS Path Modeling Approach (PLS-PM)* [183]; [166], because the estimation of the CIs plays a key role in this estimation process.

The PLS-PM approach has enjoyed increasing popularity as a key multivariate analysis method in various research disciplines in order to build a system of CIs. It has been evolving as a statistical modeling technique, with the results that there are several published articles on the method [166]; [16]; [57]; [64]; [35]. In Chapter two of the this the thesis PLS-Path Modeling Approach is reviewed, and a description of the PLS-PM algorithm, step by step, is proposed. PLS-PM allows you to estimate causal relationships, defined according to a theoretical model linking two or more latent complex concepts, each measured through a number of observable indicators. The basic idea is that the complexity inside a system can be studied by taking into account the entirety of the causal relationships among the LVs, each measured by several MVs. In this system, we are interested in including EIs on a non numerical scale, including some kind of CI relationship and testing whether there is a mediating and/or moderating effect.

For instance, when computing a CI, it could be interesting to consider demographic variables, such as religion or gender, and categorical variables defining states, such as the type of government. It would be interesting to know what the role of these variables is, if they have a moderator or mediator effect, and how considering these effects change thee estimation of the LVs considering these effects.
Moreover, applications of SEMs are usually based on the assumption that the analyzed data stem from a single population, so that a unique global model well represents all the observations. However, in many real world applications, this assumption of homogeneity is unrealistic. In modeling the real world, it is reasonable to expect that different classes showing heterogeneous behaviors may exist in the observed set of units. This is true also in CI frameworks. As a matter of fact, in developing a system of CIs, it is reasonable to suppose that different models should be applied in order to take into account differences among the units. Therefore, in recent years there have been many advances in the context of these models, with many tools being developed in order to extend the classic algorithm of the PLS-PM to the treatment of non metric data, for including and testing mediator and moderator effects, and to deal with heterogeneous data. We have addressed these developments in the third chapter of the thesis, focusing in particular on two approaches developed in recent years.

In the fourth chapter of the work we will focus on another aspect of PLS-PM concerning the construction of the hierarchical component model. As a matter of fact, in relation to the CI framework, researchers have recently been focusing their attention on a particular aspect linked to multidimensionality and a high level of abstraction, when a CI is manifold, lacks its own MVs and is described by various underlying blocks.
Higher-Order Constructs in PLS-PM are considered as explicit representations of multidimensional constructs that exist at a higher level of abstraction and are related to other constructs at a similar level of abstraction completely mediating their influence from or to their underlying dimensions [12]. In Wold's original design of the PLS-PM [186] it was expected that each construct would be necessarily connected to a set of ob-

served variables. On this basis, Lohmöller [95] proposed a procedure to treat hierarchical constructs, the so-called hierarchical component model. The hierarchical constructs or sayings are multidimensional constructs that involve more than one dimension and we can distinguish them from the one-dimensional constructs that are characterized by a single underlying dimension.
There are three main approaches existing in the literature: the Repeated Indicators Approach, the Two Step Approach and the Hybrid Approach. The Repeated Indicators Approach [95]; [186] is the most popular approach when estimating Higher-Order Constructs in a PLS-PM [175];[179]. The procedure consists of taking the indicators of the Lower-Order Constructs and using them as the MVs of the Higher-Order LV. The Two-Step Approach is divided in two phases. In the first step the LV scores of the lower-order constructs are computed without the Second-Order Construct [122]. Then, in the second step, the PLS-PM analysis is performed using the computed scores as indicators of the Higher-Order Constructs. The Hybrid Approach builds on an idea of Wold [186]. The idea behind this approach is to randomly split all the MVs of the lower-order constructs so that half are assigned to their respective construct and the other half are represented in the Second-Order Construct side [180]. Each approach presents some limitations, particularly two aspects which are taken into account in this work: the estimation of components for each block and the choice of the number of the components for each block.

In chapter five we focus on these particular aspects and we propose two new methods, called the *Mixed Two Step Approach* and the *PLS Component Regression Approach*, that allow you to estimate the System of CIs differently and optimally. The Mixed Two Step Approach begins with the implementation of the PLS-PM in the case of the Repeated Indicators Approach. In this way, the algorithm gives the scores of the Lower-Order Constructs. Next the scores of the blocks are used as indicators of the Higher-Order Construct, and at this point the PLS-PM algorithm is performed again. The PLS Component Regression Approach gives the possibility of choosing manually the number of components of the block to

be extracted, or according to a criterion, through the use of PLS Regression. Once the components have been chosen, these will be MVs of Higher-Order Construct and the PLS-PM algorithm will be performed. Since the aim of PLS-PM is to estimate the relationships between the LVs, these approaches provide components that are at the same time representative of their blocks and predictive of the Higher-Order Construct.
Finally, we will show the functioning of the proposed algorithms (implemented in an R code) through a simulation study. The performance of the proposed methods in terms of the explained variability, predictiveness and interpretation is compared to the classic Two Step Approach, using artificial data. Compared to this approach, the *Mixed Two Step Approach* and the *PLS Component Regression Approach* seem to be good methods in term of stability and predictiveness. This is confirmed by the simulation and by an application to real data, that is presented in order to show the implementation of these methods and to give some comparative empirical results.

Chapter 1

Composite Indicators

1.1 Introduction

The real world is characterized by deep complexity. Many socioeconomic phenomena are manifold and therefore difficult to measure and to evaluate. A phenomenon is defined as complex when the relevant aspects of a particular problem cannot be captured by using a single perspective [43]. It is necessary to consider the concept formed by different dimensions, each representing different aspects of it, which interact with each other. For this reason, most of the time, the complexity implies also multidimensionality [25], and this affects the measuring process of the phenomenon that we are analyzing. As a matter of fact, outcomes are determined not by single causes but by multiple causes, and these causes may, and usually do, interact in a non-additive way. In other words the combined effect is not necessarily the sum of the separate effects. The Millennium Development Goals, adopted by the United Nations General Assembly in 2000, reflect this advanced vision. The shift from a single dimension to multiple dimensions, by enlarging and enriching the scope of the analysis, represents an important theoretical progression.In last few years, the debate on the measurement of multidimensional phenomena has witnessed, within the worldwide scientific Community, a renewed interest thanks to the publication, in September 2009, of the Stiglitz report and, in March 2013, of the first report on “Equitable and Sustainable Well-being” (BES) by the Committee composed of ISTAT (the Italian National Institute of Statistics) and CNEL (Italian Council for Economics and Labour). It is well know that a number of socio-economic phenomena cannot be measured by a single descriptive indicator and that, instead, they should be represented with multiple dimensions. Phenomena such as Development, Progress, Poverty, Social Inequality, Well-Being, Quality of Life, and the Provision of Infrastructures, etc., require, in order to be measured, that the "combination" of different dimensions are considered together as the proxy of the phenomenon. This combination can be obtained by applying methodologies known as *Composite Indicator* [100]; [69]. Once the multidimensionality is recognized, measuring this phenomenon has a number of theoretical and methodological problems that are not present in the conventional unidimensional approach. The first problem concerns the choice of the dimensions: which and how many dimensions are relevant and should be considered or privileged. This is also called by Sen the problem of the appropriate "informational basis" [154], that is which information is included or excluded in the evaluation exercise. Moreover, we need to understand if there are relationships between these dimensions, and if so, to understand their nature. Therefore, in a multidimensional perspective and taking into account any relationships between the dimensions, we talk about *a system of Composite Indicators*, that measure and represent distinct dimensions of the observed phenomenon. Consequently, the system of Composite Indicators does not represent a pure and simple collection of indicators but provides researchers with information that is greater than the simple summation of the elements.

1.2 Definition of Composite Indicators

Saltelli [139] used "Composite Indicator" (CI) sensu lato, i.e. to indicate a manipulation of individual indicators. Accordingly, a CI is obviously not "the unique solution" when representing complex systems but only "a solution", (i.e. a limited exercise to take into account non-equivalent observers and observations). This is indeed the major limitation of composites. As indicated in Saisana et al. [137], the core of the non aggregators' argument is in the subjective nature of these measures. Subjectivity cannot be avoided when representing complex systems. Cherchye et al. [11] observe that the "lack of consensus" is a defining property of CIs, and that one may even hypothesize a consensus between the association of key variables with the subject of the index, the weightings will remain controversial. However, several reviews of CIs have been published in the last few years. All this interest in CIs may be attributed to a variety of reasons, which could include the following ([138]; [110]):

- CIs can be used to summarize multidimensional issues, in view of the supporting decision-makers;
- CIs offer the possibility of making the rankings between, for example, countries, companies and individuals on complex issues;
- CIs can help to synthesize a list of indicators.

In official statistics, CIs are being increasingly recognized as a useful tool for policy making and public communications in term of conveying information about a country's performance in fields such as the environment, economy, society, or technological development, and they have proven to be useful in ranking countries in benchmarking exercises. They are much easier to interpret than any attempt to find a common trend in many separate indicators. However, they can send misleading or non-robust policy messages if they are poorly constructed or misinterpreted. According to Saisana et al. [138], a *Composite Indicator* is defined as *a mathematical combination of single indicators that represent different dimensions of a concept the description of which is the objective of the analysis*. A CI is formed when individual indicators are compiled into a single index on the basis of an underlying model. CIs should ideally measure multidimensional concepts which cannot be captured by a single indicator, e.g. competitiveness, industrialization, sustainability, single market integration, or the knowledge-based society [138]. Thus, the main feature of a complex indicator is that it summarizes complex and multidimensional issues. This multiplicity implies a number of theoretical and statistical problems, especially when we need to make comparisons over time and/or space. The fundamental question is what is the best approach to (re)present complex phenomena and multidimensional realities. The construction of this kind of indicator implies a search for a suitable synthesis of a number of MVs in order to achieve a simple representation of a multidimensional phenomenon. Accordingly, a CI can be considered as a latent concept, not directly measurable, whose estimation can be obtained through the value of Elementary Indicators (EIs) or MVs. Its construction and its use involves a series of advantages and disadvantages, some of which are mentioned below. In particular, the principal advantages are that a composite indicator can be used to summarize multidimensional issues and can help to synthesize a list of indicators. On the other hand, the most serious problems are that CIs may send misleading, non-robust policy messages, if they are poorly constructed or misinterpreted, and may encourage politicians to draw simplistic policy conclusions. These pros and cons are discussed in detail in Saisana et al. [138]. To overcome these problems, studies in literature have focused on the construction of a CI through several stages that represent the basic steps of their construction, namely:

- Deciding on the phenomenon to be measured and on whether it would benefit from the use of CIs;
- Selecting the EIs. A clear selection needs to be made in terms of which sub-indicators are relevant to the phenomenon to be measured. There is no fully objective way of selecting the relevant EIs;
- Assessing the quality of the data. There needs to be high quality data for all the indicators. Otherwise, the analyst has to decide whether to drop the data or find ways of constructing the missing data points. In case of data gaps, alternative methods can be applied, e.g. mean substitution, correlation results, time series, or an assessment of how the selection of the method can affect the final result;
- Assessing the relationships between the sub-indicators. Methods such as Principal Components Analysis can provide an insight into the relationships between the EIs. It can be considered as a prerequisite for the preliminary analysis of the EIs;

- Normalising and weighting the indicators. Many methods for normalising and weighting the EIs are reported in the literature;

- Testing for Robustness and Sensitivity. Inevitably, changes in the weighting system and the choice of EIs will affect the results that the CI shows.

Each step is extremely important, but coherence in the whole process is equally vital. Choices made in one step can have important implications in others.
An OECD study [111] offers “recommended practices” for the construction of CIs [139]. In this book, Nando et al. [111] discuss in detail several stages for their construction, together with the “pros” and “cons” associated with the use of aggregated statistical information.

1.3 A quality framework for Composite Indicators

The development of a quality framework for CIs is not an easy task. In fact, the overall quality of the CIs depends on several aspects, related both to the quality of the elementary data used to build the indicator and the soundness of the procedures used in its construction. Quality is usually defined as “fitness for use” in terms of user needs. As far as statistics are concerned, this definition is broader than has been used in the past when quality was equated with accuracy. It is now generally recognized that there are other important dimensions. Even if the data are accurate, they cannot be said to be of good quality if, for example, they are produced too late to be useful, cannot be easily accessed, or appear to conflict with other data. Thus, quality is a multi-faceted concept. The most important quality characteristics depend on user perspectives, needs and priorities, which vary across user groups. Several organizations (e.g., Eurostat, the International Monetary Fund (IMF), Statistics Canada and Statistics Sweden) have been working on the identification of various dimensions of quality for statistical products.
According to these organizations, the selection of basic data should maximize the overall quality of the final result. In particular, in selecting the

data the following dimensions (drawing on the IMF, Eurostat and OECD reports) are to be considered:

Relevance. The relevance of the data is a qualitative assessment of the value contributed by these data. Value is characterized by the degree to which the statistics meet the current and potential needs of the users. It depends upon both the coverage of the required topics and the use of appropriate concepts.
In the context of CIs, relevance has to be evaluated by considering the overall purpose of the indicator. A careful selection and evaluation of the basic data has to be carried out to ensure that the right range of domains is covered in a balanced way. Given the actual availability of the data, "proxy" series are often used, but in this case some evidence of their relationships with the "target" series should be produced whenever possible.

Accuracy. The accuracy of the basic data is the degree to which they correctly estimate or describe the quantities or characteristics that they are designed to measure. Accuracy refers to the closeness between the values provided and the (unknown) true values. Accuracy has many attributes, and in practical terms it has no single aggregate or overall measure. Of necessity, these attributes are typically measured or described in terms of the error, or the potential significance of error, introduced through individual major sources of error. An aspect of accuracy is the closeness of the initially released value(s) to the subsequent value(s) of the estimates. In light of the political and media attention given to first estimates, a key point of interest is how close a preliminary value is to the subsequent estimates. In this context it is useful to consider the sources of the revision, which include the replacement of preliminary source data with later data, the replacement of judgmental projections with source data, the changes in definitions or estimating procedures and the updating of the base year for constant-price estimates. The aim is few and only minor revisions; however, the absence of revisions does not necessarily mean that the data are accurate. In the context of CIs, the accuracy of the basic data is extremely important. Here the issue of the credibility of the source becomes crucial. The credibility of data products refers to the confidence that users place in those products based simply on their image of the data producer, i.e., the brand image. One important aspect is trust in the objectivity of the data. This implies that the data are perceived to be produced professionally in accordance with appropriate statistical standards and policies and that practices are transparent (for example, the data are not manipulated, nor is their release timed in response to political pressure). All things being equal, data produced by "official sources" (e.g. national statistical offices or other public bodies working under national statistical regulations or codes of conduct) should be preferred to other sources.

Timeliness. The timeliness of data products reflects the length of time between their availability and the event or phenomenon they describe, but considered in the context of the time period that permits the information to be of value and to be acted upon. The concept applies equally to short-term or structural data; the only difference is the time-frame. Closely related to the dimension of timeliness, the punctuality of data products is also very important, both for national and international data providers. Punctuality implies the existence of a publication schedule and reflects the degree to which the data are released in accordance with it.

In the context of CIs, timeliness is especially important to minimize the need for the estimation of missing data or for revisions of previously published data. As individual basic data sources establish their optimal trade-off between accuracy and timeliness, taking into account institutional, organizational and resource constraints, data covering different domains are often released at different points of time.

Accessibility. The accessibility of data products reflects how readily the data can be located and accessed from original sources. The range of different users leads to considerations such as multiple dissemination formats and the selective presentation of meta-data. Thus, accessibility includes the suitability of the form in which the data are available, the media of dissemination, and the availability of meta-data and user support services. It also includes the affordability of the data to users in relation to its value to

them and whether the user has a reasonable opportunity to know that the data are available and how to access them.
In the context of CIs, the accessibility of basic data can affect the overall cost of the production and updating of the indicators over time. It can also influence the credibility of the CI if a poor accessibility of the basic data makes it difficult for third parties to replicate the results of the CIs. In this respect, given improvements in the electronic access to databases released by various sources, the issue of coherence across data sets can become relevant. Therefore, the selection of the source should not always give preference to the most accessible source, but should also take other quality dimensions into account.

Interpretability. The interpretability of data products reflects the ease with which the user can understand and properly use and analyze the data. The adequacy of the definitions of concepts, target populations, and variables, of the terminology underlying the data and of the information describing the limitations of the data, if any, largely determines the degree of interpretability. The range of different users leads to considerations such as the presentation of meta-data in layers of increasing detail. Definitional and procedural meta-data assist in interpretability.
In the context of CIs, the wide range of data used to build them and the difficulties due to the aggregation procedure require the full interpretability of the basic data. The availability of definitions and classifications used to produce basic data is essential to assess the comparability of data over time and across countries: for example, series breaks need to be assessed when Composite Indicators are built to compare performances over time. Therefore the availability of adequate meta-data is an important element in the assessment of the overall quality of the basic data.

Coherence. The coherence of data products reflects the degree to which they are logically connected and mutually consistent, i.e. the adequacy of the data to be reliably combined in different ways and for various uses. Coherence implies that the same term should not be used without explanation for different concepts or data items; that different terms should not be used

for the same concept or data item without explanation; and that variations in methodology that might affect data values should not be made without explanation.
In the context of CIs, two aspects of coherence are especially important: coherence over time and across countries. Coherence over time implies that the data are based on common concepts, definitions and methodology over time, or that any differences are explained and can be allowed for. Incoherence over time refers to breaks in a series resulting from changes in concepts, definitions, or methodology. Coherence across countries implies that from country to country the data are based on common concepts, definitions, classifications and methodology, or that any differences are explained and can be allowed for.

1.4 Composite Indicators from different points of view

CIs have emerged in the last few years as an alternative to a portfolio of indicators, whose scattered information is sometimes difficult to grasp, an example being the GNP per capita, which often does not correlate well with development goals. As CIs have emerged, so they have also been criticized. Points of debate relate to the selection of dimensions and indicators, their correlation (and the trade-off between redundancy and robustness), their type (input vs. output), and the normalization procedure, weighting, and aggregation of the components. Many services of the European Commission, the United Nations and regional and local Institutions have been focusing on the development and use of Composite Indicators to convey concise information to the public about several economic, environmental, technological and social domains. CIs are deemed useful because they provide "the big picture", they attract public interest and encourage the formulation of strong policy messages. However, their proliferation has been raising scepticism in relation to their accuracy and reliability. Given the seemingly ad hoc nature of their computation, the sensitivity of the results to different weighting and aggregation techniques, and the continuing problems of missing data, CIs can result in distorted findings on country performance and incorrect policy prescriptions [140]. The use of CIs is very much the subject of controversy, pitting aggregators against non-aggregators. Sharpe [155] notes that:

The aggregators believe there are two major reasons that there is value in combining indicators in some manner to produce a bottom line. They believe that such a summary statistic can indeed capture reality and is meaningful, and that stressing the bottom line is extremely useful in garnering media interest and hence the attention of policy makers. The second school, the non-aggregators, believe one should stop once an appropriate set of indicators has been created and not go the further step of producing a composite index. Their key objection to aggregation is what they see as the arbitrary nature of the weighting process by which the variables are combined.

One may note that the controversy on the use of statistical indices unfolds along an analytical versus pragmatic axis. There is abundant literature on the analytical problems associated with even well-established statistical indices such as GDP [125]. This literature hardly seems to dent the GDP's rather universal pragmatic practical acceptance. Along similar lines, in Saisana et al. [137], one reads:

[...] *it is hard to imagine that debate on the use of Composite Indicators will ever be settled* [...] *official statisticians may tend to resent CIs, whereby a lot of work in data collection and editing is "wasted" or "hidden" behind a single number of dubious significance. On the other hand, the temptation of stakeholders and practitioners to summarize complex and sometime elusive processes (e.g. sustainability, single market policy, etc.) into a single figure to benchmark country performance for policy consumption seems likewise irresistible.*

Among the list of objections to the use of CIs one reads [138]; [110]; [111]:

- *CIs may send misleading, non-robust policy messages if they are poorly constructed or misinterpreted* [*...or*] *may encourage politicians to draw* *simplistic policy conclusions.*

- *The construction of CIs involves stages where judgment has to be made: the selection of the EIs, the choice of the model, the weighting of the indicators and the treatment of any missing values etc.*
- *There could be more scope for disagreement among Member States about CIs than about individual indicators.*
- *CIs increase the quantity of data needed because data are required for all the EIs and for a statistically significant analysis.*

While the first "cons" is simply a reminder that sound practices must be used [111]; [137], and the last is an unavoidable consequence of complexity, the core of the non-aggregators' argument rest in the subjective nature of these measures. Cherchye et al. [11], observe that the "lack of consensus" is a defining property of CIs, and that while one may hypothesize a consensus between the association of key variables with the subject of the index, the weightings will remain controversial. According to Nardo et al. [111]: *CIs are much like mathematical or computational models. As such, their construction owes more to the craftsmanship of the modeler than to universally accepted scientific rules for encoding. As for models, the justification for a CI lies in its fitness for the intended purpose and its acceptance by peers* [132].

The point of these considerations is that subjectiveness and fitness need not be antithetical. They are in fact both at play when constructing and adopting a CI, where inter-subjectiveness may be at the core of the exercise, such as when participative approaches to weighting negotiations are adopted (see Nardo et al. for a review [111]). Thus, these only apparently conflicting properties underpin the suitability of CIs for advocacy. In discussing data quality issues for statistical information Funtowicz and Ravetz note [44]:

Any competent statistician knows that "just collecting numbers" leads to nonsense [...] *so in "Definition and Standards" we put "negotiation" as superior to "science", since those on the job will know of special features and problems which an expert with only a general training might miss.*

Concerning the discussion of the attraction exerted by CIs, an example is in the work of Amartya Sen, Nobel prize winner in 1998 [153]. Sen was initially opposed to CIs but was eventually seduced by their ability to put into practice his concept of "Capabilities" (*the range of things that a person could do and be in her life* [153]) in the Human Development Index.
Saltelli adds that, however good the scientific basis for a given CI, its acceptance relies on negotiation and peer acceptance [139]. However, despite their many deficiencies, they will continue to be developed due to their usefulness as a communication tool and, on occasion, for analytical purposes [138].
The evolution of CI theory has gone over the years more and more reflected on the production of the official statistics. Besides these, in the last few years a new vision has developed in all fields, many CIs have been built and used in order to deal with problems of synthesis of different latent concepts, particularly in economic and social fields. An obvious example is the construction of the ACSI (American Customer Satisfaction Index), in order to measure the Customer Satisfaction; a synthetic index that relates different aspects, such as Expectation, Perceived Quality and Perceived Value, that go to influence the Customer Satisfaction.

1.5 From Data Driven Composite Indicators to Model Based Composite Indicators

The construction of a CI implies the search for a suitable synthesis of a number of observed or MVs in order to achieve a simple representation of a multidimensional phenomenon. Accordingly, a CI can be considered as a latent concept, not directly measurable, whose estimation can be obtained through the values of EIs. There is a fundamental division in the indicators literature about indicators between those who choose to aggregate variables into CIs and those who do not, and prefer using a suite of indicators. There is no doubt that composite indicators are appealing, especially as an answer to the calls for a replacement of the single indicator approach or the use of a suite of indicators, as for example the Human Development Index

(HDI) and GDP to measure progress. As a matter of fact, using a unique measure obtained by combining indicators can indeed capture reality and can easily be used to attract the attention of policy makers and the media. Moreover, the advantages of a composite indicator over a set of indicators include the creation of a bottom line. However, composite indicators have some disadvantages, including a danger that a composite index will oversimplify a complex system and give potentially misleading signals [58]. Accordingly, the selection of the weightings and the way the indicators are combined do not seem to be methodological but, rather, empirical issues in many approaches to the aggregation of indices. For the construction of CIs three different approaches [170] are proposed in the literature:

- *Theory Based*, obtained through the combination of some variables by means of a specified function, suggested by a theory or by well established knowledge on the phenomenon to analyze;

- *Data Driven*, obtained through a suitable/optimal synthesis of the selected variables, that represent the different facets of an analyzed phenomenon;

- *Model Based*, obtained by the estimation of a multi-equations model, describing, in an optimal way, not only the relationships among the observed variables but also between the observed variables and one or more of the latent constructs to be measured.

1.5.1 Theory Based and Data Driven Composite Indicators

Theory Based CIs are computed by simple formulas that usually combine a few observed variables. This approach requires strong knowledge or assumptions about the phenomena under study, and usually considers a well defined set of variables. In contrast, a *Data Driven* approach overcomes the lack of knowledge by inserting into the building process of a CI many observed variables, that are only proxies of the concept to be measured. The absence of a prior knowledge and of a consolidated theory often necessitates the use of a data driven approach. This is an exploratory approach that falls into one of the five major principles of Benzecrì on which Data analysis has to be based [8], according to which the models have to follow the data and not viceversa. Therefore, the statement of Benzecrì is reversed in the sense that the data have to follow the model in order to build not only descriptive CIs, but in addition to enrich new interpretations and their use in supporting decisions. A first step in the construction of a CI, according to the Data Driven Approach, consists in checking the coherence between the EIs and the concept to measure, in the sense that is all EIs must have a reciprocal concordance (discordance) with respect to their relative CI. Suppose, for example, we want to build the "Quality of life" (QoL) CI that assigns a higher values to a country which enjoys a better quality of life: an indicator like "the income expected" has a positive correlation with the quality of life, whereas "infant mortality" usually presents an inverse correlation with the QoL. In order to have a set of coherent indicators we should transform it into the correspondence index "survival at birth". The coherence can be simply achieved by calculating the reciprocal of an Elementary Indicator (EI) or by using its complement to the observed maximum value. In order to homogenize the different EIs, before their aggregation for the CI building, it is necessary to adopt a transformation in the same scale often of pure numbers. In this case, transformations for homogenization can be the following:

- a ranking transformation;
- a transformation by the sign of the difference with respect to the reference mean;
- a transformation by the value of the ratio with respect to the reference value;
- a transformation by the percentage variation with respect to a previous value; or
- a transformation by the standardization.

A transformation with respect to a reference value (i.e. the arithmetic mean, maximum or minimum value) must be carried out carefully when outliers are present in the EI distribution. In this case, a trimmed mean or defined

quartiles are to be preferred. Ones the EIs have been transformed into homogeneity, the aggregation and the determination of a CI is achieved by the sum or an average of the values of the EIs for each statistical unit (e.g. a country). Some of the previous techniques have been used to build CIs at a European level, such as the Information and Communication Technologies index, the Scoreboard of DG Enterprise, the Internal Market Index and the Environmental Sustainability Index).
Alternative methods have been proposed in the literature [138] for building CIs according to the Data-Driven Approach, including Aggregation Techniques, Multiple Linear Regression Analysis, Principal Components Analysis, Factor Analysis, Cronbach's Alpha and Neutralization of Correlation Effect.

Aggregation Techiques. Before computing a composite indicator, a transformation to homogenize the various elementary indicators is needed; next, an appropriate system of weightings on which the computation of a CI is based is defined, with methods that start from the simplest to the most complex. As an example, the Information and Communication Technologies Index is based on the simplest aggregation method: it involves ranking the countries for each EI and then adding together the country rankings. The Environmental Sustainability Index is based on the standardized scores for each indicator which equal the difference in the indicator for each country and the EU mean, divided by the standard error.

Multiple Linear Regression Analysis. This has been used to combine a number of EIs to compute correlation coefficients between all of the EIs. Linear regression models can tell us something about the linkages between a large number of indicators X_1, X_2, ..., X_n and a single output indicator $\hat{Y}$. A multiple regression model is constructed to calculate regression coefficients that are the relative weightings of the EIs. This approach is used to build the National Innovation Capacity Index.

Principal Components Analysis. Applications of Principal Component Analysis (PCA) related to the development of composite indicators are

aimed at (i) identifying the dimensionality of the phenomenon (e.g. the Environmental Sustainability Index); (ii) clustering the indicators (the General Indicator of Science & Technology); and (iii) defining the weightings (e.g. the Internal Market Index).
The PCA method has been widely used in the construction of CIs from large sets of indicators, on the basis of the correlation among EIs (e.g. the Internal Market Index, and the Science and Technology Indicator). In such cases, principal components have been used with the objective of combining indicators into composite indicators to reflect the maximum possible proportion of the total variation in the set. The first principal component should usually capture sufficient variation to be an adequate representation of the original set (e.g. the Business Climate Indicator). However, in other cases the first principal component alone does not explain more than 80% of the total variance of the EIs and several principal components are combined together to create the composite indicator (e.g the Success of Software Process Implementation, and the Internal Market Index).

Cronbach's Alpha. Another way to investigate the degree of the correlations among a set of EIs is to use a coefficient of reliability (or consistency) called Cronbach's Alpha α. This coefficient measures how well a set of variables (or indicators) measures the same underlying construct. A coefficient of α = 0.80 or higher is considered in most applications as evidence that the indicators are measuring the same underlying construct. Cronbach's Alpha has been considered for example for the index of Success of software process improvement.

Neutralization of Correlation Effect. This method has been applied for the aggregation of three EIs into a composite indicator measuring the relative intensity of regional problems of the Community by the European Community in 1984. The indicators measure a) GDP per employed in ECU, b) GDP per head in PPS, and c) unemployment rate. It is based on the strong correlation between the EIs, estimating a CI as an average of the EIs compared to their correlation.

The Data Driven Approach used in literature has some limitations with respect to the number of EIs used, to the choice of the system of weightings used to aggregate the EIs and to the absence of any relationship between the EIs and the CIs. As matter of fact, the current CI practice implies that the EIs:

- are based just on a numerical scale, no use being made of ordinal and nominal data with a consequent loss of precious information;
- assume the same role, with not distinction between input, output and outcome variables. The same applies to the moderating and mediating variables whose use can improve the information carried by a CI;
- no explicit mention is made of the relationship between the EIs and their CI (the reflective or formative measurement model);
- no predictive use is allowed: their scope is essentially descriptive with, therefore, a restricted use in the decision making process.

Besides, no systemic vision is considered in their building and no relationship with other CIs is taken into account. In order to overcome the previous restrictions a Model Based Approach has been proposed.

1.5.2 Model Based Composite Indicators

The previous section shows that the approaches proposed and used in literature have some limitations with respect to the number of EIs used, to the choice of the system of weightings used to aggregate the EIs and to the absence of any relationship between the EIs and the CIs. Midway between Theory Based and Data Driven CI approaches, the *Model Based* Approach allows you to take into account some *a priori* information about the context of the phenomena by considering the relationship of the target or output CI with other CIs representing the input and outcome of the system under study in terms of a path diagram. In a *Model Based* Approach, a CI can take into account a priori knowledge of the field of interest by: i) specifying the CI measurement model (reflective, formative or both (MIMIC)); ii) defining the roles of the EIs in the model; iii) contextualizing the CI with respect to other CIs according to a given path model in a systemic vision; and iv) including any kind of CI relationship (logical, hierarchical, temporal or spatial).

In order to compute a Model Based CI, taking into account all a prior information, a relevant role is played by the *Structural Equation Modeling (SEM)* methodology, where the computation of the weightings as well the aggregation process are not subjective. Both steps are based on the statistical relationships between indicators. This is a statistical technique for testing and estimating causal relationships using a combination of statistical data and qualitative causal assumptions. SEM [84] is an extension of the general linear model that simultaneously estimates the relationships between multiple independent, dependent and LVs. According to this methodology, it is possible to define a CI as a multidimensional LV not measurable directly and related to its single indicators or MVs by either a reflective or formative relationship or by both (this defines the measurement or outer model). Each CI is related to other CIs, in a systemic vision, by linear regression equations specifying the so called Structural Model (or Inner Model). As a result a Systemic CI or a System of CIs is obtained, where the word "systemic" derives from the definition of system given by Ludwig von Bertalanffy [96], according to which "a system is a set of elements in interaction", not just an aggregation of EIs but a set of indicators related to each other by mutual relationships, expressed through functional links and, summarized in a specific model.

The choice of using the SEM as the methodological framework is particularly useful for several reasons. Specifically:

- the possibility of obtaining, simultaneously and coherently with the estimation method, a ranking of individuals for specific indicator;
- the possibility of comparing systemic indicators in space and in time;
- the possibility of estimating the hypothesized relationships without making assumptions about data distribution;
- the possibility of defining an optimal system of weightings;

- the possibility of working with a large number of variables and a few observations;
- the possibility of estimating complex models without any problems of identification of the model;
- the possibility of working with missing data and in the presence of multicollinearity.

Two different approaches exist to estimate model parameters in SEMs: the *covariance-based* [76];[77] techniques and the *Component-Based* techniques [186];[187];[95].

The first approach is primarily used to confirm (or reject) theories (i.e. a set of systematic relationships between multiple variables that can be tested empirically). It does this by determining how well a proposed theoretical model can estimate the covariance matrix for a sample data set. In contrast, in *component-based* techniques, the LV (i.e CI) estimation plays a main role. As a matter of fact, the aim of *component-based* methods is to provide an estimate of the LVs in such a way that they are the most strongly correlated with one another (according to the path diagram structure) and the most representative of each corresponding block of MVs. Among the several methods that have been developed to estimate SEMs we focus on the *Component-Based* techniques, in particular on the *PLS Path Modeling Approach (PLS-PM)* [183];[166], because the estimation of the CI plays a key role in this estimation process. In the next Chapter, the PLS-PM is described and its properties and the advantages of using this approach for the estimation of a CI are highlighted.

Chapter 2

Partial Least Squares Path Modeling

2.1 Introduction

The Partial Least Squares (PLS) approach to Structural Equation Models (SEM), also known as PLS Path Modeling (PLS-PM) has been proposed as a component-based estimation procedure different from the classic covariance-based LISREL approach. Herman Wold [181] first formalized the idea of partial least squares in his paper about principal component analysis. The first presentation of the finalized PLS approach to path models with LVs was published by Wold in 1975 [183] and other presentations of PLS-PM given by Wold appeared in the same year [182]; [184]. Wold [185] provides a discussion on the theory and the application of PLS for path models in econometrics. The main references for the PLS algorithm are Wold (1982) [186] and Wold (1985) [187]. Extensive reviews on the PLS approach to SEM with further developments are given in Chin [13] and in Tenenhaus et al. [166].

Wold opposed SEM-ML ([74]) 'hard modeling' to PLS 'soft modeling'. The two approaches to SEM have been compared in Jöreskog and Wold [79]. PLS-PM is considered as a soft modeling approach, where no strong assumptions, with respect to the distributions, the sample size and the measurement scale are required. PLS-PM follows the SEM notations and sym-

bols, including the use of a path diagram to picture the relationships among the LVs and between each MV and the corresponding LV. In the diagram, the p MVs are pictured by rectangles or squares, while circles represent the q LVs. Arrows define the relationships among LVs and/or MVs.
As in SEM, in the PLS-PM, the overall relationships between the MVs and LVs are modeled through a system of equations. The goal of PLS-PM is not the reproduction of the sample covariance matrix, unlike the classic covariance-based approach. For this reason, PLS-PM is considered more an exploratory approach than a confirmative one: it does not aim to reproduce the sample covariance matrix. [38]. Furthermore, PLS-PM provides a direct estimate of the LV scores.

2.2 The PLS path model

A PLS path model is made up of two elements, the *measurement model* (also called the *outer model*), which describes the relationships between the MVs and their respective LVs, and the *structural model* (also called the *inner model*), which describes the relationships between the LVs. Both models are described in the next subsections.

2.2.1 The Measurement Model

An LV ξ is an unobservable variable (or construct) indirectly described by a block of observable variables x_k which are called MVs or indicators. There are three ways to relate the MVs to their LVs:

- The reflective way (or outwards directed way);
- The formative way (or inwards directed way);
- The MIMIC way (a mixture of the reflective and formative ways).

\- *The reflective way*
In the reflective way, each MV reflects the corresponding LV (Figure 2.1).
A block is defined as *reflective* if the LV is assumed to be a common factor that reflect itself in its respective MVs. This implies that the relationship

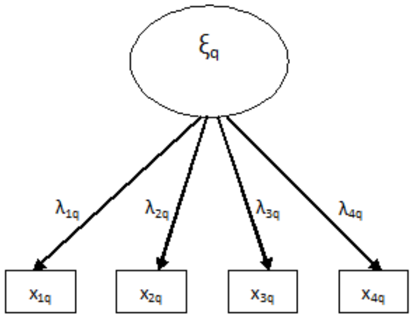


Figure 2.1: Reflective model in a path diagram

between each MV x_{ij} (with *i* from *1* to *q*) and the corresponding LV is modeled as:

$$x_{pq} \quad = \quad \lambda_{pq}\xi_{pq} + \epsilon_q \tag{2.1}$$

where ξ_{pq} is the exogenous LV, and λ_{pq} is the simple regression coefficient between the MV and the LV, the so called *loading*.
In the reflective case, the MVs should be highly correlated, due to fact that they are correlated with the LV of which they are expression. In other words, the block has to be homogeneous. There are several tools for checking the homogeneity and unidimensionality of a reflective block:

- Cronbach's Alpha;

- Dillon- Goldstein's Rho; and

- Principal Component Analysis of a block.

Cronbach's Alpha. A block is considered homogeneous if this index is larger than 0.7.

$$\alpha_q = \frac{\sum_{p \neq p'} cor(x_{pq}, x_{p'q})}{P_q + \sum_{p \neq p'} cor(x_{pq}, x_{p'q})} \times \frac{P_q}{P_q - 1} \tag{2.2}$$

where P_q is the number of MVs in the q-th block, and x_{pq} and $x_{p'q}$ are two MVs of the $q - th$ block.

Cronbach's Alpha is sensitive to the number of items in the scale and generally tends to underestimate the internal consistency reliability.

Dillon- Goldstein's Rho. This measures the composite reliability of the block. A block is considered homogeneous if its composite reliability is larger than 0.7.

$$\rho_q = \frac{(\sum_{p=1}^{P_q} \lambda_{pq})^2}{(\sum_{p=1}^{P_q} \lambda_{pq})^2 + \sum_{p=1}^{P_q}(1-\lambda_{pq}^2)} \tag{2.3}$$

According to Chin [13] *Dillon-Goldstein's Rho* is considered to be a better indicator of the homogeneity of a block than *Cronbach's Alpha*.

Principal Component Analysis rule. A block is considered homogeneous if, according to Kaiser's rule, the first eigenvalue of the correlation matrix is higher than 1, while the others are smaller [166].
The first statistic assumes that each MV is equally important in defining the LV.
In *Dillon-Goldstein's* ρ, in contrast, this assumption does not hold because it is based on the loadings of the model rather than the correlations observed between the MVs in the dataset. This type of reliability takes into account the different outer loadings of the indicator variables. λ_{pq} symbolizes the standardized outer loading of the indicator variable *i*. The composite reliability varies between 0 and 1, with higher values indicating higher levels of reliability. It is generally interpreted in the same way as Cronbach's Alpha. All of these rules assume, without any loss of generality, that LVs are standardized and all correlations between the MVs of the block show the same sign. In the case that the hypothesis of unidimensionality is rejected, it is possible to identify some groups of unidimensional sub-blocks by considering the variable-factor correlations displayed on the loading plots. PLS-PM is a mixture of a priori knowledge and data analysis. In the reflective way, the a priori knowledge concerns the unidimensionality of the block and the signs of the loadings and the data have to fit this model. If they do not, they can be modified by removing some MVs that

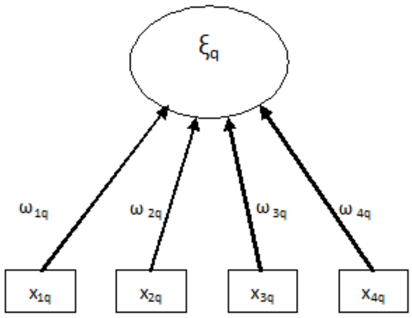


Figure 2.2: Formative model in a path diagram

are far from the model. Another solution is to change the model and use the formative way.

- *The formative way*

In the formative case, the LV is supposed to be generated by its own MVs (Figure 2.2).

$$\xi_q = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} + \delta_q \tag{2.4}$$

where ω_{pq} is the coefficient linking each MV to the corresponding LV and δ_q is the error that represents the part of the LV not explained by the block of MVs.

The assumption behind this model is the following predictor specification:

$$\mathrm{E}(\xi_q \mid x_{pq}) = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} \tag{2.5}$$

which implies that the residual vector $\mathrm{E}(\delta_q) = 0$ and is uncorrelated with the MVs. Each MV or every set of MVs represents a different level of the underlying latent concept. This model does not assume any homogeneity or unidimensionality of the block, and for this reason the block of MVs can be multidimensional and the indicators do not need to covary. Unlike reflective indicators, which are essentially interchangeable, high correlations are not expected between items in formative measurement models.

In fact, a high correlation between two formative indicators, also referred to as *collinearity*, can prove problematic from a methodological and interpretational standpoint. When more than two indicators are involved, this situation is called *multicollinearity*. Collinearity may occur because the same indicator is entered twice or because one indicator is a linear combination of another indicator. High levels of collinearity between formative indicators are a crucial issue because they have an impact on the estimation of weighs and their statistical significance, in particular boosting the standard errors and thus reducing the ability to demonstrate that the estimated weights are significantly different from zero. High collinearity can result in the weighs being incorrectly estimated, as well as in their signs being reversed. To assess the level of collinearity, researchers should compute the *tolerance*. The *tolerance* represents the amount of variance of one formative indicator not explained by the other indicators in the same block. It can be obtained in two steps:

1. first, we take the first formative indicator x_1 and regress it on all the remaining indicators in the same block and calculate its proportion of variance associated with the other indicators ($R^2_{x_1}$);

2. then, compute the tolerance for this indicator (TOL_{x_1}):

$$TOLx_1 = 1 - R^2_{x_1} \tag{2.6}$$

A related measure of collinearity is the *Variance Inflation Factor (VIF)*, defined as the reciprocal of the tolerance:

$$VIF = \frac{1}{TOL_{x_1}} \tag{2.7}$$

A tolerance value of 0.20 or lower and a VIF value of 5 and higher respectively indicate a potential collinearity problem [57]. If the level of collinearity is very high, one should consider removing one of the corresponding indicators [55].

- *The MIMIC way*

The MIMIC way is a combination of the reflective and formative ways. The scores of the standardized LV $\widehat{\xi}_q$ associated with the $q-th$ LV ξ_q are computed as a linear combination of its own block of MVs by means of the weight relation defined as:

$$\widehat{\xi}_q = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} \tag{2.8}$$

where the variables x_{pq} are centred and ω_{pq} are the outer weighs.

2.2.2 The Structural Model

In the PLS-PM framework, the structural model specifies the relationships between the LVs; an LV, if it is supposed to depend on other LVs, is called exogenous, and, otherwise, endogenous. In the structural model each endogenous LV is linked to the other LVs by the following multiple regression model:

$$\xi_j = \sum_{(q:\xi_q \rightarrow \xi_j)} \beta_{qj} \xi_q + \zeta_j \tag{2.9}$$

where ξ_j is an endogeneous LV, β_{qj} is the path coefficient linking the exogenous $q-th$ LV to the $j-th$ endogenous one (Figure 2.3), expressing the impact on the endogenous LV ξ_j of the connected exogenous LVs, and ζ_j is the error in the inner relationship.

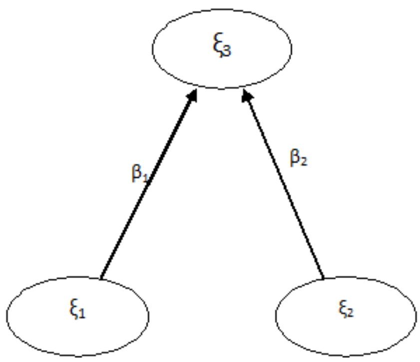


Figure 2.3: Structural model in a path diagram

The only hypothesis of this model is what Wold named the *prediction specification hypothesis* [186]: the residual vector ζ_j has a zero mean and is not correlated with the predictor.

2.3 The Partial Least Squares Algorithm

The PLS-PM [186]; [187]; [166] approach to SEM consists of an iterative algorithm that computes the estimation of the LVs, measured by a set of MVs, and the relationships between them, by means of an interdependent system of equations based on multiple and simple regression. The idea is to determine the scores of the LVs through a process, that, iteratively, computes, first, an outer and, secondly, an inner estimation.
The algorithm alternates the outer estimation with the inner estimation. It performs the estimation of the LVs separately for each block, and then updates the estimation with an inner estimation. So, in the *outer estimation* phase the algorithm computes the weighs w_{pq}, according to the relationship between the LVs and MVs, where q represents the *q-th* latent blocks associated with each MV for the estimation of the LV. The algorithm performs the estimation of the LVs separately for each block, and then it updates the estimation of the LVs, by the inner estimation.
In particular, the PLS algorithms includes three stages:

- an Iterative Approximation of LVs;
- an Estimation of the LVs scores;
- an Estimation of the path coefficients.

2.3.1 The first stage: the Iterative Approximation of LVs

The first stage of the algorithm consists of fours steps [166]:

- Initial arbitrary assignment of outer weights;
- Computing the external approximation of the LVs and obtaining the inner weights;

- Computing the internal approximation of the LVs;
- Calculating the new outer weights;
- Repeating step 2 to step 4 until convergence of the outer weights.

Step 1: Initial arbitrary assignment of outer weights
The procedure starts by choosing arbitrary weights ω_{pq} (for example all 1). The iterative process by assigning any arbitrary non-trivial linear combination of indicators can serve as an outer proxy of a LV [61].

Step 2: Computing the external approximation of the LVs and obtaining the inner weights
In this step, the outer proxies of the LVs are calculated as a linear combination of their own centred MVs (the outer estimation):

$$\nu_q = \sum_{p=1}^{P_q} w_{pq} x_{pq} \tag{2.10}$$

where ν_q is the standardized outer estimate of the $q-th$ LV ξ_q; and the x_{pq} are centred MVs. In the *inner* or *structural model* estimation, the algorithm updates the estimation of the LVs, called z_q, by the computation of the inner weights $e_{qq'}$ (q' is a generic LV associated with the q-th LV). These weights are calculated for each LV in order to reflect how strongly the other LVs are connected to it, considering the existing links with other Q' adjacent LVs:

$$z_q = \sum_{q'=1}^{Q} d_{qq'} e_{qq'} \nu_{q'} \tag{2.11}$$

$d_{qq'}$ is the generic element of the square matrix D of order Q, where $d_{qq'}$=1 if the LV ξ_q is connected to $\xi_q^{'}$ in the path diagram and $d_{qq'}$=0 otherwise. The inner weights $e_{qq'}$ are computed according to three different alternatives:

- the *centroid scheme*, (Wold's original scheme), where the weights are computed as:

$$e_{qq'} = sign[cor(v_q, v_{q'})] \tag{2.12}$$

This choice shows a drawback in a case where the correlation is approximately zero as its sign may change for very small fluctuations. However, this does not seem to be a problem in practical applications.

- the *factorial scheme*, (Lohmöller scheme) where the weights are computed as:

$$e_{qq'} = cor(v_q, v_{q'}) \tag{2.13}$$

Compared to the previous method, the factorial scheme is suggested in all cases in which the correlations between the LVs are weaker.

- the *path weighting scheme*, or structural scheme, where the LVs connected to ξ_q are divided into two groups:

$$e_{qq'} = cor(v_q, v_{q'}) \quad if\ v_{q'}\ predicts\ v_q \quad or \tag{2.14}$$

$$e_{qq'} = \ regression\ coefficient \quad if\ v_{q'}\ is\ predicted\ by\ v_q \tag{2.15}$$

Step 3: Computing the internal approximation of LVs
Inner proxies of the LVs are calculated as linear combinations of the outer proxies of their respective adjacent LVs, using the inner weights previously determined.

Step 4: Calculating the new outer weights Once a first inner estimation of the LVs is obtained, the algorithm proceeds by updating the outer weights ω_{pq}. The estimation of the outer weights depends on the chosen model. There are two ways to estimate these weights: *Mode A* and *Mode B*.

- *Mode A*: each outer weights ω_{pq} is the the regression coefficient in the simple regression of the p-th MV of the q-th block (x_{pq}) on the inner estimate z_q of the q-th LV. As a matter of fact, since z_{pq} is standardized, the generic outer weight ω_{pq} is obtained as:

$$\omega_{pq} = cov(x_{pq}, z_q) \tag{2.16}$$

In this case, the LV is reflected in its respective MVs. In the path diagram the arrows start from the LV and proceed to the MVs.

- *Mode B*: the vector ω_q of the weights ω_{pq} associated with the MVs of the q-th block is the regression coefficient vector in the multiple regression of the inner estimate z_q of the q-th LV on MVs X_q

$$\omega_q = \left(X_q' X_q\right)^{-1} X_q' z_q \tag{2.17}$$

  In this case, the latent concept is formed by its MVs. In the path diagram the arrows start from the MVs and proceed to the LV.

PLS-PM with *Mode A* tends to optimize a covariance criterion [163], and PLS-PM with *Mode B* optimizes a correlation criterion [59]. A small modification of the PLS algorithm is needed to actually maximize a covariance criterion, but simulation shows that both approaches are in very close correspondence [163]. The choice of a certain mode is subject to statistical and theoretical reasoning and typically results from a decision to define an outer model as reflective or formative [40]. In particular, it is closely related to the nature of the model. For a *reflective model Mode A* is more appropriate, while *Mode B* is better for the *formative model*. Furthermore, *Mode A* is suggested for endogenous LVs, while *Mode B* is preferable for exogenous LVs. *Mode A* and *Mode B* can be used simultaneously when the measurement model is the MIMIC one. *Mode A* is used for the reflective part of the model and *Mode B* for the formative part. A general PLS-PM seems not to optimize any criterion, as Kramer showed that *Mode A* of Wold's algorithm is not based on stationary equations related to the optimization of a twice differentiable function. However, in 2011, Tenenhaus and Tenenhaus [163] slightly adjusted *Mode A* in that a normalization constraint was put on the outer weights rather than on the LV scores. In particular, they showed that Wold's procedure, applied to a PLS-PM where the *new Mode A* is used in all the blocks, monotonically converges to the criterion:

$$argmax_{\|\omega_q=1\|} \sum_{q \neq q'} c_{qq'} cov^2(\mathbf{X}_q \omega_q, \mathbf{X}_{q'} \omega_{q'}) \tag{2.18}$$

when the factorial scheme is used for the inner estimation of the LVs. In a completely Data Driven approach, a further alternative for the updating of the outer weights is *Mode PLS* [38]; [37]. In this mode ω_q is the regression coefficient vector in a PLS regression of z_q on $\mathbf{X}_q$. If the PLS-PM algorithm converges on a single component PLS-R, then the *Mode PLS* weights will equal the *Mode A* weights: the data are definitively the expression of a reflective model. If the PLS-PM algorithm converges on a PLS-R with several components, the data are interpreted in a formative model: each sub-block of MVs represents a different dimension of the concept underlying the LV. These three steps are repeated until the change in the outer weights between the two iterations drops past a predefined limit.

Step 5: The convergence algorithm
The convergence of the iterative PLS-PM algorithm is verified according to a stopping rule, most often defined as:

$$max|\omega_{pq}^{(s)} - \omega_{pq}^{(s-1)}| < 10^5 \tag{2.19}$$

where s refers to the $s - th$ iteration.

2.3.2 The second stage: the estimation of the LV scores

Once the final weights ω_{pq} are obtained, the LVs scores are finally calculated as normalized weighted aggregates of the MVs:

$$\hat{\xi}_q \propto X_q \omega_q \tag{2.20}$$

2.3.3 The third stage: the estimation of the path coefficients

In the last stage of the PLS-PM algorithm, the path coefficients are estimated through OLS multiple regressions among the estimated LV scores, according to the path diagram structure. Denoting with ξ_j the generic endogenous LV score vector and with $\hat{\Xi}_{\rightarrow j}$ the matrix of the corresponding latent predictors, the path coefficient vector for each ξ_j is:

$$\hat{\beta}_j = (\hat{\Xi}'_{\rightarrow j}\hat{\Xi}_{\rightarrow j})^{-1}\hat{\Xi}'_{\rightarrow j}\hat{\xi}_q \tag{2.21}$$

In the case of multicollinearity among the estimated LV scores, in order to reduce the estimation variability, PLS regression can be used instead of OLS regression [38].
So, in summary, the PLS-PM estimation proceeds according to the following iterative scheme:

The PLS-PM algorithm

Initializing the algorithm with the matrix X of raw MVs
Step1: Compute a first random vector of weights w_{pq}
repeat
Step2: Compute the first estimate of the LVs
  for (q in 1:Q)
    $v_q = \sum_{p=1}^{P_q} w_{pq} x_{pq}$
  end for
Step3: Update the previous estimation of LVs
  for (q in 1:Q)
    $z_q = \sum_{q=1}^{Q} e_{qq'} v_q$
  end for
Step4: Update the estimation of the weights w_{pq}
    for (q in 1:Q)
      for (p in 1:P_q)
        $w_{pq} = cov(x_{pq}, \mathbf{z}_q)$
        $\mathbf{w}_q = (X_q' X_q)^{-1} X_q' z_q$
      end for
    end for
Check the convergence
  Until $\sum |w_{pq}^{old} - w_{pq}^{new}| < \epsilon$

The convergence[1] of the algorithm is achieved if the sum of the absolute differences of the weights of the two outer successive estimations is less than ϵ (a small positive real value). Finally the inner estimation of the path coeffi-

[1]The convergence of the PLS-PM algorithm is demonstrated for two blocks. In the case of a greater number of blocks the convergence is demonstrated only empirically.

cients and the loadings among the LVs, according to the supposed relationship between them, are computed by the classic OLS for multiple/single regressions.
From the inferential point of view the PLS-PM does not make any reference to the distribution hypothesis on data, making use of computational inference based tools such as resampling techniques. In particular the Bootstrap technique based on the extraction, with the replacement of m samples of size n (n is the original sample size) is considered. The model is estimated on each m-th Bootstrap sample, in order to obtain an empirical distribution for the parameters (weights, path coefficients and loadings) and to compute a suitable confidence interval. This procedure is performed for the parameters of both the outer model (the weights and loadings), and the inner model (the path coefficients). The intervals including the zero suggest eliminating the MVs or LVs from the model. To compare the parameters estimated and the mean of the bootstrap replications, a ratio between their deviation and the standard deviation of the resembling distribution is computed as a classic test statistics.

2.4 Model Validation

Model estimation delivers empirical measures of the measurement models (the relationships between the indicators and the constructs), as well as of the structural models (the relationships between the constructs). The empirical measures enable us to compare the theoretically established measurement and structural models with reality, as represented by the sample data. In other words, we can determine how well the theory fits the data. More precisely, the evaluation of the measurement and structural model results in PLS-PM builds on a set of non-parametric evaluation criteria and uses procedures such as bootstrapping and blindfolding. This process involves a separate assessment of the measurement model and the structural model.
Initially, the model assessment focuses on the measurement models. An examination of PLS-PM estimates enables the researcher to evaluate the

reliability and validity of the construct measures. When evaluating the measurement models, we must distinguish between reflectively and formatively measured constructs. The two approaches are based on different concepts and therefore require a consideration of different evaluative measures. Reflective measurement models are assessed on their internal consistency reliability and validity. The specific measures include the composite reliability (as a means to assess the internal consistency reliability), convergent validity, and discriminant validity. The criteria for reflective measurement models cannot be universally applied to formative measurement models. With formative measures, the first step is to ensure content validity before collecting the data and estimating the PLS-PM. After the model estimation, the formative measures are assessed for their convergent validity, significance and relevance and the presence of collinearity among the indicators. The structural model estimates are not examined until the reliability and validity of the constructs have been established. If the assessment of reflective and formative measurement models provides evidence of the measures' quality, the structural model estimates are evaluated. The PLS-PM assessment of the structural model involves the model's ability to predict. Hence, after the reliability and validity have been established, the primary evaluation criteria for the PLS-PM results are the coefficients of determination (R^2 values) as well as the level and significance of the path coefficients. The assessment of the PLS-PM outcomes can be extended to more advanced analyses (e.g., examining the mediating and/or moderating effects, considering any unobserved heterogeneity, multi-group testing, and common method variance).

2.4.1 Assessing the results of reflective measurement models

The assessment of reflective measurement models includes composite reliability to evaluate the internal consistency, individual indicator reliability, and Average Variance Extracted (AVE) to evaluate the convergent validity. In addition, the Fornell-Larcker criterion and cross loadings are used to assess the discriminant validity.

Regarding the first two assessment, the *internal consistency* and *individual* *indicator reliability*, these have already been described in detail above.

Convergent Validity. This is the extent to which a measure correlates positively with alternative measures of the same construct. Using the domain sampling model, the indicators of a reflective construct are treated as different approaches to measure the same construct. Therefore, the items that are indicators (measures) of a specific construct should converge or share a high proportion of variance.

To establish convergent validity, researchers consider the outer loadings of the indicators, as well as the AVE. High outer loadings on a construct indicate that the associated indicators have much in common, which is captured by the construct. This characteristic is also commonly called indicator reliability. At a minimum, all indicators outer loadings should be statistically significant.

A common measure to establish convergent validity on the construct level is the AVE [41] that expresses the degree of variance of the block explained by $\hat{\xi}_q$:

$$AVE_q = \frac{\sum_{p=1}^{P_q} \hat{\lambda}_{pq}^2}{\sum_{p=1}^{P_q} var(x_{pq})} \tag{2.22}$$

This criterion is defined as the grand mean value of the squared loadings of the indicators associated with the construct (i.e., the sum of the squared loadings divided by the number of indicators). An AVE value of 0.5 or higher indicates that, on average, the construct explains more than half of the variance of its indicators. Conversely, an AVE of less than 0.5 indicates that, on average, more error remains in the items than the variance explained by the construct. Therefore, the AVE is equivalent to the *communality* of a construct. In a good measurement model, each MV is well summarized by its own LV. So, for each block, a *Communality Index* is computed as:

$$Com_q = \frac{1}{P_q} \sum_{p=1}^{P_q} cor^2(x_{pq}, \hat{\xi}_q) = \frac{1}{P_q} \sum_{p=1}^{P_q} \hat{\lambda}_{pq}^2 \tag{2.23}$$

that is the average of the communalities between each MV of the $q-th$ block and $\hat{xi}_q$. The communality index measures the capacity of the LV to explain the variance of its MVs. If we work on standardized MVs, AVE and Communality coincide for less than the constant $1/P_q$

Discriminant validity. This is the extent to which a construct is truly distinct from other constructs by empirical standards. Thus, establishing discriminant validity implies that a construct is unique and captures phenomena not represented by other constructs in the model. Alternative measures of discriminant validity have been proposed. One method for assessing discriminant validity is by examining the cross loadings of the indicators. Specifically, an indicator′s outer loading on the associated construct should be greater than all of its loadings on other constructs (i.e., the cross loadings).

$$H_0 : cor(\xi_q, \xi_{q'}) = 1 \;\; against \;\; the \;\; H_1 : cor(\xi_q, \xi_{q'}) < 1 \tag{2.24}$$

The presence of cross loadings that exceed the indicators' outer loadings represents a discriminant validity problem. This criterion is generally considered rather liberal in terms of establishing discriminant validity [57]. This means it is very likely to indicate that two or more constructs exhibit discriminant validity.

The Fornell-Larcker criterion is another approach for assessing discriminant validity. It compares the square root of the AVE values with the LV correlations. Specifically, the square root of each construct's AVE should be greater than its highest correlation with any other construct. The logic of this method is based on the idea that a construct shares more variance with its associated indicators than with any other construct.

$$(AVE_q \; and \; AVE_{q'}) > cor(\hat{\xi_q}, \hat{\xi_{q'}}) \tag{2.25}$$

This means that the LVs better explain the MVs than other LVs.

2.4.2 Assessing the results of formative measurement models

Many researchers incorrectly use reflective measurement model evaluation criteria to assess the quality of formative measures in PLS-PM, as revealed by the review of PLS-PM studies in the strategic management and marketing disciplines by Hair et al. [56].
The statistical evaluation criteria for reflective measurement scales cannot be directly transferred to formative measurement models where the indicators are likely to represent the construct independent causes and thus do not necessarily correlate highly. Researchers should focus on establishing content validity before empirically evaluating formatively measured constructs. This makes it necessary to ensure that the formative indicators capture all (or at least major) facets of the construct. In creating formative constructs, content validity issues are addressed by the content specification in which the researcher clearly specifies the domain of content the indicators are intended to measure. Researchers must include a comprehensive set of indicators that fully exhausts the formative construct domain. Failure to consider all facets of the construct (i.e., the relevant formative indicators) entails an exclusion of important parts of the construct itself. The evaluation of formative measurement models makes it necessary to establish the measures' convergent validity, assess the indicators' collinearity, and analyze the indicators' relative and absolute contributions, including their significance.

Convergent Validity. This is the extent to which a measure correlates positively with other measures (indicators) of the same construct. When evaluating formative measurement models, we have to test whether the formatively measured construct is highly correlated with a reflective measure of the same construct. This type of analysis is also known as *redundancy analysis* [12]. The term redundancy analysis stems from the information in the model being redundant in the sense that it is included in the formative construct ξ_1 and again in the reflective one ξ_2 (see Figure 2.4).
The strength of the path coefficient linking the two constructs is indicative of the validity of the designated set of formative indicators in tapping the

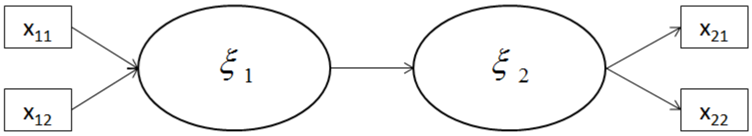


Figure 2.4: Redundancy Analysis for Convergent Validity Assessment

construct of interest. If the analysis exhibits a lack of convergent validity (i.e. the R^2 value of ξ_2 < 0.64), then the formative indicators of the construct ξ_1 do not contribute at a sufficient level to its intended content. The formative constructs need to be theoretically/conceptually refined by exchanging and/or adding indicators. Regarding the former, the *collinearity among indicators*, this has been described in detail above.

Significance and Relevance of the Formative Indicators. This is another important criterion to evaluate the contribution of a formative indicator. The values of the outer weights can be compared with each other and can therefore be used to determine each indicator's relative contribution to the construct, or its relative importance. We must test if the outer weights in formative measurement models are significantly different from zero by means of the bootstrapping procedure. It is important to note that the values of the formative indicator weights are influenced by other relationships in the model (the PLS-PM algorithm above). Non-significant indicator weights should not automatically be interpreted as indicative of poor measurement model quality. Rather, researchers should also consider a formative indicator's *absolute contribution* to its construct-that is, the information an indicator provides without considering any other indicators. The absolute contribution is given by the formative indicator's outer loading, which is always provided along with the indicator weights. Differently from the outer weights, the outer loadings stem from single regressions of each indicator on its corresponding construct. When an indicator's outer weight is non-significant but its outer loading is high (i.e., above 0.5), the indicator should be interpreted as absolutely important but not as relatively important. In this situation, the indicator would generally be retained. But when an indicator has a non-significant weight and the outer loading is below 0.5, the researcher should decide whether to retain or delete the indicator by examining its theoretical relevance and potential content overlap with other indicators of the same construct.

2.4.3 Assessing the results of structural models

Once we have confirmed that the construct measures are reliable and valid, the next step addresses the assessment of the structural model results. This involves examining the model's predictive capabilities and the relationships between the constructs The key criteria for assessing the structural model in PLS-PM are the significance of the path coefficients, the level of the R^2 values, the f^2 effect size, the predictive relevance Q^2, and the q^2 effect size.

Structural model path coefficients. The paths represent the hypothesized relationships among the constructs. Whether a coefficient is significant ultimately depends on its standard error that is obtained by means of bootstrapping. The bootstrap standard error allows a computation of the *empirical t value*:

$$t = \frac{p_{qj}}{se^*_{p_{qj}}} \tag{2.26}$$

when the empirical t value is larger than the *critical value*, the coefficient is significant at a certain error probability (i.e., significance level); commonly used critical values for two-tailed tests are 1 .65 (significance level= 10%), 1.96 (significance level = 5%), and 2.57 (significance level = 1%). Instead of t values, researchers routinely report p values that correspond to the probability of erroneously rejecting the null hypothesis, given the data at hand. In addition to calculating the t and p values, the bootstrapping confidence interval for a pre-specified probability of error can be determined.

***Coefficient of Determination* R^2.** R^2 is a measure of the model's predictive accuracy and is calculated as the squared correlation between a specific endogenous construct's actual and predicted values. It represents the amount of variance in the endogenous constructs explained by all of the exogenous constructs linked to it. The R^2 value ranges from 0 to 1 with higher levels indicating higher levels of predictive accuracy; the acceptable R^2 value depends on the model complexity and the research discipline. [56].

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

$$f^2 = \frac{R^2_{included} - R^2_{excluded}}{1 - R^2_{included}} \tag{2.27}$$

where $R^2_{included}$ and $R^2_{excluded}$ are the R^2 value of the endogenous LV when a selected exogenous LV is included in or excluded from the model. Guidelines for assessing f^2 are proposed by Cohen [22]:

- if $f^2 \approx 0.02 \rightarrow$ small impact
- if $f^2 \approx 0.15 \rightarrow$ medium impact
- if $f^2 \approx 0.35 \rightarrow$ large impact

***Predictive Relevance* Q^2.** This last indicator concerns the model's predictive relevance developed by Stone [159] and Geisser [47]. The PLS-PM adaptation of this approach follows a blindfolding procedure. Given a block of n cases and P MVs, the procedure extracts a portion of the considered block during parameter estimations and then attempts to estimate the omitted part using the estimated parameters. To estimate the model, the omitted value is typically replaced with the variable mean, (though other imputation techniques may be used [13]). Based on the estimated model, the estimates for the omitted value are compared to the observed values, using the squared difference (E). At the same time, the difference between the variable mean (or otherwise imputed value) and the observed values are also compared using the squared difference (O). This procedure is repeated until every data point has been omitted and estimated. The predictive measure for these MVs is then calculated as:

$$Q^2 = 1 - \frac{\sum_m E_m}{\sum_m O_m} \tag{2.28}$$

where m is the number of times the procedure is repeated to ensure that every data point is omitted.
Q^2 represents a measure of how well-observed values are reconstructed by the model and its parameter estimates [15]. When PLS-PM exhibits predictive relevance, it accurately predicts the data points of indicators in reflective measurement models of endogenous constructs and endogenous single-item constructs (the procedure does not apply for formative endogenous constructs). $Q^2 > 0$ implies that the model has predictive relevance whereas $Q^2 < 0$ represents a lack of predictive relevance. In the structural model, Q^2 values greater than zero for a certain reflective endogenous LV indicate the path model's predictive relevance for this particular construct. In contrast, values of 0 and below indicate a lack of predictive relevance. Similar to the f^2 effect size approach for assessing R^2 values, the relative impact of predictive relevance can be compared by means of the measure to the q^2 effect size, formally defined as follows:

$$q^2 = \frac{Q^2_{included} - Q^2_{excluded}}{1 - Q^2_{included}} \tag{2.29}$$

where $Q^2_{included}$ and $Q^2_{excluded}$ are the Q^2 values of the endogenous LV when a selected exogenous LV is included in or excluded from the model. As a relative measure of predictive relevance, values of 0.02, 0.15 and 0.35 indicate that an exogenous construct has a small, medium or large predictive relevance for a certain endogenous construct [56]. Different forms of Q^2 can be obtained with different procedures for predicting observations from the model. In the *cross-validated communality* Q^2 the prediction of observations is made by the computed composite and the estimated loadings. The *cross-validated redundancy* Q^2 is still based on the estimated loadings but the composites are predicted from the structural model using the estimated path coefficients. The redundancy-based Q^2 is applicable only to observations of MVs of the endogenous blocks, while the communality-based Q^2 can be applied to all MVs [15].

Tenenhaus et al. [165]; [166] proposed a PLS *Goodness-of-Fit (GoF)* as *an operational solution to this problem as it may be used as an index for validating the PLS model globally*. The GoF can be proposed as the geometric mean of the average communality and the average of R^2:

$$GoF = \sqrt{\overline{Com} \times \overline{R^2}} \tag{2.30}$$

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

The GoF is a compromise between the quality of the outer model and the quality of the inner model, so the normalized index is obtained by bringing each part to its maximum value. In particular, for the outer estimation (the first part of the formula is the average communality) for each block the maximum is the first eigenvalue, because the first principal component explains the maximum variability, while for the inner estimation the maximum is given by the first canonical correlation squared. To verify the GoF significance it is possible to build an interval confidence with the Bootstrap technique, as also for the R^2.

Henseler and Sarstedt [65] criticize the usefulness of the GoF both conceptually and empirically. Their research shows that the GoF does not represent a goodness-of-fit criterion for PLS-SEM. Using simulated data, they have illustrated that the GoF is not suitable for model validation. For some specific types of model validation, though, the application of the GoF does make sense. This is the case when it comes to validating models that differ not in their structure but in their (reflective) indicators; in such models, the GoF is the statistic of choice. If the structural model remains constant, the GoF can indirectly assess relative changes in convergence validity as expressed by the average variance extracted [41]. The GoF is also very useful for data comparisons (i.e., varying the data while keeping the model constant). As a consequence, the GoF is best applied in group comparisons [148] and assessments of unobserved heterogeneity, as is the case with the REBUS-PLS procedure. In these cases, the GoF can answer questions on how well different subsets of the data can be explained by a particular model. However, since the GoF is also not applicable to formative measurement models and does not penalize over-parametrization efforts, researchers are advised not to use this measure. For a formative block, one might replace in the GoF formula the block communality by the R^2 between the inner proxy of the formative block and the block's MVs. Another point of departure could be assessing a formative block's weights. Future research should make more concrete suggestions of how to improve the GoF, and demonstrate the viability of the improvements by means of both conceptual reasoning and Monte Carlo simulations [65].

2.5 A CI Decision Matrix

A key characteristic of the PLS-PM method is the extraction of CI scores. One of the greatest advantages of PLS-PM is these CI scores. In the System of CIs built with PLS-PM, you can obtain the scores for each CI, exogenous or endogenous, and for each CI you can make a ranking among units. Moreover, PLS-PM provides information on the relative importance of constructs in explaining other constructs in the structural model. Information on the importance of constructs is relevant for drawing conclusions. For this reason, a CI Decision Matrix is a valuable decision making tool. It is useful in extending the findings of the basic PLS-PM outcomes using the LV scores [66]. The results of PLS-PM take into account the performance of each construct. In addition, CI average values are considered. For a specific endogenous CI, this Matrix contrasts the structural model's total effects (the importance) and the average values of the CI (the performance). As a result, conclusions can be drawn on two dimensions (i.e., both importance and performance), which is particularly important in order to prioritize actions. The analysis is based on a scatter plot where each CI is positioned according to its mean and its path coefficient with respect to the target CI.

The x-axis represents the total effects of the CIs on the target CI (i.e. their importance). The y-axis depicts the average construct scores of these LVs. (i.e. their performance). In this way the scatter plot is divided into four areas (Table 2.1):

- the first area is the most critical area, because the CIs have a high impact but a low mean value;
- the second is the area of the monitoring, in which the CIs have a low value for the mean and the path coefficient;
- the third is the area to improve because the CIs have a high mean value and a low path coefficient;
- the fourth is the area to be maintained, in which the CIs have a high value for the mean and the path coefficient.

Table 2.1: A CI Decision Matrix

<table>
<tr><th></th><th></th><th colspan="2">Mean Scores</th></tr>
<tr><th></th><th></th><th>Low</th><th>High</th></tr>
<tr><td rowspan="2">Total Impact</td><td>Low</td><td>Area of monitoring</td><td>Area to improve</td></tr>
<tr><td>High</td><td>Area of immediate intervention</td><td>Area to maintain</td></tr>
</table>

A similar scatter plot can be considered also for the MVs. In this kind of matrix, we have the possibility to analyze the strengths, weaknesses, opportunities, and threats of constructs, that are considered in the model in order to estimate a latent concept.

2.6 The Predictive Power of PLS-PM

Composite-Based approaches, such as PLS-PM, are preferred to Covariance-Based approaches, since the objective of the research is to develop a predictive model. PLS-PM is a powerful method for predictive purposes, and it is certainly an important technique which deserves a prominent place in research applications when the aim of the analysis is prediction [7]. The PLS-PM evaluation criteria should include the predictive ability and, therefore, further criteria and evaluation techniques for PLS-PM are needed [150]. Thus, an interesting topic for further research in PLS-PM is the extension and development of further measures and evaluation criteria for the assessment of PLS-PM in terms of predictive capability. Based on the proposed criteria, further extensions and modifications should be made to the basic PLS-PM algorithm in order to improve the predictive capabilities of the model estimation. The *Non-Symmetrical Approach for Component-Based Path Modeling* proposed by Dolce et al. [31] and Dolce [30] is an example of work in this direction. In their opinion, prediction in Composite-Based Methods could refer to different concepts. The predictive ability could be interpreted as either the ability to explain variance in the endogenous LVs or the ability to predict individual observations. Moreover, individual observations may refer to either individual LV score observations or individual observations for MVs of the endogenous blocks. The predictive capability of the model depends on several aspects, including the sample size and the way the outer weights are calculated. Furthermore, the predictive capability of a Component-Based Method can also be improved by extracting more than one component for each block. PLS-PM generally considers one component for each block of variables. In some cases we can lose information in predictor blocks that may be of extreme importance for the predicting of endogenous composites or the MVs related to them. The latter consideration is examined in chapter five, where we will deal with new methods for the estimation of Higher-Order Constructs in PLS-PM, particularly when we will propose PLS Component Regression as a method to extract more than one component for each block, in accordance with the Predictive Relevance Q^2 Index.

2.7 Available software for PLS Path Modeling

For a long time *LVPLS* 1.8 [95] was the only available software for PLS Path Modeling. The DOS-based program includes two different modules

for estimating path models. The LVPLSC method analyzes the covariance matrix of the observed variables, whereas the LVPLSX module is able to process raw data. In order to specify the input file an external editor is necessary. The input specification requires that the program parameters are defined at specific positions in the file. The results are reported in a plain text file. The program offers blindfolding and jackknifing as resampling methods in cases where raw data has been analyzed. When analyzing covariance/correlation matrices, resampling techniques cannot be applied [102]. Over the years other PLS path modeling software have been developed.
The list includes *SmartPLS* [130], *XLSTAT-PLSPM* [35] in co-operation with Addinsoft France, (http://www.xlstat.com/en/products/xlstat-plspm/) - and the *plspm* package [146]. *SmartPLS* and *XLSTAT-PLSPM* are closed source and *plspm* is licensed under the General Public License (GPL$\geq$2). All differences in model parameters due to the used software were in line with the predefined tolerance for the outer weights.

SmartPLS. SmartPLS is a stand alone software specialized for PLS path models. It is built on a Java Eclipse platform making it operating system independent. The model is specified via drag and drop by drawing the structural model for the LVs and by assigning the indicators to the LVs. Data files of various formats can be uploaded. After fitting a model, coefficients are added to the plot. More detailed output is provided in plain text, in the LATEX and HTML formats. The graph representing the model can be exported to PNG. Besides bootstrapping and blindfolding methods it supports the specification of interaction effects. A special feature of SmartPLS is the finite mixture routine (FIMIX), a method to deal with unobserved heterogeneity [131];[149];[148].

XLSTAT-PLSPM. XLSTAT [1] is a modular statistical software relying on Microsoft Excel for the input of data and the display of results, but the computations are performed using autonomous software components.
XLSTAT-PLSPM is integrated in XLSTAT as a module for the estimation of PLS path models. It has been developed by a research team from the

Department of Mathematics and Statistics of the University of Naples in Italy and Addinsoft in France and implements all the methodological features and most recent findings of the PLEASURE (Partial LEAst Squares strUctural Relationship Estimation) technology by Esposito Vinzi et al. [35]. Special features of XLSTAT-PLSPM are multi-group comparisons [18] and the REBUS segmentation approach [38] for the treatment of unobserved heterogeneity.

plspm in R. The plspm package implements the PLS method with emphasis on structural equation models in R. The fitting method 'plspm.fit' returns a list including all the estimated parameters and almost all the statistics associated with PLS path models. The print method gives an overview of the following list elements: the outer model, inner model, scaled LVs, LVs for scaled = FALSE, outer weights, loadings, path coefficients matrix, R^2, outer correlations, inner model summary, total effects, unidimensionality, goodness-of-fit, bootstrap results (only if activated) and data matrix. For the treatment of observed heterogeneity, *pathmox* and *rebus.pls* [145] are provided as a companion package [102].

Chapter 3

Some developments in PLS - PM for the building of Composite Indicators

3.1 Introduction

The PLS-PM approach has enjoyed increasing popularity as a key multivariate analysis method in various research disciplines in order to build a system of Composite Indicators. The model allows you to estimate causal relationships, defined according to a theoretical model linking two or more latent complex concepts, each measured through a number of observable indicators. The basic idea is that the complexity inside a system can be studied by taking into account the entirety of the causal relationships among LVs, each measured by several MVs. Nowadays, complex phenomena such as Development, Progress, Poverty, Social Inequality, Welfare and Quality of Life require, to be measured, the combination of different dimensions, to be considered together as the proxy of the phenomenon.This combination can be obtained by applying methodologies based on CIs [100]. As is well known, the main feature of a CI is that it summarizes this type of complex and multidimensional issue.

In building a CI, we are interested in (i) including elementary indicators on a non numerical scale, (ordinal and nominal data); (ii) including some kind of CI relationship (logical, hierarchical, temporal or spatial); (iii) defining the roles of the EIs (MVs) as mediator and moderator variables; and (iv) defining the roles of the CIs (LVs) in the inner model (mediator and moderator LVs). For instance, when computing a CI, it could be interesting to consider demographic variables, such as religion or gender, categorical variables defining states, such as type of government. It would be interesting to know what is the role of these variables, is if they have a moderator or mediator effect, and if a consideration of these effects change the estimation of the LVs. Moreover, applications of SEMs are usually based on the assumption that the analyzed data stem from a single population, so that a unique global model represents all the observations effectively. However, in many real world applications, this assumption of homogeneity is unrealistic. In modeling the real world, it is reasonable to expect that different classes showing heterogeneous behaviors may exist in the observed set of units. This is true also in CI frameworks. As a matter of fact, in developing a system of CIs, it is reasonable to suppose that different models, i.e. different systems of weightings, should be applied in order to take into account differences among the units. Furthermore, in these frameworks also, it is of great importance to obtain clusters of units that are homogenous with regard to the weights to be applied in computing the CIs. For this reason, many improvements, in order to extend the classic algorithm of PLS-PM to the treatment of particular data, have been made, in particular to non-metric data, mediator and moderator data and hierarchical data. Furthermore, several clustering techniques have been developed in PLS-PM to look for latent classes.

In the following sections these developments are presented.

Next, a chapter will be included developed on dealing with a hierarchical model.

3.2 Non Numerical Models for data measured on different measurement scales

PLS-PM is a technique devised to handle quantitative variables. However, in practice categorical indicators could be used to measure complex concepts as well. When we study complex phenomena in various research disciplines, some elementary indicators are not on a numerical scale (nominal and ordinal variables). This kind of MV can play several different roles in PLS-PM, in particular it can have an active role in the analysis. An active categorical variable directly participates in the construction of the system of CIs. In other words, it is a categorical indicator impacting on a CI jointly with other indicators. In order to deal with this type of variable, the existing literature provides new algorithms to quantify and use the MVs for the estimation of an SEM, according to the PLS-PM algorithm.

3.2.1 Partial Alternating Least Squares Optimal Scaling Path Modeling

One of these is *Partial Alternating Least Squares Optimal Scaling-Path Modeling (PALSOS-PM)* [109]. This algorithm allows us to quantify optimally while, at the same time, proceeding with the estimation of the model parameters. Until now the quantification has been achieved internally according to a suitable Optimal Scaling technique. In particular, in the quantification step, with the aim of taking into account nominal, ordinal and numerical MVs in the model, PALSOS uses the *MORALS (Multiple Optimal Regression by Alternating Least Squares)* algorithm by Young et al. [189] belonging to the *Alternating Least Squares Optimal Scaling family (ALSOS)*. The MORALS algorithm estimates the parameters of a regression between LVs and MVs, by introducing a quantification step into the process of estimation. A relevant feature of MORALS is that the step of quantification is performed individually for each MV, taking into account the type of relationship with the LV. MORALS bases the quantification of the nominal variables on the orthogonal projection of the LV in the space spanned by the columns of the indicator matrix G_i generated by the j categories of the MV x_i (no constraints are imposed on the admissible values for the new variable quantified). The quantification of an ordinal variable is based on the use of a monotone regression [87], that consists in a non-linear regression problem (the categories, of the new variable quantified, must have the same order as the categories of the original variable). After the quantification step, the algorithm estimates the regression coefficients by the minimization of a quadratic loss function. It is worth noticing that, in MORALS, the loss function introduced into the third step of the classic PLS-PM algorithm depends on the reflective or formative relationships between the LVs and MVs. In the reflective mode, MORALS estimates the vector of optimal scaling and the parameters of a simple regression, while in the formative mode it estimates the parameters of a multiple regression. The final objective of this technique is to obtain the optimal quantification of the nominal/ordinal variables, optimizing the regression parameters. In fact, once the vector x_i^{os} (o.s. is the acronym of Optimal Scaling) for the $i - th$ MV has been computed, the parameters of simple/multiple regression are just updated using as MVs the new ones obtained in the previous step, by reiterating the regression until convergence. The PALSOS-PM algorithm is initialized with a particular quantification obtained by the PRINCALS [174]; [23] algorithm that develops a Principal Component Analysis for Non Linear MVs where the term non-linear relates to the non-linear transformation of the observed variables. This initialization of the LVs that remain in the ALSOS frame is also in line with a typical choice in the classic algorithm of PLS-PM. The algorithm proceeds with the inner estimation of the LVs, and when it returns to the external estimation, uses MORALS to update the outer estimation. The above algorithm also estimates a model with all the quantitative variables, in this case being equivalent to the classic PLS-PM algorithm. As in the PLS-PM algorithm, the PALSOS-PM algorithm stops when the estimation of the weights is stabilized. The algorithm proceeds with the estimation of the path coefficients by simple/multiple OLS regression and, if necessary, by PLS regression. For the validation of the outer and inner model, the Bootstrap technique is used to create a suitable interval confidence. Therefore, information about the variability of the parameter estimates and hence their significance has to be generated by means of resembling procedures like Bootstrap. PALSOS-PM, as in the PLS-PM algorithm, solves the problems on the signs of the weights by comparing the signs of the eigenvectors [139]. In contrast to the other internal quantification approaches, in PALSOS-PM the weights, associated with the MVs, are computed in the same way for all kinds of variable. With respect to the other proposals, PALSOS-PM quantifies the MVs both for reflective and formative relationships between MVs and LVs. For further details, see [109].

3.2.2 Non-Metric PLS Path Modeling

There is another new algorithm called the *Non-Metric PLS Path Modeling* algorithm [135]. This algorithm extends the applicability of PLS methods to data measured on different measurement scales, as well as to variables linked by non-linear relationships. The Non-Metric PLS (NM-PLS) approach extends the covariance-based PLS criteria to the treatment of non-metric variables and non-linearity. This approach is based on the concept of Optimal Scaling [48]; [24] The OS principle sees observations as categorical, and represents each observation category by a scaling parameter. This parameter is subject to constraints deriving from the measurement characteristics of the variables. This is a valid tool to obtain coherent models when we observe variables measured on a variety of measurement scales, as well as when we want to discard the linearity hypothesis with regards to relationships between the MVs and the corresponding LV. In fact, a milder hypothesis of monotonicity can be adopted in a non-metric approach. In general, Non-Metric PLS Path Models provide better models, since MV are transformed in such a way as to make relationships between the MVs and LVs linear. In this process each variable x is transformed as $\hat{\mathrm{x}} \propto \tilde{\mathrm{X}}\phi$, where $\phi' = (\phi_1, ..., \phi_K)$ is a vector of the numeric values (the scaling parameters) associated with the K different values or categories of the variable x, and the matrix $\tilde{\mathrm{X}}$ defines a space in which the constraints imposed by the scaling level are respected. The symbol $\propto$ means that the left side of the equation corresponds to the right side normalized to unitary variance.

Non-Metric PLS-PM loops differ from the standard PLS-PM loops in the sense that they start by initializing the inner estimate of each LV, used to obtain a first scaling of the MVs. Each raw MV x_pq is quantified so as to be maximally correlated to the corresponding LV. The Non-Metric PLS-PM algorithm supports three levels of scaling analysis: (i) variables quantified at a nominal level preserve the grouping property; (ii) variables quantified at an ordinal level follow the secondary Kruskal's monotonic quantification; (iii) variables transformed at a functional level are related to the corresponding LV inner estimate by a polynomial relation (for further details, see Russolillo [134]).

3.3 The importance of modeling heterogeneity in PLS-PM: Mediator and Moderator Variables

Another important topic in PLS-PM is the mediation and moderation effect. A significant mediator variable or moderator variable may to some extent absorb a cause-effect relationship. Examining these variables enables researchers to better understand the relationships between dependent and predictor constructs. Mediation and moderation are two important topics in the context of PLS-SEM. The mediation function of a third variable represents the generative mechanism through which the focal independent variable is able to influence the dependent variable of interest. The moderator function of the third variable splits up a focal independent variable into sub-groups that establish its domains of maximal effectiveness with regard to a given dependent variable. Mediation focuses on a theoretically established direct path relationship between ξ_q and ξ_j, as well as on an additional theoretically relevant component μ, which indirectly provides information on the direct effect via the indirect effect from ξ_q to ξ_j via μ. Thereby, the indirect relationship via the μ mediator affects the direct relationship from ξ_q to ξ_j in the mediator model.

Moderator variables are variables influencing the relationship, in terms of strength and/or direction, between an exogenous and an endogenous variable.

3.3.1 Mediator Variables

Mediator variables address issues of how or why such effects occur (Figure 3.1).

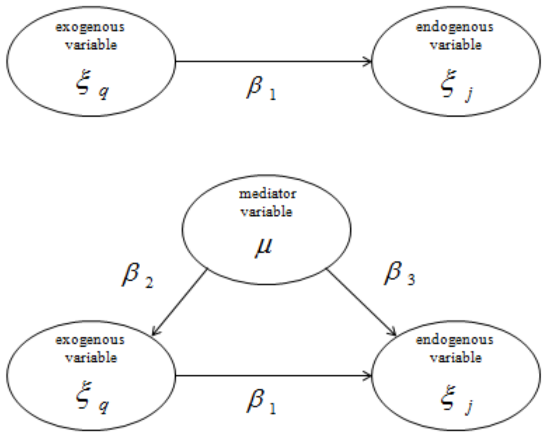


Figure 3.1: Simple Cause - Effect Relationship and General Mediator Model

The relationship of the exogenous variable ξ_q to the endogenous variable ξ_j is influenced by another LV called the Mediator Variable μ. Therefore, in addition to the direct effect β_1 we must also consider the indirect effects β_2 and β_3.
Technically, a variable function is a mediator when it satisfies the following conditions [5]:

- Variations in the levels of the independent variable account significantly for the variations in the presumed mediator;

- Variations in the mediator account significantly for the variations in the dependent variable;

- When paths β_2 and β_3 are controlled, a previously significant relationships between the independent and dependent variables changes its value significantly.

Consequently, empirical tests must answer the following questions: Is the direct effect β_1 significant when the mediator variable is excluded from the PLS path model? Is the indirect β_2 and β_3 effect via the mediator variable

significant after this variable has been included in the PLS path model? A necessary (but not sufficient) condition for the significance of the product of paths β_2 and β_3 is that the two paths themselves are both significant. How much of the direct effect β_1 does the indirect effect absorb? Do we have a situation of full or partial mediation?
A commonly used approach for testing mediating effects is the Sobel test [156], which examines the relationship between the independent variable and the dependent variable compared with the relationship between the independent variable and dependent variable, including the mediation construct [60]. However, this test relies on distributional assumptions, which usually do not hold for the indirect effect β_2 and β_3.
Furthermore, the Sobel test requires unstandardized path coefficients as the input for the test statistics and lacks statistical power, especially when applied to small sample sizes. Preacher and Hayes [119]; [120] proposed another approach for testing mediating effects. They bootstrap the sampling distribution of the indirect effect, which works for simple and multiple mediator models. Bootstrapping makes no assumptions about the shape of the variables distribution or the sampling distribution of the statistics and can be applied to small sample sizes with more confidence. The approach is therefore perfectly suited for the PLS-PM method, and, in addition, it exhibits higher levels of statistical power compared with the Sobel test.
It starts to consider the direct effect, that should be significant if the mediator is not included in the model. When including the mediator, the indirect effect must be significant. If the indirect effect is significant, the mediator absorbs some of the direct effect. For example, in a PLS path model without the mediator variable, a positive direct effect would become smaller after the inclusion of the mediator variable. The question is how much the mediator variable absorbs. To answer this question the authors introduce the *Variance Accounted For (VAF)*, that determines the size of the indirect effect in relation to the total effect. Making reference to the diagram in Figure 3.1, VAF is calculated as follows:

$$VAF = \frac{\beta_2 * \beta_3}{(\beta_2 * \beta_3) + \beta_1} \tag{3.1}$$

If the indirect effect is significant but does not absorb any of the exogenous LV effect on the endogenous variable, the VAF is rather low. This occurs when the direct effect is high and declines only very slightly after a mediator variable with a significant but very small indirect effect is included. In this situation, the VAF would be less than 20%, and we can conclude that (almost) no mediation takes place. In contrast, when the VAF has very large outcomes of above 80%, we can assume a full mediation. A situation in which the VAF is larger than 20% and less than 80% can be characterized as partial mediation.

3.3.2 Moderator Variables

Besides the examination of direct effects, researchers are also interested in moderating effects. Moderating effects are evoked by variables whose variation influences the strength or the direction of a relationship between an exogenous and an endogenous variable (Figure 3.2) [63].

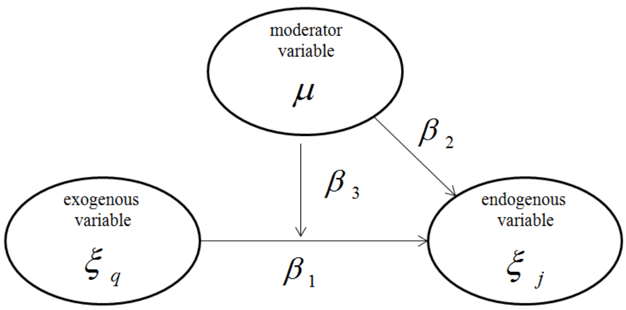


Figure 3.2: A simple model with a moderating effect

Such moderator variables can be metric (e.g. age or income) or categorical (e.g. race, gender or social class) in nature. It could be a single MV or LV, and, moreover, may be observed or unobserved.
The identification and quantification of moderating effects in complex causal structures is possible by means of PLS-PM. The moderating effect in the context of PLS-PM means a moderated relationship within the structural model. This means that we are interested in the moderating effects of the LVs on the direct relationships between the LVs.

Basically, there are two main methods to study moderating effects depending on the nature of the moderator variable:

- *Group Comparisons*. This approach applies when the moderator is an *observed* MV, and it is a qualitative variable or can be categorized. In this case, the sample is split into two or more groups relating to the codes of the qualitative variable and the path coefficient of the moderated relationship is estimated for each of the sub-samples;

- *Moderator Constructs*. This approach applies when the moderator variable is an LV; MVs of a latent moderator variable are *observed* and quantitative. Under this approach, moderator variables are considered in the inner model.

Group Comparisons. Researchers are often interested in comparing PLS path models across two or more groups of data to see whether different parameter estimates occur for each group. For example, a researcher may aim at finding out whether the path coefficients in a PLS path model differ significantly across observations. Different groups of observations represent a special case in term of moderating effects in that they hae the grouping variable as a categorical moderator variable. In this case, there is a categorical moderator variable that splits the data set into two or more groups and thus requires the estimation of two separate models. Usually, such a (categorical) moderator variable captures some observable trait of the respondents such as their gender (male vs. female) and is known a priori. Path coefficients based on different samples are almost always different (in a mathematical sense), but the question is whether these differences are statistically significant. An example to show how a categorical variable can split the data into groups is given by Russet [133], with the aim of measuring a Political Instability CI.The basic hypothesis in Russet' s paper is that economic inequality leads to political instability. In particular, in the Russet model political instability is a function of inequality of land distribution and of industrial development. This dataset has already been analyzed in Gifi [48] and in Tenenhaus [164]. In particular, Tenenhaus had modeled the Russet dataset in a PLS-PM framework, creating three reflective blocks of

LVs. The first LV is "Agricultural Inequality" , the second is "Industrial Development" and the third is "Political Instability". All MVs are numeric. The model supposes a positive relationship between "Agricultural Inequality" and "Political Instability", while it considers as negative the impact of "Industrial Development" on the "Political instability". In the original dataset another qualitative variable is measured: it is the EI Democracy that classifies countries in three groups: stable democracy, unstable democracy and dictatorship. This MV is introduced in the block of Political Instability, in order to evaluate the impact of its modality in the determination of the LV. In this way it is possible to use qualitative information to estimate the CI Political Instability. The introduction of the qualitative MV not only causes an improvement in the quality of the model, and so of the estimation of the CI, but also gives more information for the interpretation of the results obtained. It has highlighted the political instability of the countries: for example some countries have two different scores in the model with and without democracy.

To find out whether there is a significant difference between coefficients, researchers need to run a PLS-SEM multi-group PLS-MGA analysis with a parametric approach [82]. Hence, more comprehensive approaches for PLS-MGA have been introduced by Chin and Dibbern [18], Henseler et al. [64] and Sarstedt et al. citeart:rif.93, who propose non-parametric procedures to execute PLS-MGA. Parallel with the concept of an F test in regression, Sarstedt et al.[149] outlined a technique to compare more than two groups. In R software resampling methods have been developed to test the difference between groups [145]: the bootstrap t-test and permutation procedure. The bootstrap $t-test$ consists of separating the data into groups and then running bootstrap samples with replacement for each group. Path coefficients are calculated in each resampling and the standard error estimates are treated in a parametric sense via a $t-test$. This method is a resampling parametric approach. The bootstrap t-test supposes two groups G_1 and G_2 with sample sizes of n_1 and n_2, respectively. It is possible to compare path coefficients or other parameters (outer weights, loadings, R^2, the GoF index). If we want to compare path coefficients between both groups: $\beta_j^{G_1}$ against $\beta_j^{G_2}$, the steps are the following:

- Calculate a PLS path model for each group to obtain path coefficients: $\beta_j^{G_1}$ and $\beta_j^{G_2}$;

- Separate the data into groups and run bootstrap samples for each group;

- For each sample, calculate a PLS path model to obtain resampling path coefficients;

- After running all the resamples (say 200 times), calculate the standard error estimates;

- Use the standard error estimates in a parametric sense via a $t - test$.

  The bootstrap procedure still depends on the assumptions of a $t-test$ which relies on two major conditions: a normal distribution of data and a similar sample size of the groups.

It is true that t procedures are useful in practice because they are robust. However, when the data have less symmetric distributions and the size of the groups is very different, the application of the bootstrap t-test will be limited. Another type of resampling approach is based on randomization or permutation procedures. Compared to bootstrap samples (which are drawn with replacement), permutation resamples are drawn without replacement. The permutation test assumes that it is possible that all of the groups are equivalent, and that every member of the group is the same as before the sampling began. Suppose we have two groups G_1 and G_2 with path coefficients $\beta_j^{G_1}$ and $\beta_j^{G_2}$ and sample sizes of n_1 and n_2, respectively. The permutation test is designed to determine whether the observed difference between the path coefficients is large enough to reject the null hypothesis H_0 that the two groups can be considered identical. The steps are the following:

- First, we calculate the test statistic for the data. In our case the test statistic is the difference between the path coefficients of the two - groups.

- Then we combine the observations of groups G_1 and G_2 into a single large group.

- Next, the data are permuted (divided or rearranged) repeatedly in a manner consistent with the random assignment procedure. Each permutation implies dividing the data into two groups of size n_1 and n_2; estimating the PLS models for each group; and calculating and recording the test statistic. The set of calculated differences is the distribution of possible differences under the null hypothesis that the group label does not matter.

- Next, we sort the recorded differences and we check if the original test statistic is contained within say the middle 95% of the sorted values. If it is not, we reject the null hypothesis of identical groups at the 5% significance level.

The main attraction of the permutation procedure is that it is a distribution free test that requires no parametric assumptions: it does not require specific population shapes such as Normality; it applies to a variety of statistics; and it can give very accurate *p-values*, regardless of the shape and size of the population.

Moderator Constructs. When the moderator variables are considered in the inner model, the moderating effects are treated as LVs. In the case of quantitative moderator variables, the product of two variables is used to represent the interaction effect [62]. For a structural model, the regression equation would have the following form:

$$\xi_j = \beta_0 + \beta_1 \xi_q + \beta_2 \mu + \beta_3 \xi_q \mu + \epsilon \tag{3.2}$$

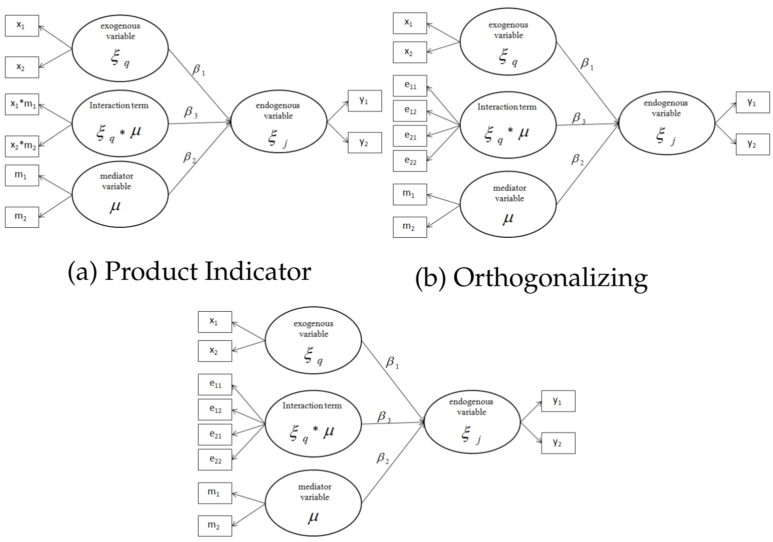
Here, ξ_j is the endogenous variable that will be explained by the exogenous variable ξ_q, the moderator variable μ, and the interaction of the two. The β_s represent the regression parameters, where β_0 stands for the constant. The unexplained variance is captured by the error term ϵ. Note that ξ_j, ξ_q and μ are LVs, and thus are supposed to be measured with error. The previous equation can be rearranged into a different form, representing a regression of ξ_j on ξ_q having the constant as well as the slope of the exogenous variable ξ_q depending on the level of the latent moderator variable μ:

$$\xi_j = (\beta_0 + \beta_2\mu) + (\beta_1 + \beta_3\mu)\xi_q + \epsilon \tag{3.3}$$

This form provides an intuitive appeal for the interpretation of interaction effects: An increase in the moderator variable μ of 1 implies a change of the effect of ξ_q on ξ_j by β_3. For instance, if μ is standardized and increased from 0 to 1, the slope of ξ_q changes from β_1 to $\beta_1 + \beta_3$. In the literature related to PLS path modeling, many approaches for the analysis of interaction effects between variables have so far been presented. The most important are:

- the Product Indicator Approach [170];
- the Two-Stage Path Modeling Approach [63];
- the Orthogonalizing Approach [92].

They are graphically represented in the Figure 3.3.



(a) Product Indicator (b) Orthogonalizing

(c) Two Stage

Figure 3.3: Approaches for Modeling Interaction

Chin et al. [170] were the first to transfer the Product Indicator Approach to PLS path modeling. First, they introduced a new LV, the latent interaction term. Further, they suggested creating the so-called product indicators p_{ij};

that is, all possible pairwise products of the centred indicators of the exogenous variable (x_i) and of the moderator variable (m_j). The product indicators p_{ij} become the indicators of the latent interaction term. If the exogenous LV ξ_q has I indicators and the latent moderator variable μ has J indicators, then the latent interaction variable will have $I * J$ product indicators (Figure 3.3 (a)). Note that Chin et al. recommended using the *centred* original indicators to produce the product indicators. Although such a practice does not necessarily diminish the multi-collinearity resulting from building the product, it does facilitate the interpretation of the interaction model results. In this approach both the LVs (ξ_q, μ_j) have a *reflective* measurement model.
When the exogenous LV or the moderator variable has a formative measurement model, the product indicator approach cannot be applied. Instead, researchers should use the two-stage approach [116] that extends the product indicator approach to formative measures by making explicit use of PLS-SEM's advantage in estimating the LV.
The Two Stages are as follows:

- Stage 1: The main effects model is estimated without the interaction term to obtain the scores of the LVs. These are saved for further analysis in the second stage.

- Stage 2: The LV scores of the exogenous LV and moderator variable from Stage 1 are multiplied to create a single-item measure used to measure the interaction term. All other LVs are represented by means of single items of their LV scores from Stage 1.

The Two-Stage Approach (Figure 3.3 (c)) is not restricted to models that include formative measurement approaches but can also be used when all constructs are measured by reflective indicators. Henseler and Chin's simulation study on the use of these alternative approaches in PLS-PM [62] shows that the product indicator approach performs favorably when the parameter accuracy is a major issue of concern. Thus, it is the best choice for hypothesis testing. When prediction represents the major or only purpose of an analysis, however, researchers should use the two-stage approach.

Little et al. [93] suggested an Orthogonalizing Approach for modeling interactions among LVs (Figure 3.3 (b)). The underlying idea of residual centring is that,*(ideally), an interaction term is uncorrelated with (orthogonal to) its First-Order effect terms*. They introduced a modification to the product indicator approach. As in the latter case, product indicators are first created as element-wise products of the indicators of the independent and the moderator variables. Each of the preliminary product indicators is then regressed on all indicators of the exogenous and the moderator variable. The residuals of these regressions (e_{ij}) are then used as indicators of the interaction term, in analogy with the product indicator approach. This way, it is ensured that the indicators of the interaction term do not share any variance with any of the indicators of the exogenous or the moderator variable. From the fact that PLS calculates the LV scores as linear combinations of the respective indicators, it can be derived that the interaction term is orthogonal to its constituting LVs.
Researchers have proposed many other PLS-based approaches for modeling interaction and non-linear terms, but Henseler and Chin [62] comparing approaches for modeling interactions in terms of point estimate accuracy, statistical power, and prediction accuracy, concluded that the orthogonalizing approach is to be recommended in almost all circumstances.

3.4 An Example: Building an Italian Social Cohesion Composite Indicator (SC-CI)

To illustrate the importance of mediation and quantification in PLS-PM, we will examine a Social Indicator (the Social Cohesion CI), based on Higher-Order Construct [1], in which we will analyze the dimensions, the mediating relationships between the dimensions and the nature of the EI and CIs.

[1]The Higher-Order Construct in PLS-PM is described in detail in the fourth Chapter

3.4.1 A brief history of Social Cohesion

Social cohesion is a term used in sociology and political science *to describe the links, or "glue", that bring people together in society. Social Cohesion is a multi-faceted notion covering many different kinds of social phenomenon.*

The social cohesion concept has been the subject of discussion both in politics and in the academic context. In contrast to the political field, in which there is the tendency to identify social cohesion with the social problems that the various governments are facing, in the academic field, there is no homogenous discussion about this topic. To measure social cohesion five different dimensions are usually considered in literature [97]:

1. Material conditions are fundamental to social cohesion, particularly employment, income, health, education and housing;

2. Social order, safety, freedom and tolerance for other people;

3. Social relationships, networks and interactions between individuals and communities;

4. The extent of social inclusion or the integration of people into the mainstream institutions of civil society. This dimension also includes people's sense of belonging to a country or community;

5. Social equality referring to the level of fairness or disparity in the access to opportunities or material circumstances, such as to income, health, quality of life, or future life chances.

Bernard [89] completes the proposal of Jenson by introducing the essential dimension of equality/inequality with regard to social justice and equity in the economic domain. He considers Social Cohesion as a dialectic balance between three values: freedom, equality and solidarity. These three elements are related and at the same time stand in contradiction. According to this theory a model is derived to compute the Social Cohesion CI ([29]), that is applied to the fourth wave of the European Values Study (EVS) [2]of 2008

[2]The first wave of the survey was launched in 1981 in ten European countries. To explore the dynamics of value changes, a second wave of surveys was launched in 1990 in all

conducted in 47 countries, The authors have estimated the Social Cohesion CI only for the citizens of Luxembourg. The model is a Second-Order hierarchical Structural Equation Modeling, estimated according to the covariance approach: LISREL [78]. The CI is determined by the concepts of trust, political interest, political participation and involvement in organizations and social relationships. In this model only the impact of each LV on Social Cohesion is measured, omitting the relationships between the other LVs.

3.4.2 The Social Cohesion Path Modeling Estimation

Starting from Bernard's theory and from the existing model for the estimation of this CI, we propose a new model to compute Social Cohesion (SC), in which not only the impact on SC is considered but also the relationships between the other LVs. We have used the same database as the EVS survey, but the model is estimated only for Italy in order to evaluate the social cohesion of our country.

The sample is constituted by 1,519 Italian adults (aged 18 years and over). This database contains a great number of subjective and objective items that measure attitudes towards and behavior regarding social relations, participation, and trust at many levels of social reality as well as in many domains of everyday life, which more or less correspond to the dimensions of social cohesion in the literature.

With regard to the proposal of Dickes et al., two new LVs are introduced representing the economic-social condition, the impact of which on all LVs of the model is estimated, and Italian Sentiment.

European countries, including Switzerland, Austria and countries in Central and Eastern Europe, as well as the US and Canada. About ten years later (1999/2000), the third EVS survey was launched, the fieldwork being conducted in almost all European countries. The fourth wave was launched in 2008 (www.europeanvaluesstudy.eu).

3.4.3 The model

The LVs considered in the model are:

- with the role of *mediator* LV: *Economic Status* (the MVs are nominal and ordinal);

- with the role of *input* (*exogenous* LVs): *Participation* (the MVs are all ordinals with 5 levels); *Solidarity* (all MVs are ordinal with 5 levels); and the *Institutional trust* (all MVs are ordinal with 5 levels);

- with the role of *output* (or *target* or *endogenous LV*): the multi-block *Social Cohesion* (the MVs are all the other LVs);

- with the role of *outcome*: *Italian Sentiment* (its MVs are ordinal and expressed on 5 levels).

The LVs Participation, Solidarity and Institutional Trust are multi-blocks, i.e. they are determined by other LVs. In particular, Participation is estimated by two LVs (Participation in Legal and in Illegal Associations), Solidarity by two LVs (Proximal and Distal Solidarity) and Institutional Trust by two LVs (Trust in National and Organizational Institutions). The MVs are expressed on an ordinal scale with different levels. The major contributions of this example are the following:

- the use of a Higher-Order Construct Model;

- the use of nominal and ordinal elementary indicators for the construction of a CI with a suitable quantification;

- the use of some Mediating LVs.

In Table 3.1 the MVs are reported, highlighting their nature (nominal, ordinal or numerical) for each LV.

LVs (CIs)	**MVs (basic indicators)**	**Nature of MVs**
Economic status (ECS)	Annual householder income	Ordinal, 12 levels
	Educational level	Ordinal, 7 levels
Participation in legal activities (LEG)	Signing a petition	Ordinal, 3 levels
	Joining in boycotts	Ordinal, 3 levels
	Attending lawful demonstrations	Ordinal, 3 levels
Participation in illegal activities (ILLEG)	Joining in boycotts	Ordinal, 3 levels
	Attending lawful demonstrations	Ordinal, 3 levels
Participation (PART)	All the MVs of the Participation	
Trust in National Institutions (NAT)	Education system	Ordinal, 4 levels
	Social security system	Ordinal, 4 levels
	Health care system	Ordinal, 4 levels
	Justice system	Ordinal, 4 levels
Trust in Organizational Institutions (ORG)	Trade unions	Ordinal, 4 levels
	Press	Ordinal, 4 levels
	Parliament	Ordinal, 4 levels
	Civil service	Ordinal, 4 levels
Institutional Trust (ISTT)	All the MVs of the Trust in Institutions	
Proximal solidarity (PROX)	Immediate family	Ordinal, 5 levels
	People - neighborhood	Ordinal, 5 levels
	People - own region	Ordinal, 5 levels
	Fellow countrymen	Ordinal, 5 levels
Solidarity Distal (DISTAL)	Elderly people	Ordinal, 5 levels
	Unemployed people	Ordinal, 5 levels
	Immigrants	Ordinal, 5 levels
	Sick and disabled	Ordinal, 5 levels
	Poor children	Ordinal, 5 levels
Solidarity (SOL)	All the MVs of the Solidarity	
Social Cohesion (SC)	All the MVs of Interpersonal and Institutional trust	
Italian Sentiment (ITA)	Important to be born in Italy	Ordinal, 4 levels
	Important to respect political institutions and laws	Ordinal, 4 levels
	Important to have ancestry	Ordinal, 4 levels
	Important to be able to speak Italian	Ordinal, 4 levels
	Important to have lived in Italy for a long time	Ordinal, 4 levels

Table 3.1: LVs and MVs of the Social Cohesion model

So, SC is here conceived as a third order latent construct affecting Second-Order dimensions, which in turn shape First-Order LVs underlying specific aspects of the Second-Order dimensions.
The study focuses on a reflective-formative measurement model, a model resulting from the combination of reflective Lower-Order and formative Higher-Order Constructs.
Sanchez's 'plspm' package in the R programming language [142], with Russolillo's quantification [135] was used in order to estimate the model.
The model is presented in Figure 3.4.

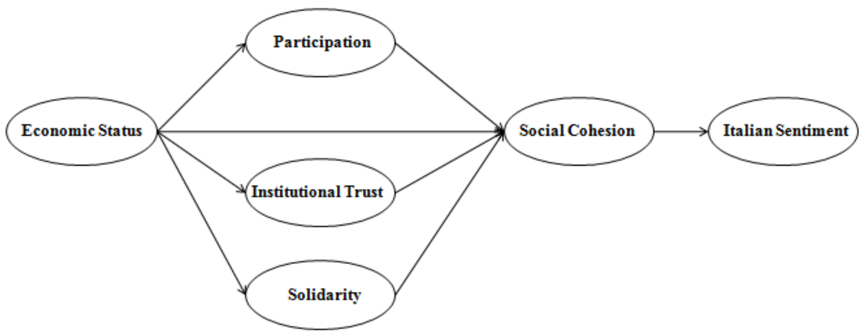


Figure 3.4: The model for the Social Cohesion Composite Indicator

In the following section, we present three estimated models:

- the estimated model without the use of mediating LVs and quantification;
- the estimated model with the use of mediating LVs but no quantification;
- the last completed estimated model with the use of mediating LVs and quantification.

3.4.4 Statistical Analysis and Main Results

The first important result is the confirmation of the unidimensionality property for each latent block.
In this case all the blocks are unidimensional, as it is possible to verify from Table 3.2 in which the values of Cronbach's Alpha and Dillon-Goldstein's

Table 3.2: The outer estimation of the model

LV	Cronbach	Dillon-Goldstein	First eigenvalue	Second eigenvalue
ECS	0.778	0.793	1.31	0.686
LEG	0.741	0.848	1.47	0.529
ILLEG	0.703	0.871	2.16	0.702
PART	0.713	0.823	1.54	0.457
PROX	0.810	0.888	2.18	0.573
DISTAL	0.859	0.905	2.82	0.519
SOL	0.847	0.884	3.67	1.347
NAT	0.759	0.787	1.30	0.702
ORG	0.762	0.816	1.79	0.670
ISTT	0.762	0.816	1.79	0.670
SC	0.732	0.761	4.02	1.724
ITA	0.583	0.842	1.71	0.928

Rho are reported (the values of Dillon-Goldstein' Rho are greater than 0.7, and the first eigenvalues are greater than 1 for all LVs).
This result shows that the outer model is well specified and that the LVs are well measured by the MVs, their synthesis being good.

Table 3.3 reports communality, an index that measures the goodness of the models of measurement, for each considered model.

Table 3.3: Communality index for latent blocks for each estimated model

LV	Non-Mediating Non-Quantification	Mediating Non-Quantification	Mediating Quantification
ECS	0.755	0.754	0.757
PART	0.639	0.638	0.644
SOL	0.623	0.624	0.625
ISTT	0.510	0.578	0.575
SC	0.370	0.372	0.473
ITA	0.461	0.348	0.357

The values for communality are appreciably higher for all blocks except for the construct SC that is much lower than the commonly accepted threshold of 0.7. However, if we consider the completed model with the use of the mediating LVs and quantification, the communality of the SC block increases. Table 3.4 reports the path coefficients linking the constructs to the SC-CI.

Table 3.4: Path coefficients for each model

	No mediating No quantification	Mediating No quantification	Mediating Quantification
ECS $\rightarrow$ PART		0.243 [0.185;0.298]	0.261 [0.213;0.321]
ECS $\rightarrow$ ISTT		0.121 [-0.121;0.177]	0.148 [0.098;0.217]
ECS $\rightarrow$ SOL		-0.052 [-0.113;0.065]	0.178 [0.150;0.305]
ECS $\rightarrow$ SC	0.287 [0.254;0.315]	0.254 [0.217;0.281]	0.259 [0.219;0.305]
PART $\rightarrow$SC	0.382 [0.348;0.522]	0.430 [0.371;0.496]	0.440 [0.380;0.494]
SOL $\rightarrow$ SC	0.416 [0.376;0.548]	0.528 [0.472;0.686]	0.610 [0.593;0.669]
ISTT $\rightarrow$ SC	0.353 [0.320;0.395]	0.306 [0.262;0.441]	0.404 [0.367;0.453]
SC $\rightarrow$ ITA	-0.148 [-0.210;-0.110]	-0.195 [-0.257;-0.220]	0.420 [0.364;0.480]

Without considering the quantification, the mediating effect improves the estimation of the model.

If we look at the completed model with the mediating effect and quantification, the estimation greatly improves, making some path coefficients significant that previously were not. In order to measure SC, Solidarity is the most important dimension, with a good impact of 0.61, followed by Participation (0.44) and Institutional Trust (0.40); this shows that to have a cohesive society Solidarity is important as indeed is Trust in Institution. Economic Status proves to be less influential among all facets with an impact of 0.26. This is not very important and not instrumental to the creation of SC. The outcome of the model is Italian Sentiment: this variable is considered a result of SC, and, as a matter of fact, SC has a good impact on it (0.42); this path in previous models proves to be negative. In the last estimated model, with mediating effects and quantification, all the path coefficients are significant, having positive Bootstrap confidential intervals.

The results of the inner estimation and of the impact of the CIs on SC are reported in Figure 3.5:

In Figure 3.5, the average values for each LV are also reported; the scale is

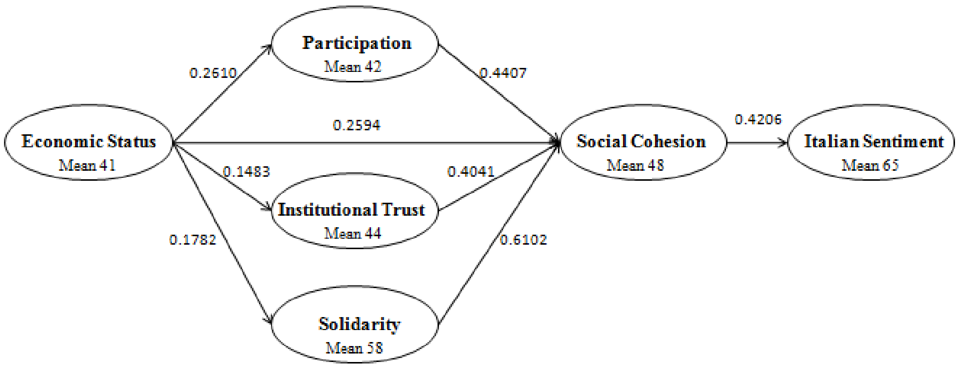


Figure 3.5: The estimated model for the Social Cohesion Composite Indicator

transformed in order to obtain a range between 0 and 100, so Solidarity has a high average (greater than 50) showing a good SC for the Italian people. At the same time Italian individuals prove to have a good Italian Sentiment, as a result of a strong SC.
In order to test the significance of the indirect effect, we calculate the VAF index, according to the Formula (3.1), that determines the size of the indirect effect in relation to the total effect.

- VAF(Participation)=0.30719
- VAF(Institutional Trust)=0.187558
- VAF (Solidarity)=0.295391

In this situation, the VAFs of Institutional Trust and Solidarity are less than 20%, so we can conclude that no mediation takes place; instead Participation, in which the VAF is larger than 20% and less than 80% is characterized as a partial mediation.

3.4.5 Conclusions for Italian Social Cohesion Composite Indicator Example

The example presents three estimated models (the estimated model without the use of mediating LVs and quantification, the estimated model with the use of mediating LVs but no quantification and the last completed estimated model with the use of mediating LVs and quantification) in order to understand how researchers can, by using a suitable quantification and entering the effect of mediation into the model, significantly improve the estimate of the Composite Indicator.

3.5 Unobserved Heterogeneity in PLS-PM

Heterogeneity among units is an important issue in statistical analysis. Treating the sample as homogeneous, when it is not, may seriously affect the quality of the results and lead to a biased interpretation. Since human behaviors are complex, looking for groups or classes of units having similar behaviors will be particularly hard [38].

Because heterogeneity is often present in empirical research, researchers should always consider potential sources of heterogeneity, for example, by forming groups of data based on observable characteristics such as demographics (e.g. age or gender). When heterogeneous data structures can be traced back to observable characteristics, we refer to this situation as observed heterogeneity. Unfortunately, the sources of heterogeneity in data can never be fully known a priori. Consequently, situations arise in which differences related to unobserved heterogeneity prevent the PLS path model from being accurately estimated. Since researchers never know if unobserved heterogeneity is causing estimation problems, they need to apply complementary techniques for response-based segmentation (so-called *latent class techniques*) that allow for the identification and treatment of unobserved heterogeneity.

Heterogeneity can hardly be detected using external information, (i.e. using an *a priori* clustering approach, especially in social, economic and marketing areas). Moreover, in several application fields more attention is being given to clustering methods able to detect groups that are homogeneous in terms of their responses [176]. Two types of heterogeneity could be affecting the data: observed and unobserved heterogeneity ([167]; [63]; [17]). Traditionally, heterogeneity in an SEM is taken into account by assuming that observations can be assigned to segments a priori, on the basis of observable characteristics such as geographical or demographic traits [177]. Alternatively, sequential procedures have been proposed in which a researcher can partition the sample into segments by applying a clustering algorithm such as k-means on manifest or LV scores. However, different clustering algorithms yield different results, and, to date, there has been little guidance on choosing the best procedure [72].

Usually heterogeneity in SEMs is handled by first forming classes on the basis of external variables or on the basis of standard clustering techniques applied to MVs and/or LVs, and then by using the multi-group analysis introduced by Jöreskog [75] and Sörbom [157]. However, heterogeneity in the models may not be necessarily captured by well-known observed variables playing the role of moderating variables [54]. Moreover, post-hoc clustering techniques on MVs, or on LV scores, does not take into any account the model itself. Hence, while the local models obtained by cluster analysis on the LV scores will lead to differences in the group averages of the LVs but not necessarily to different models, the same method performed on the MVs is unlikely to lead to different and well-separated models. This is true for both the model parameters and the means of the LV scores. In addition, a priori unit clustering in SEM is not conceptually acceptable since no structural relationship among the variables is postulated: when information concerning the relationships among variables is available, classes should be looked for while taking into account this important piece of information.

Empirical studies and numerical experiments show that these "sequential" procedures – exploratory clustering followed by multiple group analysis – are not robust and perform poorly in terms of parameter recovery [149]. Therefore, if researchers do not have an a priori rationale for distinguishing subgroups within a population, then latent class approaches, which allow for the identification and treatment of unobserved heterogeneity, seem to be a better choice. However, researchers may certainly be interested in differences between sub-groups defined a priori, so there is certainly a place for a priori multiple group analysis in PLS-PM [126].

The availability of tools for dealing with heterogeneous data within PLS-PM has grown rapidly, with many new developments appearing only in

specialized literature devoted to PLS methods [126]. Several latent class techniques, designed to capture and treat unobserved heterogeneity in PLS path models, have been proposed lately and reviewed by Sarstedt [147]: Finite Mixture PLS, proposed by Hahn et al. [54] and modified by Ringle et al. [131]; PLS Typological Path Model presented by Squillacciotti [158] and modified by Trinchera and Esposito Vinzi [169] and Trinchera et al. [171]; PATHMOX by Sanchez and Aluja [143]; PLS-PM based Clustering (PLS-PMC) by Ringle and Schlittgen [127]; and Response Based Unit Segmentation in PLS-PM (REBUS-PLS) proposed by Trinchera [168] and Esposito Vinzi et al. [39].
The Figure 3.6 shows the available latent class approaches for capturing heterogeneity in PLS-PM.

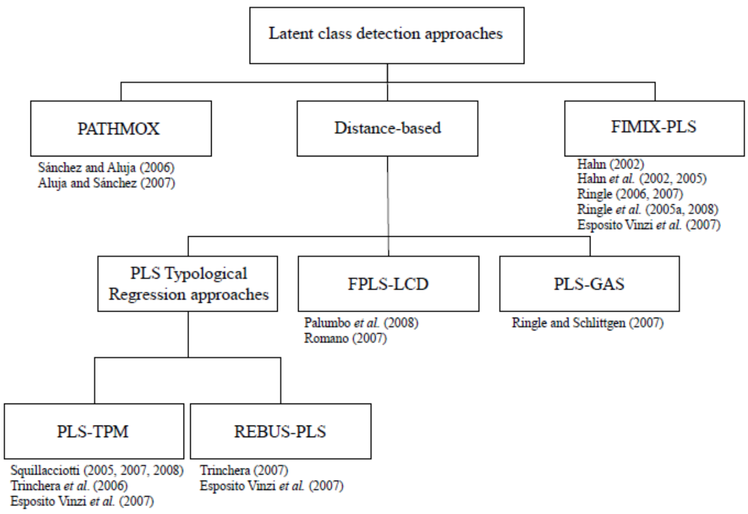


Figure 3.6: Methodological taxonomy of latent class approaches to capture unobserved heterogeneity in PLS path models

In the following sections the PATHMOX and REBUS-PLS approaches are discussed in detail.

3.5.1 The PATHMOX Approach

In the context of PLS-PM, Sanchez and Aluja [143] introduced a decision tree–like structure approach in which segments are represented by the outer

nodes of a segmentation tree. It represented a new point of view in observing heterogeneity in PLS-PM models.
Their *Path Modeling Segmentation Tree (PATHMOX)* algorithm had been specifically designed to take into account external information, such as demographic variables, whose values are used to identify and differentiate segments, thus enhancing segment profiling. The idea is to build a path models tree having a decision tree-like structure with models for different segments in each of its nodes. The segment identification not only takes into account the available a prior information, in the form of external variables (such as socio-demographic variables), but also considers the structural relationships between the variables. The iterative process starts with the estimation of a global PLS path model, taking the entire sample into account. Using the external variables, PATHMOX makes two-way splits and estimates the PLS model for each sub-group thus defined. Just as a decision tree seeks to maximally discriminate, PATHMOX looks for the largest differences between sub-groups in terms of the model parameter estimates [168]. Among all possible splits, the best model is selected by means of a modified F-test for comparing regression models. The partition resulting with the most significant p-value is considered as a candidate for the best split. This process is applied for each external explicative variable selecting the partition with the minimum p-value among all the candidates as the optimal split. Subsequently, a Ryan-Joiner [136] correlation test is initiated to compare each identified segment and its parent model. The Ryan-Joiner test is an objective way of judging normal probability plots used for testing normality on a set of data. In other words, this test is used to measure the straightness of a probability plot. By using a Ryan-Joiner test we do not pretend that we are performing any normality test; instead, we use it as a tool for assessing how close to unity the correlations between the LVs in the parent node and the LVs in the child node are. It may be argued that this test is being misused the way it is applied in the PATHMOX algorithm, but, in fact, we are using it as a first (although primitive) tool for outer models comparison. After an optimal first split has been chosen, the algorithm then looks for further splits of those initial sub-groups that again maximize differences in the parameter estimates within the sub-groups.

Finally, the stop rule evaluates two conditions: (i) a fixed number of individuals in a node, and/or (ii) the p-value significance level. The first condition is used to avoid the presence of small size segments which are not useful in practice. The second criterion avoids the identification of segments with low significance levels.
Once a PATHMOX tree has been constructed and the final nodes have been obtained, it is necessary to identify the differences among segments. Since the PATHMOX approach is based on the inner structural model, we focus only on the path coefficients. This implies comparing the path coefficients of the different segments. Sanchez proposes the use of bootstrapping to validate the results of the final segments. The bootstrap samples are built by resampling with replacement from the original sample. The samples consist of the same number of units as in the original sample, and the number of resamples is fixed to 100. Moreover, bootstrap confidence intervals of the path coefficients can be obtained from the resampling procedure. Hence, confidence intervals allow an identification of those coefficients in a segment that may be different to the rest of the segments. With this information, we can identify those structural relationships in which some path models differ from the other segments [141].
The aim of the PATHMOX algorithm is to select, among a set of segmentation variables (i.e. observed sources of heterogeneity), those having superior discriminant capacity in the sense that they separate the path models as much as possible. The split criterion in this case is used to decide whether two confronted structural models can be considered to be different. For this purpose, the F-global test comparison method is introduced. Sanchez [141] proposed the F-global test as a criterion for comparing two different PLS path models by extending the test for comparing two linear regressions introduced by Lebart et al. [91]. This test focuses on the relationships between the path coefficients of the structural model, and it is based on the consideration that comparing two structural models can be framed in terms of comparing two regression models. Structural models are in fact nothing more than a set of regressions among LVs, one regression for each endogenous variable. The F-global test comparison is based on the global model comparison at the structural level. Each binary split defines a pair of nodes,

each of which will have its associated structural model, (i.e. its associated set of path coefficients). Then, we perform a global comparison test on the identity of the two models, meaning that the sets of path coefficients in the two child nodes are equal to those of the parent node. The model of the parent node corresponds to a homogeneous situation, and the model of the child nodes corresponds to a heterogeneous situation. To achieve that objective, Sanchez [141] adapted the identity test of two regression models by Lebart et al. [91] and Chow [21], and used it to detect the most significant split.

PATHMOX thus requires additional external data [168], and depends on the heterogeneity within the sample conforming to straightforward differences in the values of those external variables [126].

Several problems arise when applying the PATHMOX algorithm. In order to produce distinct segments based on the modalities of explanatory variables, the algorithm tests for the equality of segment-specific coefficients of the structural and measurement models. These tests rest on the assumption of normally distributed error terms which may not apply in practice [143]. Furthermore, even though PATHMOX does not rely on predefined segments, the decision tree structure depends on external explanatory variables which need to be specified by the researcher beforehand and which are, as mentioned earlier, often insufficient to capture heterogeneity adequately. A more serious problem is the dependence of the segmentation on the ordering of the explanatory variables. As a consequence, PATHMOX should rather be viewed as a data mining approach which enables the discovery of “unexpected” models in population segments [144].

3.5.2 The REBUS-PLS Approach

A new method for unobserved heterogeneity detection in a PLS-PM framework was presented by Trinchera [168] and Esposito Vinzi et al. [39], as an improvement of PLS-TPM: Rebus-Based Unit Segmentation in PLS-PM (REBUS-PLS), which has been designed to overcome some methodological problems of the PLS-TPM approach [126]. It is a distribution-free approach which allows a classification taking into account heterogeneity in

the structural and the measurement models of endogenous and exogenous LVs. REBUS-PLS is an iterative algorithm that permits to estimation at the same time both of the unit membership to latent classes and of the class specific parameters of the local models. The approach follows a similar procedure to PLS-TPM but applies a different distance measurement. In fact, it is based on the distance measurement, labeled the "Closeness Measure" (CM) between units and models based on residuals. The idea behind the definition of this measurement is that, if latent classes exist, units belonging to the same latent class will have similar local models. Moreover, if a unit is assigned to the correct latent class, its performance in the local model computed for that specific class will be better than the performance of the same unit considered as supplementary in the other local models. Coherent with the PLS-PM features, REBUS-PLS does not require distributional hypotheses. Moreover, REBUS-PLS may lead to local models that are different both in terms of structural and measurement models.
The CM distance is a function of the average communality and average structural R^2 across the whole model. The CM used in the REBUS-PLS algorithm represents an extension of the distance used in PLS-TPM by Trinchera et al. [171], aiming at taking into account both the measurement and the structural models in the clustering procedure. In order to obtain local models that fit better than the global model, the chosen closeness measure is defined according to the structure of the Goodness of Fit (GoF) index, the only available measure of global fit for a PLS Path Model. In accordance with the DmodY distance used in PLS Regression [164] and the distance used by Esposito Vinzi and Lauro [36] in PLS Typological Regression all the computed residuals are weighted by quality indexes: the importance of the residuals increases while the quality index decreases. That is why the communality index and the R^2 values are included in the CM computation [38].
The choice of the CM distance as a criterion for assigning units to classes has two major advantages. First, the unobserved heterogeneity can now be detected in both the measurement and the structural models. If the two models show identical structural coefficients, but differ with respect to one or more outer weights in the exogenous blocks, REBUS-PLS is able to iden-

tify this source of heterogeneity, which might be of major importance in practical applications. Moreover, since the closeness measure is defined according to the structure of the GoF index, the identified local models will show a better prediction performance [38]. The number of classes (K) to be taken into account during the successive iterations and the initial composition of the classes are obtained by performing a hierarchical cluster analysis on the computed residuals (both from the measurement and the structural models). Once the number of classes to consider and the initial composition of the classes have been obtained, a PLS-PM analysis is performed on each formed class and K provisional local models are estimated.

Once stability on the class composition has been reached, the final local models are computed. The class-specific parameters are then compared in order to explain differences among the detected latent classes. Moreover, the quality of the obtained partition can be evaluated through a new index (i.e. the Group Quality Index (GQI)) expressly developed. A permutation test procedure applied on the GQI, can be used to validate the detected latent classes. The GQI is a reformulation of the GoF index in a multi-group optics, and, like the CM used in REBUS-PLS algorithm, it is based on residuals. If local models performing better than the global model are detected, the GQI index will be higher than the GoF value computed for the global model. As a matter of fact, local models performing better than the global model mean working with residuals that are smaller than the one computed for the global model. This directly entails obtaining a higher GQI index than the one obtained for the global model.

REBUS-PLS is limited to reflective measurement models because the measurement residuals come from the simple regressions between each MV in a block and the corresponding LV.

This alternative is included in the *plspm* package [146] for the R open source statistical programming language [126].

3.6 An example: Treating the Heterogeneity of the Legitimacy of Violence Higher-Order CI

The example of an analysis of the concept *Legitimacy of Violence among teenagers* is now presented in order to illustrate the implementation and results of two latent class techniques implemented in PLS-PM described above. The latent concept of Legitimacy of Violence among teenagers is not present in literature; it was constructed ad hoc at a high level of abstraction, built on Higher-Order construct PLS-PM, formed by two dimensions that until now have always been considered and analyzed separately: an aptitude for violence and ambivalent sexism.
This higher construct derives from the data analysis of a study conducted by a research group of the Department of Social Science, investigating the behavior of teenagers in Naples in March and April 2014. Initially, it was believed that the phenomenon of gender violence concerns only adults. Today there are numerous empirical studies that have shown that it is also perpetrated within relationships described as relating to protagonist teenagers. For this reason, a questionnaire was administered to a group of 300 teenagers, aged between 16 and 20 years, attending the last two years of several high schools in Naples, in order to investigate the experiences of young people and the asymmetries between men and women. The questionnaire was also designed to detect if their way of thinking about and experiencing emotional relationships includes a space where there is a possibility of violence ([50];[101]). Several studies have found a direct relationship between violence and sexism ([45];[173];[46];[88]) converging in considering the latter a major cause of gender inequality [103]. Of the participants, 56 percent were women; and 76 percent were aged 17 or 18. Glick and Fiske [49] define "hostile sexism" as a conflicting vision of gender relations, according to which women are perceived as those who seek control over men, both through sexuality, and a feminist ideology. Hostile sexism is composed of beliefs and negative attitudes directed against women, who are seen as undermining the power of men. "Benevolent sexism", conversely, sees women as "pure creatures" who should be protected, supported and idolized by men, in their "natural" roles of mother and wife;

their love is needed to make a man complete. Benevolent sexism consists of sexist attitudes that are offering a stereotypical view of women, although subjectively manifesting themselves as positive.

3.6.1 Measurement Instruments (questionnaires)

A semi-structured questionnaire was used, composed of scalar items, checklists and open-ended questions, useful to investigate the dimensions listed above. Socio-demographic information was requested: gender, age, school, class, father and mother's occupation, and religious and political orientation. In order to measure the attitudes of the participants towards diversity and violence, a CADV scale was administered, in accordance with the version of De Lemus et al. [27]. The CADV questionnaire consisted of 35 items, measuring attitudes towards diversity and violence, operationalized in three dimensions: i) justification of peer violence; ii) sexist beliefs and justification of domestic violence; iii) justification of intolerance and violence against minorities. All CADV items were measured in relation to a Likert Scale with scores ranging from 1 (strongly disagree) to 7 (totally agree). In order to measure the Hostile, Benevolent and Ambivalent Sexism dimensions, the Ambivalent Sexism Inventory for teenagers, in the version of De Lemus et al. [27] was used. The ISA- Adolescents is an adaptation of ASI and consists of 20 items: the first 10 items measure Hostile Sexism and the last 10 Benevolent Sexism. All ISA items were measured in relation to a Likert scale with scores ranging from 1 (strongly disagree) to 6 (totally agree).

3.6.2 The model

We have considered the dimensions of the questionnaire as five logical blocks: three of which refer to the higher concept of *Aptitude for Violence (A-Violence)* (*Justification of Peer Violence (J-Peer Violence)*; *Sexist Beliefs and Justification of Domestic Violence (J-Domestic Violence)*; *Justification of Intolerance and Violence against Minorities (J- Intolerance*), while the other two blocks refer to the higher concept of *Ambivalent Sexism (A-Sexism)* (*Hostile Sexism (H-Sexism)* and *Benevolent Sexism (B-Sexism)*).

Since the three blocks of *Aptitude for Violence* are in a single CADV scale and the two blocks of *Ambivalent Sexism* are in a single ISA scale, our model is reflective at a first Higher-Order, precisely because the two concepts represent a synthesis of the two scales. Next, these two first Higher-Order scales merge to form a single scale of the latent concept of *Legitimacy of Violence (L-Violence)*. Consequently, we have constructed the latent concept *Legitimacy of Violence* with a hierarchical model of a formative third-order. The graphical representation of the third-order *Legitimacy of Violence* construct is reported in Figure 3.7.

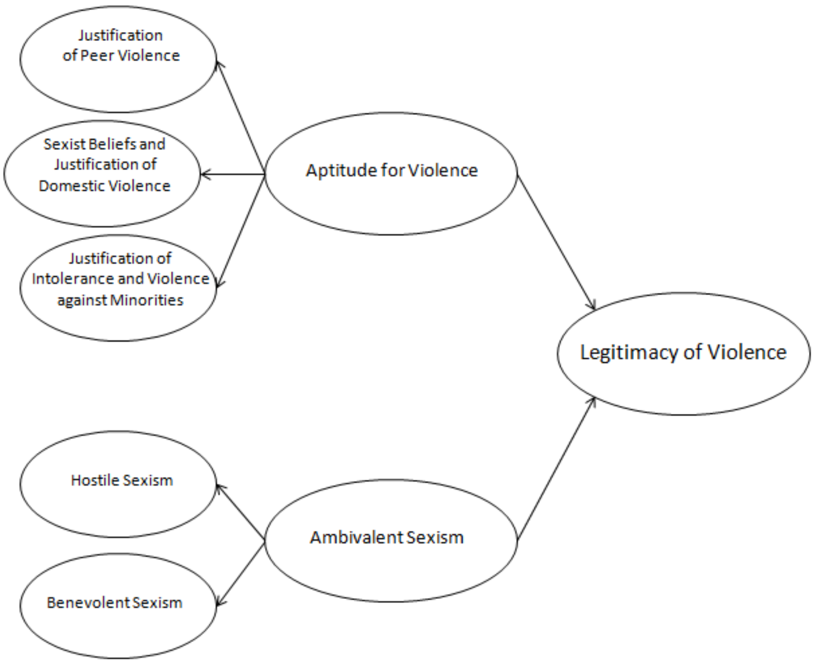


Figure 3.7: The third-order *Legitimacy of Violence* construct

3.6.3 Pre-treatment of data

Before making the PLS-PM analysis, a pre-treatment of the data was performed. First of all, the two scales were normalized with scores from 0 to 100 to make them homogeneous. Since the questionnaire was composed of CADV items in a Likert Scale with a range from 1 to 7, and ISA items in a Likert Scale with a range from 1 to 6, the normalization made comparable the data belonging to the different variables. Next, the variables that had a low average and low correlation with the other variables in the block were eliminated from the analysis. The final database was composed of 50 variables on 300 individuals.

3.6.4 Statistical Analysis and Main Results

The new proposed Mixed Two Step Approach (presented in detail in the fifth chapter of this dissertation) to the estimation of Third-Order LV models has been implemented in order to measure the *Legitimacy of Violence*. The analysis was performed with a path weighting scheme for the inner structural model, while the measurement model is reflective in each block. Table 3.5 reports the main quality measures of each lower-order construct. All Cronbach's Alpha and Dillon-Goldstein's Rho indices are acceptable in each block, close to the conventional acceptability threshold of 0.7 for all blocks. This table shows that the outer model is well specified and that the LVs are well measured by their MVs, their synthesis being effectively performed.

Table 3.5: Reliability measures for Lower-Order Constructs

	MVs	Cronbach Alpha	Dillon Rho	Communality
J-Peer Violence	10	0.783	0.838	0.333
J- Domestic Violence	10	0.739	0.811	0.300
J-Intolerance	10	0.726	0.805	0.319
H-Sexism	10	0.789	0.840	0.324
B-Sexism	10	0.709	0.792	0.282

Concerning the Higher-Order Constructs, Table 3.6 shows the Cronbach's Alpha and Dillon-Goldstein's Rho for the latent concepts *Aptitude for Violence, Ambivalent Sexism* and *Legitimacy of Violence*. Both Second-Order latent constructs and third order latent constructs are unidimensional with a high value on the Cronbach's Alpha and Dillon-Goldstein's Rho scales.

Table 3.6: Reliability measures for Higher-Order Constructs

	Cronbach Alpha	Dillon Rho	Communality
A-Violence	0.764	0.865	0.721
A-Sesixm	0.608	0.848	0.770
L-Violence	0.806	0.872	0.811

Another important index is Communality, that measures the goodness of the model of Measurement (the third column of Table 3.6). The amount of variability of the MVs captured by the higher concepts is sufficiently good, in particular that captured by *Ambivalent Sexism*, that presents a Communality Index higher than the other two higher concepts. In Table 3.7 the structural coefficients, linking the Lower-Order Constructs to the first Higher-Order Constructs *Aptitude for Violence* and *Ambivalent Sexism*, and the structural coefficients, linking the first to the second Higher-Order Construct *Legitimacy of Violence*, are reported.

Table 3.7: Path coefficients

	Path Coefficients
A-Violence → J-Peer Violence	0.826 [0.705;0.951]
A-Violence → J-Domestic Violence	0.922 [0.870;1.010]
A-Violence → J-Intolerance	0.869 [0.788;0.989]
A-Sexism → H-Sexism	1.141 [1.013;1.227]
A-Sexism → B-Sexism	0.662 [0.534;0.925]
A-Violence → L-Violence	0.693 [0.651;0.747]
A-Sexism → L-Violence	0.315 [0.315;0.356]

Looking at Table 3.7, the Second-Order *Aptitude for Violence* Construct is reflected more in the block of *Sexist Beliefs and Justification of Domestic Violence* (0.922), while the Second-Order *Ambivalent Sexism* Construct is reflected more in the *Hostile Sexism* block (1.141), showing even a low correlation path with the *Benevolent Sexism* block (0.662) As regards the third order construct, *Aptitude for Violence*, this has a higher impact (0.693) on *Legitimacy of Violence* than *Ambivalent Sexism* (0.315). The estimated Third-Order *Legitimacy of Violence* construct is graphically presented in Figure 3.8, where the path coefficients and means of each block are reported.

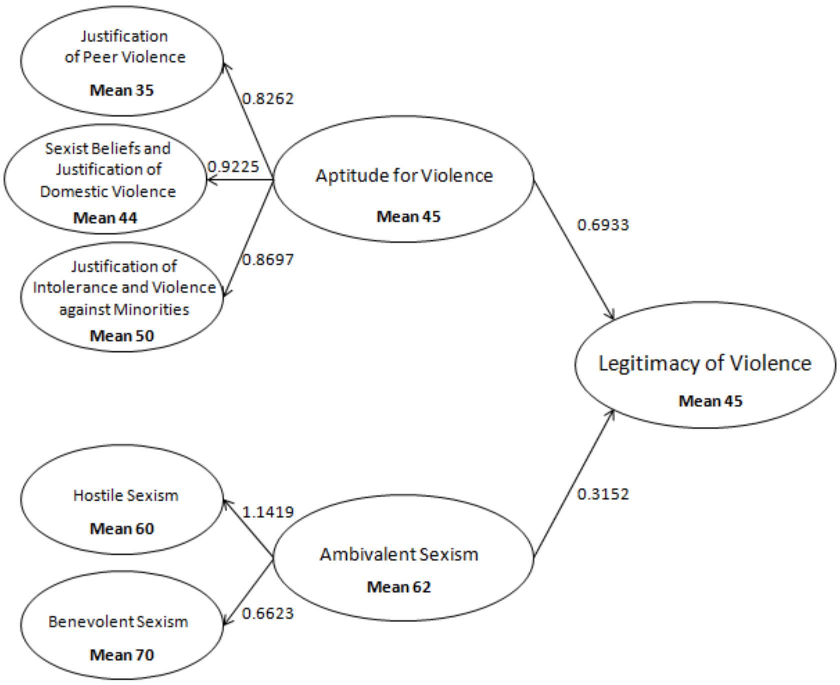


Figure 3.8: The estimated third-order *Legitimacy of Violence* construct

Regarding the Third-Order Construct, *Aptitude for Violence* has a higher impact on *Legitimacy of Violence* than *Ambivalent Sexism*, but this latter block presents a higher mean than the former. This means that, although *Aptitude for Violence* has a high impact on the endogenous construct, having a low average, it represents a critical block, that needs an immediate intervention. Instead, *Ambivalent Sexism*, which has a high mean but a low impact on the latent construct, needs to be addressed, especially by reducing *Hostile Sexism* levels.

3.6.5 Heterogeneity through PATHMOX Approach

In this kind of context we cannot assume that all the students have the same aptitude of Legitimacy to Violence, but we can say that there are groups, or clusters, of students that follow the same model.
The PATHMOX algorithm has been specifically designed to take into account external information, such as demographic variables, whose values are used to identify and differentiate segments, thus enhancing segment profiling. As has been said above, the iterative process starts with the estimation of a global PLS path model, taking the entire sample into account. Using the external variables, PATHMOX makes two-way splits and estimates the PLS model for each sub-group thus defined.
In order to calculate the PATHMOX segmentation tree, it is necessary to specify the scale (i.e., binary, ordinal, or nominal) of the segmentation variables (Table 3.8).

Table 3.8: Codification of segmentation variables according to their type of scale and level

	Scale	**Number Levels**	**Levels Description**
Gender	Binary	2	Male / Female
Age	Ordinal	2	<18 / >=18
School	Nominal	4	I.P.S.S.C.T Fortunato Liceo S.L.S. Mazzini Liceo Classico Pansini I.T.I.S Giordani

In addition, we had to determine the parameters and stop conditions of the algorithm. We decided to establish a value of 0.05 for the threshold of the p-value in looking for those partitions that are highly significant. Given that we have a total sample of 300 students, it seemed to us that 30 students (10% of the total sample) is a reasonable minimum number to stop the growth of a node.
The depth level (depth = 2) was selected with the aim of obtaining a simple segmentation tree with a possible maximum number of four final segments.

Figure 3.9 illustrates the segmentation tree obtained. The main characteristic of the obtained tree is that each node corresponds to a different segment with its own particular path model. The number of students forming each segment is shown inside each node, and the segments in the final nodes are numbered from 4 to 7. In fact, we can observe that there are four distinct models. Additionally, every split is characterized by its corresponding explanatory partition.

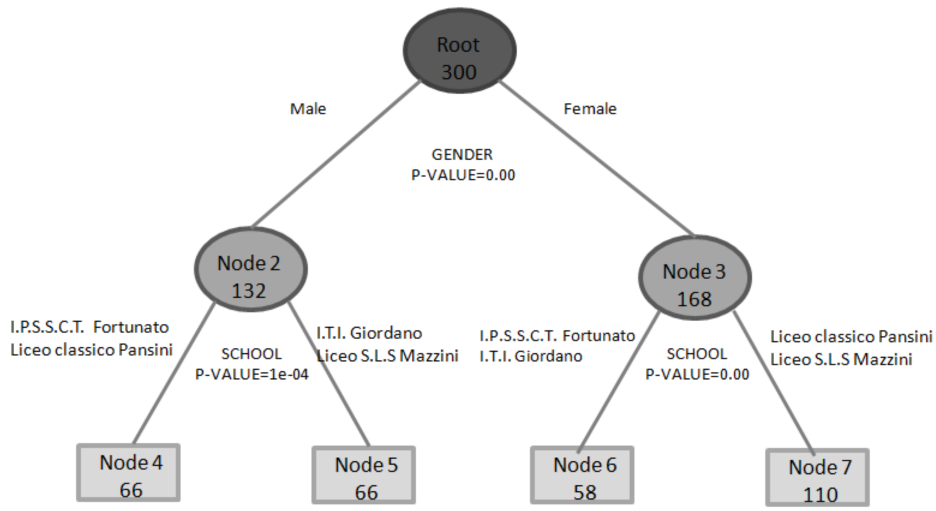


Figure 3.9: PATHMOX Regression Tree

At the first split, PATHMOX defines two different models for students according to gender: male students and female students. As we can see in the Table 3.9, the first split produced is highly significant, giving an F-statistic of 23.08 with a p-value of 0.00. The tree continues by splitting node two and node three. The most significant split for node two is obtained by the segmentation variable School, giving an F-statistic of 4.29 with a p-value of 0.00. This variables splits node three also, with an F-statistic of 8.71 and p-value of 0.00. So, we now divide the male and female students according to the type of school. This ends the splitting process, as the maximum depth of two levels has been reached. Hence, at the end, we have four final segments, each one corresponding to a distinct model: node four, the model of male students who attend I.P.S.S.C.T "Fortunato" and

Liceo Classico "Pansini"; node five, the model of male students who attend Liceo S.L.S. "Mazzini" and I.T.I.S "Giordani"; node six, the model of female students who attend I.P.S.S.C.T "Fortunato" and I.T.I.S "Giordani"; and finally, node seven, the model of female students who attend Liceo Classico "Pansini" and Liceo S.L.S. "Mazzini".
The F-global statistics, the p-values and the obtained partitions for each node are summarized in Table 3.9.

Table 3.9: F-global values and partitions - Least Squares Method

		F-statistic	p-value
Root	Gender	23.08402	0.000000
	Age	5.951494	0.000001
	School	4.437927	0.000066
Node 2	School	4.29068	0.000114
Node 3	School	8.715006	0.000000

However, unbalanced segments and differences in the variance of the endogenous constructs may affect the sensitivity of the F-statistic.
The final part of the analysis consists of the comparison between the terminal nodes of the tree. The coefficients calculated with the p-values associated with each coefficient for each node are shown in Table 3.10.
From Table 3.10 we can see some differences between the global model and the identified segments according to the three endogenous constructs. Male students have high values for the three blocks of Aptitude for Violence, giving much importance to Sexist Beliefs and Justification of Domestic Violence; female students are influenced mainly by the endogenous construct of Ambivalent Sexism, in particular, Hostile Sexism influences female students attending the professional institutes, while Ambivalent Sexism influences female students attending the lyceum.

Table 3.10: Coefficients estimate computed for each terminal node

	Root	Node 4	Node 5	Node 6	Node 7
A-Violence $\rightarrow$ J-Peer Violence	0.841	0.884	0.829	0.829	0.786
St.Error	0.015	0.024	0.034	0.050	0.034
A-Violence $\rightarrow$ J-Domestic Violence	0.908	0.947	0.905	0.822	0.866
St.Error	0.009	0.009	0.024	0.040	0.021
A-Violence $\rightarrow$ J-Intolerance	0.798	0.844	0.871	0.712	0.780
St.Error	0.022	0.036	0.023	0.061	0.040
A-Sexism $\rightarrow$ H-Sexism	0.889	0.889	0.892	0.896	0.889
St.Error	0.009	0.023	0.023	0.015	0.017
A-Sexism $\rightarrow$ B-Sexism	0.865	0.854	0.854	0.880	0.867
St.Error	0.013	0.040	0.045	0.030	0.029
A-Violence $\rightarrow$ L-Violence	0.569	0.572	0.568	0.568	0.589
St.Error	0.005	0.014	0.016	0.0130	0.011
A-Sexism $\rightarrow$ L-Violence	0.546	0.538	0.555	0.534	0.576
St.Error	0.006	0.020	0.015	0.020	0.013

3.6.6 Conclusions for PATHMOX Approach

In conclusion, this work deals with the problem of modeling heterogeneity through the PATHMOX approach. We can see that PATHMOX follows a data mining approach for discovering heterogeneity in the PLS-PM context. It remains as a working issue the validity of the emerged segments in order to avoid false positives; this can be solved as a first attempt by bootstrap [142]. Also, the validity of the measurement model across the segments needs to be assessed in order to make meaningful comparisons across segments. Finally, the F of Fisher splitting criterion, even if it relies on the normality assumption of intangibles and the homoschedastic assumption over the segments, showed in all applications performed a clear interpretability of the results.

3.6.7 Heterogeneity through REBUS-PLS Approach

The aim of REBUS-PLS is to detect sources of heterogeneity in both the structural and the measurement model. It is obtained through the definition of an ad hoc distance based on the sum of squared residuals. For each cluster the LVs are estimated. The model has been estimated using the software R and the package 'plspm' implementing the REBUS-PLS method [146].

Performing REBUS-PLS on that dataset allows us to detect three different classes of units showing homogeneous behavior. As a matter of fact, the cluster analysis performed on the residuals from the global model (Figure 3.10) suggests that we to look for three latent classes.

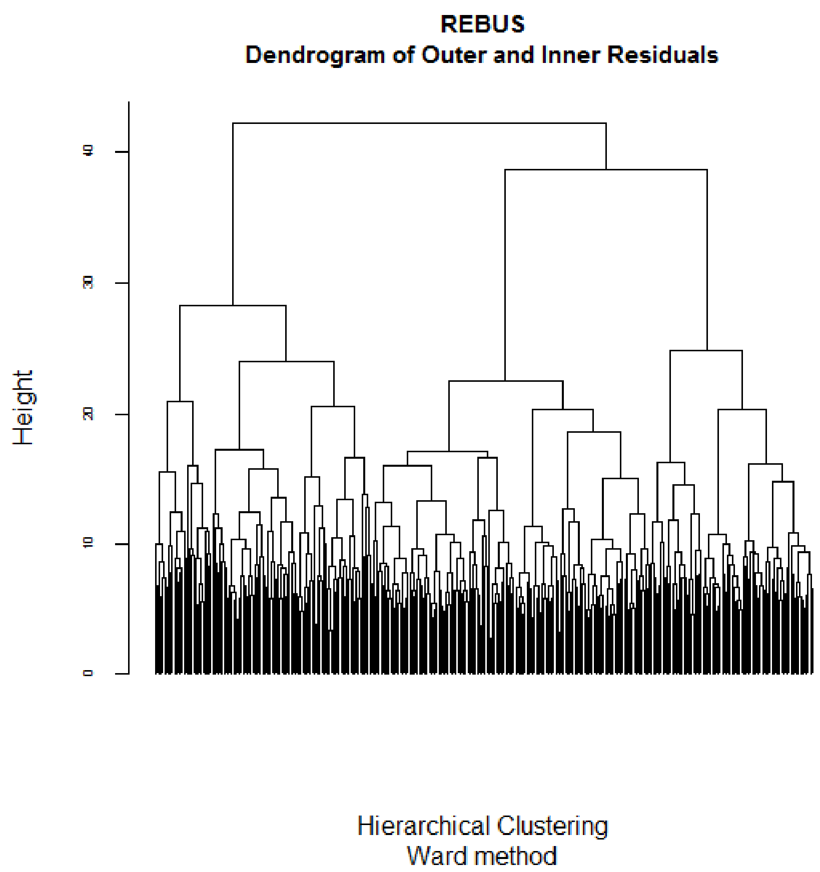


Figure 3.10: Dendrogram of students

Thanks to the REBUS-PLS algorithm the 300 units have been clustered in three classes (Table 3.11) that are more homogeneous as regards the model parameters.

Table 3.11: REBUS segments

	Cluster 1	Cluster 2	Cluster 3
Number of units	75	118	107
Proportions %	25	40	36

For each cluster the quality of the global model is very high. The results are shown in Table 3.12.
The reliability of each LV is measured by the communality. The communality measures the percentage of variance, in a given variable, explained by all the factors jointly.
Taking into account the LVs on the Higher-Order Construct, the communality is never under 40%. The quality of the model is high.

Table 3.12: Quality measures

	Global	Cluster 1	Cluster 2	Cluster 3
J-Peer Violence	0.333	0.274	0.202	0.279
J-Domestic Violence	0.300	0.302	0.213	0.291
J-Intolerance	0.319	0.240	0.309	0.229
H-Sexism	0.324	0.278	0.275	0.310
B-Sexism	0.282	0.279	0.245	0.320
A-Violence	0.721	0.784	0.734	0.774
A-Sexism	0.770	0.882	0.792	0.797
L-Violence	0.811	0.818	0.781	0.800

The contribution of each LV to the Legitimacy of Violence for each cluster can be seen in Figure 3.11.

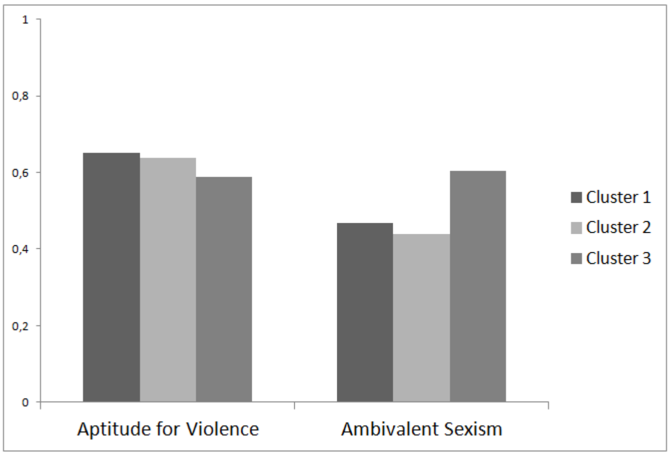
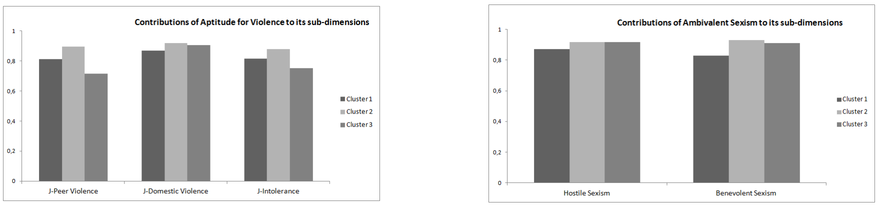


Figure 3.11: Contribution of each LV to Legitimacy of Violence for each cluster

Generally, the contributions of the LVs to Higher-Order CI keep the same structure in all three clusters.
Cluster 1 gives slightly more importance to the Aptitude to Violence while Cluster 3 give highest importance to Ambivalent Sexism. But if we analyze the individual blocks, we see how the LVs are reflected differently in their sub-dimensions (Figure 3.12).



(a) Aptitude to Violence (b) Ambivalent Sexism

Figure 3.12: Contribution of each LV to its own sub-dimensions for each cluster

The Aptitude to Violence is very strongly reflected in all Cluster for each dimension, especially in Sexist Beliefs and Justification of Domestic Violence; the same situation occurs for Ambivalent Sexism, which is reflected slightly more in Cluster 2.
The test on the differences among coefficients reveals a significant differ-

ence between clusters 1-2 and 1-3.
Regarding the discriminatory power for LV in the clusters, Table 3.13 presents for each cluster the mean, standard deviation and t-test of the LVs.

Table 3.13: Characterization of the LVs for each cluster

		Global	Cluster 1	Cluster 2	Cluster 3
J-Peer Violence	Mean	32.96	27.47	46.03	51.02
	St. Dev	23.62	0.82	3.34	3.70
	T-Test		-6.72	**3.91**	**4.88**
J-Domestic Violence	Mean	37.88	33.57	52.89	46.44
	St. Dev	22.75	0.79	3.22	3.56
	T-test		-5.48	**4.66**	**2.40**
J-Intolerance	Mean	51.83	50.17	59.79	52.55
	St. Dev	23.86	0.82	3.37	3.74
	T-test		-2.02	**2.36**	0.19
H-Sexism	Mean	51.78	49.24	58.85	58.99
	St. Dev	21.71	0.75	3.07	3.40
	T-test		-3.40	**2.30**	**2.12**
B-Sexism	Mean	69.49	70.85	66.89	64.25
	St. Dev	17.60	0.61	2.49	2.76
	T-test		**2.23**	-1.04	-1.90
A-Violence	Mean	43.72	41.58	54.76	43.67
	St. Dev	21.66	0.75	3.06	3.39
	T-test		-2.85	**3.60**	-0.01
A-Sexism	Mean	61.49	60.55	67.65	59.87
	St. Dev	19.18	0.66	2.71	3.00
	T-test		-1.41	**2.27**	-0.54

The Cluster 1 is characterized by the Benevolent Sexism, with a T-test value of 2.23, while all LVs, except Benevolent Sexism, characterize the Cluster 2. Justification of Peer Violence is the LV that strongly characterizes the Cluster 3 (T-test value of 4.88), followed by the Sexist Beliefs and Justification of Domestic Violence and Hostile Sexism, which respectively have a T-test value of 2.40 and 2.12.
Finally, the three class solution shows a Group Quality Index (GQI) equal

to 0.531, as we can see in Table 3.14.

Table 3.14: Group Quality Index

Number of iterations	100
Rate of unit change	0.118840
Group Quality Index	0.524749

The GQI value obtained for the REBUS-PLS based partition is the highest obtained value. This allows us to assess that the REBUS-PLS based clustering of the units is better than a random assignment of the units, and is definitely better than the global model solution. This means that a partition of units in latent classes surpassed the performance of the global model in every case. In other words, the global model definitely has to be definitely considered as affected by heterogeneity.

3.6.8 Conclusions for REBUS-PLS Approach

In summary, the same application deals with the problem of modeling heterogeneity through the REBUS approach. It was demonstrated that there are differences in the groups of students that follow the same model, so the model initially assumed is not uniquely adaptable to clusters. To conclude, a permutation test performed on the Group Quality Index has proved that the REBUS-PLS based partition is the best one according to the prediction capability of the model.

3.7 Conclusions

In this Chapter, we have considered a CI system formed by EIs on a non numerical scale, including some kind of CI relationship, and testing whether there is a mediating and/or moderating effect. We have shown how the estimation of LVs changes, and so the entire descriptive and predictive power of the model, if we consider the indicators according to their real nature and if we include mediating relationships among the constructs. Moreover, we have treated the problem of the heterogeneity of data. We have seen how a unique model for the construction of CIs is not always well suited to the entire population that we are studying, but that are local models for each population according to its own characteristics; we have experienced this phenomenon through two approaches known in the literature, the PATHMOX and REBUS-PLS Approaches, that, as they are constructed from two different perspectives, lead to different results. It is important to point out the main difference between REBUS-PLS and PATHMOX: REBUS-PLS Approach does not require the identification of a target variable and it allows us to obtain units classification taking into account units performance for both the structural and the measurement model, while in PATHMOX Approach the available external information is used to identify different segments and to cluster units.

Chapter 4

Higher-Order Constructs in PLS-PM

4.1 Introduction

As has been said in the first Chapter, many phenomena are complex and based on different levels of abstraction. Just think of the concept of poverty, that for many years was measured by referring only to the country's income. Sen [152] was the first person to recognize that the concept of poverty requires a multidimensional approach that focuses its attention not only on the strictly monetary characteristics of the phenomenon, but also on other aspects of people's daily lives, such as labor, environment, social relations, knowledge and health, which represent its sub-dimensions. Therefore, PLS-PM is a suitable tool for the investigation of this kind of model with a high level of abstraction, in cases where the building of a system of CIs depends on different levels of construction.
Almost 25 years ago Noonan and Wold [115] observed: *"Path analysis with hierarchically structured LVs within the framework of PLS is at an early stage of development, and research is still under way"*. Fortunately, in the last few years, research into the use of Higher-Order Construct Models using PLS-PM has been undertaken and several applications developed. The use of Higher-Order Construct Models has allowed researchers to extend the application of PLS-PM to more advanced and complex models.

In the content of PLS-PM models, Higher-Order Construct have shown an increasing popularity in the last few years. Several authors have discussed both the theoretical and empirical contributions hierarchical models can make [33];[71];[73];[97];[178]. Both Covariance-Based structural equation modeling (CB-SEM) and PLS-PM can be used to estimate the parameters in Higher-Order Construct models [178]. For Covariance-Based SEM, guidelines and empirical illustrations are generally available [33]. For PLS-PM, guidelines are mainly available for Higher-Order Construct models with reflective relationships ([94];[178];[186]). However, Ringle et al. [73] show that Higher-Order Construct models with reflective relationships in the First-Order and Second-Order of the hierarchy represent only a minority (20%) of the models applied in *MIS Quarterly*. Thus, there is a great need for guidelines on using hierarchical construct models with formative relationships in PLS-PM, as the Second-Order model for social capital by Koka and Prescott [85] clearly exemplifies.
Higher-Order Constructs Models, also known as *Hierarchical Models*, or *Multidimensional Constructs* are explicit representations of multidimensional constructs that exist at a higher level of abstraction and are related to other constructs at a similar level of abstraction completely mediating the influence from or to their underlying dimensions [13]; [12]. Law et al. [90] define *"[...] a construct as multidimensional when it consists of a number of interrelated attributes or dimensions and exists in multidimensional domains. These dimensions can be conceptualized under an overall abstraction, and it is theoretically meaningful and parsimonious to use this overall abstraction as a representation of the dimensions."* Establishing such a higher model component, usually required in the context of PLS-PM [94], most often involves testing Second-Order Constructs that contain two layers of constructs. This kind of model is often limited to a Second-Order hierarchical structure, and can be defined as a construct involving more than one dimension [33]; [71]; [89]; [97]; [113]; [118]. As such, it can be distinguished from unidimensional constructs, which are characterized by a single underlying dimension [113].
There are three main reasons for the inclusion of a Higher-Order Constructs Model in PLS-PM.

- First, by establishing Higher-Order Constructs Models, researchers can reduce the number of relationships in the structural model, making the PLS-PM more parsimonious and easier to grasp.

- Secondly, Higher-Order Constructs Models prove valuable if the constructs are highly correlated; the estimations of the structural model relationships may be biased as a result of collinearity issues, and discriminant validity may not be established. In situations characterized by collinearity among the constructs, a Second-Order Construct can reduce such collinearity issues and may solve discriminant validity problems.

- Thirdly, establishing Higher-Order Constructs Models can also prove valuable if formative indicators exhibit high levels of collinearity. Provided that theory supports this step, researchers can split up the set of indicators and establish separate constructs in a Higher-Order structure.

The utility of these models is based on a number of theoretical and empirical grounds [33]. Proponents of the use of Higher-Order Constructs have argued that they allow for more theoretical parsimony and reduce model complexity [33]; [90]; [97]. Edwards [33] summarizes this argument as theoretical utility; theory requires general constructs consisting of specific dimensions. This is closely related to the trade-off between accuracy and generalization as suggested by Gorsuch [51], who argues that *"factors are concerned with narrow areas of generalization where the accuracy is great [whereas] higher-order factors reduce accuracy for an increase in the breadth of generalization*. Law et al. [90] even state that *"treating dimensions as a set of individual variables precludes any general conclusion between a multidimensional construct and other constructs"*.

4.2 Estimation of Higher-Order Construct Models

Edwards [33] proposed an integrative analytical framework on the basis of structural equation modeling, which allows for the simutaneous inclusion of higher-order constructs and their dimensions as LVs. In a structural model, the Higher-Order Constructs may serve as either cause or effect by being embedded in a nomological network. This approach also allows us to derive the (indirect) effects of Lower-Order constructs, or dimensions, on outcomes of the Higher-Order Construct as the pairwise product of the loadings (or weights for formative constructs) and coefficients of the outcomes. Moreover, SEM allows for the explicit specification of the direction of the relationships between MVs and LVs [34].

4.2.1 Molecular and Molar Higher-Order Construct Models

Due to the determinate nature of the PLS algorithm that explicitly weights measurement indicators to create construct scores, two types of Higher-Order Construct can be modeled: what Chin and Gopal termed as *Molecular* and *Molar Higher-Order Constructs* [19]. Essentially, these two models can be distinguished on the basis of the directions of the relationships between the MVs and LVs [89].

For the Molecular Higher-Order Constructs, or reflective construct models, the MVs are affected by the LVs ($LV_j \rightarrow MV_i$), whereas for the Molar Higher-Order Constructs, or the formative construct models, the relationship is reversed ($LV_j \leftarrow MV_i$).

4.2.2 Types of Higher-Order Construct Models

Each of the Higher-Order Construct Model (HCM) types is characterized by different relationships between the Higher-Order Constructs and the LVs: the reflective relationship and the formative relationship. As we can see in Figure 4.1, there are four main types of Higher-Order Construct Model discussed in the extant literature ([71]; [178]) and used in applications [73]. These types of model have two elements: the *Higher-Order Construct (HOC)*, which captures the more abstract entity, and the *Lower-Order Construct (LOC)* which captures sub-dimensions of the abstract entity.

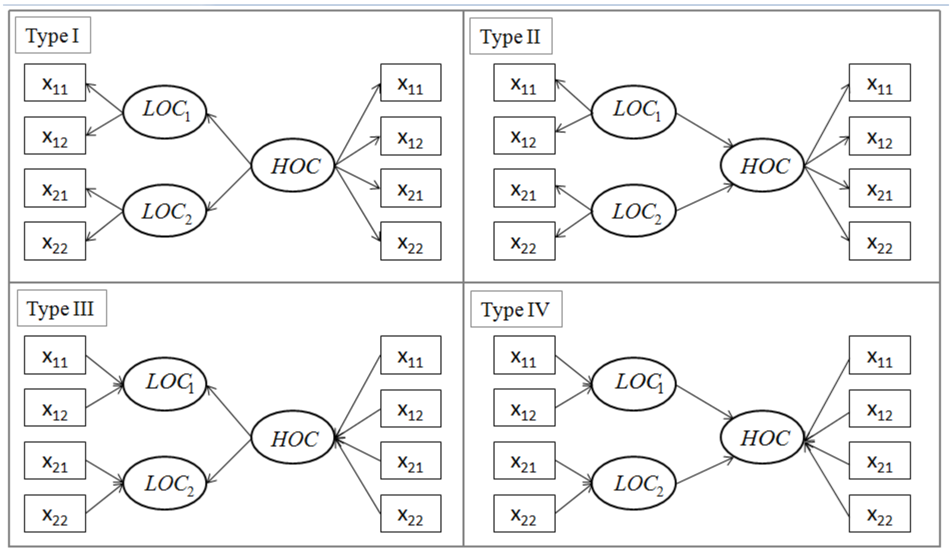


Figure 4.1: Types of Higher-Order Construct

- One of the models most frequently applied in SEM among researchers nowadays is the *Reflective-Reflective Measurement Model* known as the *Second-Order Construct Type I*.

- Secondly, the *Reflective-Formative Measurement Model Type II* is slightly different compared to the previous HCM, in which the HOC is automatically formative constructs playing a double role. This model comprises reflective and formative measurement models and is a structural model. According to Chin's clarification the LOCs are selectively measured constructs that do not share a common cause but rather form a general concept that fully mediates the impact on subsequent endogenous variables [13].

- Thirdly, the *Formative-Reflective Measurement Model Type III* is slightly different compared to the Reflective-Formative Type II in the explanation above. In this instance, a higher construct model will be imposed by each MV (indicator) and at the same time the causal effect from the HOC will be exerted on the LOCs that comprise the indicator.

- Finally, the *Formative-Formative Measurement Model Type III* is the least frequently implemented in the structural model. This application is appropriate when both the HOC and LOCs are in the form of formative constructs.

4.3 PLS-based Approaches to Estimating Path Models with Higher-Order Constructs

In the frame of the PLS-PM, three main approaches are presented in literature for dealing with Higher-Order LV models. These approaches are described in detail in the next sub-sections.

4.3.1 The Repeated Indicators Approach

Wold's original design of PLS path modeling does not consider Higher-Order LVs; each construct has to be necessarily related to a set of observed variables in order to be estimated. On this basis, Lohmöller [94] proposed a procedure for the case of hierarchical constructs, the so-called *Hierarchical Component Model* [186] or *Repeated Indicators Approach* [186];[94], or Super-block Approach [166], which is the most popular approach when estimating Higher-Order Constructs through PLS [175];[179];[190].
The procedure is very simple: *"a Second-Order factor is directly measured by observed variables for all the First-Order factors. While this approach repeats the number of MVs used, the model can be estimated by the standard PLS algorithm"* [124]. The manifests indicators, measuring each First-Order LV, are simply repeated in order to represent the Higher-Order Construct. For example, if a Second-Order LV consists of two underlying First-Order LVs, each with two MVs, the Second-Order LV can be specified using all the MVs of the underlying First-Order LVs, and thus the Second-Order LV will be formed by four MVs.
Consequently, the MVs are used twice: for the First-Order LV (*primary loadings*) and for the Second-Order LV (*secondary loadings*). Having thus specified the outer model (the measurement model), the inner model (the structural model) accounts for the hierarchical component of the model, as it represents the loadings of the Second-Order LV on the First-Order LVs.

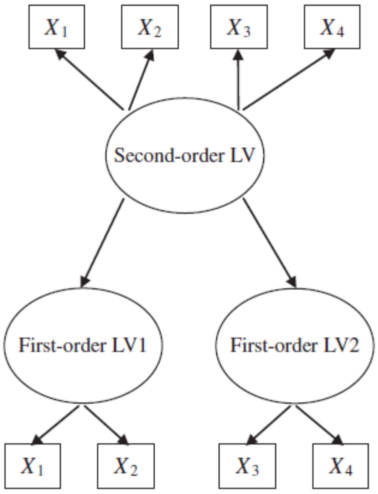


Figure 4.2: Model building: the Repeated Indicators Approach

Obviously, this approach can easily be extended to Higher-Order models [115]. As LV scores are determinate in PLS path analysis, LV scores for Lower-Order LVs can be obtained [13], which can subsequently be used as MVs for the Higher-Order LVs [178].
The Repeated Indicators Approach can be specified by considering the following three equations:

$$\xi^{I}_{q,1} = \mathbf{B}_{q,q} * \xi^{II}_{q,1} + \zeta_{q,1} \tag{4.1}$$

$$\mathbf{x}_{p,1} = \Lambda^{I}_{p,q} * \xi^{I}_{q,1} + \delta_{p,1} \tag{4.2}$$

$$\mathbf{x}_{p,1} = \Lambda^{II}_{p,q} * \xi^{II}_{q,1} + \epsilon_{p,1} \tag{4.3}$$

where the subscripts m and p are the number of, respectively, First-Order LVs and MVs in the model, and the subscript q is the number of Second-Order LV. The vectors ξ^{I}, ξ^{II}, x, ζ, δ and ϵ indicate respectively the first and the Second-Order LVs, the MVs, and the structural and measurement errors terms. The matrices B, Λ^{I} and Λ^{II} define the path coefficients linking the LVs and the factor loadings linking, respectively, the MVs to the First-Order and Second-Order LVs.The structural or inner model (4.1) specifies the relationships among the First-Order and the Second-Order LVs. Equations 4.2 and 4.3 denote the measurement models, where the MVs, measuring

each First-Order LV, are repeated in order to represent the Higher-Order Construct.
This approach is the one most favored by researchers when using PLS for modeling Higher-Order Constructs, due to its simplicity and also to the fact that it has been presented most clearly by prominent PLS methodologists (e.g. Wold and Lohmöller).
The advantage of the Repeated Indicators Approach is its ability to estimate all constructs simultaneously instead of estimating Lower-Order and Higher-Order dimensions separately. Thus, it takes the whole nomological network, not only the lower level or the higher level model, into account, thereby avoiding interpretational confounding. When using the Repeated Indicators Approach, researchers have to make decisions regarding the mode of measurement for the Higher-Order Construct and the inner weighting scheme. Some authors list guidelines for using different model types [6]. First, as for any construct in a PLS-PM model, the mode of measurement for the Higher-Order Repeated Indicators needs to be specified (i.e. Mode A or Mode B). Usually, Mode A measurement is associated with reflective constructs and Mode B is associated with formative constructs [64]; [166]. The standard approach for repeated indicators on a Higher-Order Construct Model is to use Mode A [186] which generally suits reflective-reflective type models best. Therefore, formative type models are often also estimated using Mode A for the repeated indicators, especially when the First-Order Constructs are reflective (i.e., the reflective-formative type) [16];[73], although the formative nature of the Higher-Order Construct might suggest Mode B measurement. Therefore, most researchers think it is more appropriate to use Mode B for the repeated indicators of a formative type hierarchical LV model (i.e., the reflective-formative and the formative-formative types). However, the importance of the mode of measurement is usually not discussed in research papers presenting the Repeated Indicators Approach, but only indirectly inferred from the direction of the arrows in the path diagram [16];[73]. Secondly, besides the mode of measurement, Lohmöller [94] analytically discusses how setting the inner weighting scheme (factor or path weighting) together with the mode (Mode A or Mode B) leads to different (or equal) results for the dif-

ferent types of hierarchical LVs. Thus, researchers have to be aware that the type of inner weighting scheme they choose can make an important difference to the results of a Repeated Indicator Model. However, Lohmöller [94] does not provide any guidelines on which setting is more suitable for each type. In addition, it is frequently mentioned that the Repeated Indicators Approach is only advisable if the Lower-Order Constructs have an equal number of indicators, because, otherwise, it will lead to biased loadings/weights for the Lower-Order Construct on the Higher-Order Constructs ([20];[94];[73]). However, to the best of our knowledge, an assessment of this general assumption is missing in the literature.
A disadvantage of this approach is that there is a perceived effect of possibly biasing the estimates by relating variables of the same type together by means of the PLS estimation. According to Rajala and Westerlund [122], the Repeated Indicators Approach may be applied provided that all the measurement relationships are of the reflective type. Formative structural relationships from the First-Order to the Second-Order LVs can also be hypothesized, as has been shown in different studies [53]; [99]. Moreover, the repeated use of the same indicators can cause artificially correlated residuals [6].

4.3.2 The Two Step Approach

Another way to build a Higher-Order model is to use the Two Step Approach: the LV scores are initially estimated in a model without the Second-Order construct [2]. Once the First-Order LV scores are computed, they are subsequently used as indicators in a separate higher-order structural model analysis. The First-Order LVs are then a linear combination of the Higher-Order Construct, while the observed variables are directly related only to the specific dimensions. Hence, it is termed a Two Step Approach. This is typical of how analysts previously used factor scores prior to running further regression analyses.
Such an approach may offer advantages when estimating Higher-Order models with formative indicators [28]; [124]. The implementation is not performed through a single PLS run; this implies that any Second-Order

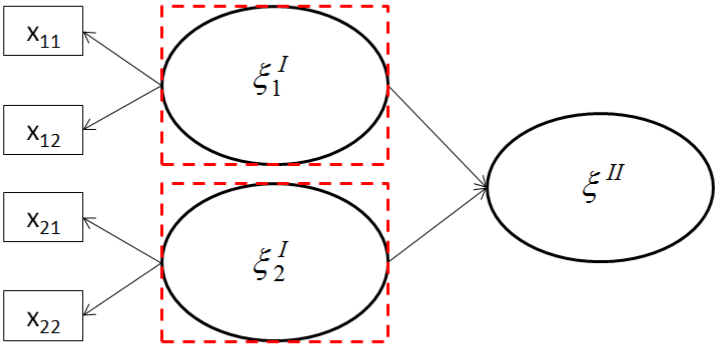


Figure 4.3: Model building: the Two Step Approach

Construct, investigated in stage two, is not taken into account when estimating LV scores in stage one. The first step of estimation is made by considering only the measurement model which provides the estimation of the First-Order Constructs, as reported in the following equation:

$$x_{p,1} = \Lambda^I_{p,q} * \xi^I_{q,1} + \delta_{p,1} \tag{4.4}$$

In the second step, the estimated scores $\hat{\xi^I}$, obtained in the first step, are used as indicators of the Second-Order Construct:

$$\hat{\xi}^I_{q,1} = \mathbf{B}_{q,1} * \xi^{II}_{1,1} + \zeta_{q,1} \tag{4.5}$$

Sanchez [142] suggests this way of computing scores for the LVs of Lower-Order: we can obtain a score for a First-Order Construct by taking the first principal component of its indicators. Next, the PCA scores of the Lower-Order Constructs are subsequently used as indicators for the Higher-Order Construct in a separate PLS path model.

When using the Two Step Approach, you usually use the mode of measurement for the Higher-order Construct in the second stage that matches the construct's operationalization, (i.e., Mode B for a formative and Mode A for a reflective construct). The Two-Stag Approach has the advantage of estimating a more parsimonious model on the higher level analysis without needing the Lower-Order Constructs. On the downside, a clear disadvantage of any Two Step Approach is that any construct that is investigated in stage two is not taken into account when estimating the LV scores at stage one. This could encourage "interpretation confounding" [9]; [180]. Similar arguments have followed the use of the Two Step modeling approach advocated by Anderson and Gerbing [3] in the CB-SEM literature. The implementation is not one simultaneous PLS run.

Another important difference between the approaches emerges when hierarchical LVs are used in a nomological network of LVs as an endogenous construct (i.e., a consequence or criterion). When the Repeated Indicator Approach is used, regardless of the type of measurement, Mode A or Mode B, and the Higher-Order Construct is formative (i.e., reflective-formative or formative-formative), the Lower-Order constructs already explain all the variance of the Higher-Order Construct (i.e., R^2 equals 1.0). Therefore, other antecedent constructs cannot explain any variance of the Higher-Order Construct and consequently, their paths to the Higher-Order Construct will be zero (non-significant) [73]; [178]. This problem does not occur when the Two Step Approach is used for formative Higher-Order Constructs [73]; [6].

A few studies have focused on a comparison of the two approaches and they are limited to the case of reflective measurements [98]; [180]. From a theoretical perspective, the two approaches lead to different definitions of the Second-Order Construct. The difference lies in the level of the distinction between the measurement and structural models. While in the Repeated Indicators Approach the Higher-Order LV is directly measured by the whole set of MVs (which, in turn, measure the First-Order-specific factors), in the Two-Step Approach the Second-Order Construct is directly measured by means of the First-Order LVs. In the former case, the general construct can be seen as a context variable and its meaning is independent of the relationships with the First-Order Factors. This formalization could apply when, for instance, you want to evaluate the effects of a perception change that had happened in the Second-Order LV on the First-Order LVs or, in the case of formative relationships, the effects of a perception change in the First-Order LVs on the Second-Order LV. Therefore, the Repeated Indicators Model measures the intensity of the causal relationships between sub-dimensions (the First-Order LVs) and the context. On the contrary, with the Two Step Approach, the meaning of the Second-Order Construct is defined by the relationships with the sub-dimensions; that is, it is measured and cannot exist before the estimation of the First-Order LVs. The relationships reflect, or form, the composition of the Higher-Order LV; indeed, they do not represent how much the First-Order LVs affect the Second-Order LV, but the extent to which the First-Order Constructs reflect, or form, the higher level of abstraction. So, the difference is in the directness of the impact of the Second-Order LV on the observed variables. While the Repeated Indicators Approach links directly the Second-Order LV both to the First-Order LVs and the MVs, in the Two Step estimation the general construct has direct effects on the sub-dimensions and only indirect effects on the MVs. In a recent study, Wilson et al. [179] showed that the Second-Order Constructs reliability does not depend on the approach adopted; anyway, the Repeated Indicators Approach produces biased and less consistent estimates (in the case of small samples) compared to the Two Step Approach.

4.3.3 The Hybrid Approach

The third option for modeling Higher-Order Constructs is the Hybrid Approach. The Hybrid Approach works in a similar way to the Repeated Indicators Approach, but uses each indicator only once in a model to avoid artificially correlated residuals. The idea behind this approach is to randomly split all the MVs of the First-Order Constructs, so that half of their indicators are represented on their respective First-Order Construct side and the other half on the Second-Order Construct side. Thus, it uses half to estimate the First-Order Construct and the other half to estimate the Second-Order Construct, therefore avoiding the repeated use of indicators in the model [180]. A clear disadvantage of this approach is the reduced reliability of the measures having only half the number of indicators. This could be a particular problem as PLS-PM is known to be "consistent at large", meaning that the estimates are consistent if the sample size and number of indicators increase [94]. Using the Hybrid Approach, there are no clear guidelines on whether Mode A or Mode B should be used for the formative Second-Order Construct. Wilson and Henseler [180] believe this approach has not been trialed in PLS and could overcome the criticism that is directed towards the Higher-Order Constructs in that the indicators are repeated and therefore via PLS iteration and estimation the analyst could be in some way relating the same items together. Naturally, the Hybrid Approach circumvents this criticism. During the runtime of the algorithm, the Second-Order Construct is generated by a proxy which is then assigned to the Second-Order Construct (to derive the LV scores and path coefficients).

4.4 A Multidimensional Poverty Composite Indicator based on Higher-Order Constructs

World poverty has always been considered to be one of the most serious global problems and one that requires an immediate solution. Over the years, national commissions and European and International organizations have drawn up many proposals and implemented many attempts to combat the incidence and persistence of this phenomenon, initiatives that often involve inquiring into the most suitable measurement methods to be taken.

4.4.1 A brief history of Poverty Indices

For many years poverty was measured by using a purely economic approach, which involves the use of a single variable (income or consumption). It is now universally recognized that the concept of poverty requires a multidimensional approach that focuses its attention not only on the strictly monetary characteristics of the phenomenon, but also on other aspects of people's daily lives, such as labor, environment, social relations, affective, knowledge and health.

The multidimensional approach to poverty owes much to Amartya Sen [152] according to whom poverty must be identified not only as an individual material deprivation but also as a loss of real opportunities, a failure to realize the fundamental goals and functions of human life such as: living as long a life as possible, having sufficient food and shelter, enjoying good health and the access to a system of education, and actively participating in community life.

In this regard, an important role is played by the United Nations Development Programme (UNDP), which with the publication in 1990 of its first Human Development Report (Human Development Report - HDR), introduced the Human Development Index (HDI), a simple composite indicator that measures, for each country, human development based on three dimensions: (i) a long and healthy life, as measured by life expectancy at birth; (ii) education level, measured by adult literacy rate (with a 2/3 weighting), and the gross enrolment in primary, secondary and tertiary education (with a 1/3 weighting); and (iii) a decent standard of living as measured by Gross Domestic Product per capita in Purchasing Power Parity. The HDI corresponds to the simple arithmetic average of the indices of the three dimensions.
In 1997 the HDI was combined with another indicator, which had been for years the most comprehensive tool for measuring poverty, the Human Poverty Index (HPI). While the HDI measures average achievements in basic dimensions of human development, the HPI measures deprivations in the same dimensions. Poverty is then evaluated by referring to the exclusion parameters. The HPI focuses on deprivation in the three essential dimensions already taken into account by the HDI: longevity, education and a decent standard of living. The formula used to calculate the HDI index is the following:

$$HPI = \Big[\frac{1}{3} * (P_1^{\alpha} + P_2^{\alpha} + P_3^{\alpha})\Big]^{\frac{1}{\alpha}} \tag{4.6}$$

where P_1 is the probability at birth of not reaching 40 years of age, P_2 is the adult illiteracy rate, and P_3 is the unweighted average of people without access to drinking water and the percentage of malnourished children under 5 years. The α value has an important influence on the IPU index construction, as it serves to encourage a consideration of the value of the three individual indices. In fact, if α = 1, the index would correspond only to the average of the dimensions that constitute it, and the impact of the size of this, since the increase is of one unit for each EIs, would be the same regardless of the level of deprivation for each dimension. Considering a value of α> 1, it will assign a higher weight to the dimension in which the level of deprivation is greater The value of α = 3 is chosen because this value allows you to attribute a greater impact to the dimension that has the greatest deprivation, but without that impact being too great. The HPI is derived separately for developing countries (HPI_1) and a group of select high-income OECD countries (HPI_2) to better reflect socio-economic differences and also the widely different measures of deprivation in the two groups. For OECD countries the HPI_2 index takes account also of social exclusion:

$$HPI_2 = \left[\frac{1}{3} * (P_1^{\alpha} + P_2^{\alpha} + P_3^{\alpha} + P_4^{\alpha})\right]^{\frac{1}{\alpha}} \tag{4.7}$$

where P_4 is the rate of long-term unemployment (lasting 12 months or more).

In 2010 The Multidimensional Poverty Index (MPI) was developed by the Oxford Poverty & Human Development Initiative and the United Nations Development Programme. It uses different factors to determine poverty beyond income-based lists.

4.4.2 The Higher-Order Multidimensional Poverty Composite Indicator (MP-CI)

Grassia et al. [52] propose the PLS-Path Modeling Approach to derive a measure of poverty taking into account its multidimensional nature. The model, shown in the Figure 4.4, uses the four dimensions considered by the index HPI_2: (i) Health; (ii) Education; (iii) Employement and (iv) Living Standards.

They have chosen a super-block model where the CI of Multidimensional Poverty is the endogenous variable, while Health, Education, Employement and Living Standards are exogenous variables. The basic indicators (MVs) have been transformed into a scale from 0 to 100, where 100 represents the worst evaluation.

Each of these four dimensions was measured by EIs and the relationship between them and the respective LV is assumed to be reflective: every LV is the reflection of the MVs to which it is connected.

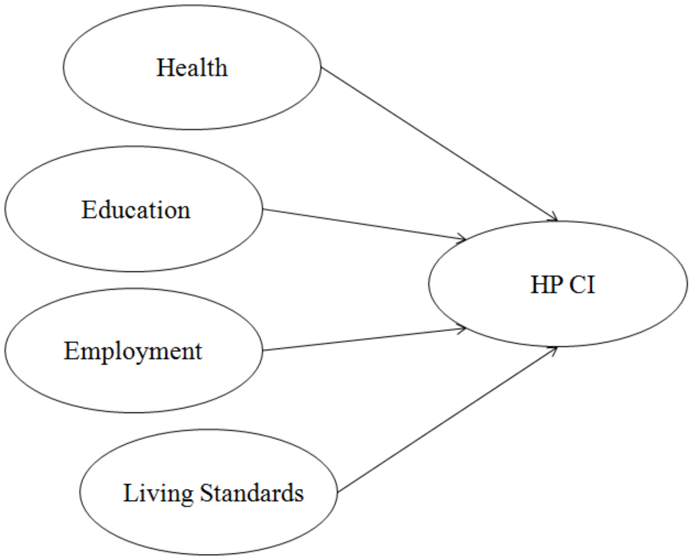


Figure 4.4: Human Poverty Composite Indicator Model Based

The MVs, in relation to the respective latent construct, are shown in Table 4.1.
The data are related to the year 2007; note that for some variables, because of the lack of data for that year, the previous or the following year was taken as the reference.
The model was developed with reference to the European Community countries. Malta and Luxembourg were excluded from the analysis, while Norway, which is not part of the European community, was considered instead. Therefore, the number of countries considered is 28.
The descriptive statistics analysis for each variable allowed to identify outliers. These values were been replaced with the maximum value of the distribution. Next, the variables were been normalized in order to "standardize" their units of measurement; the following transformation was applied on each variable:

$$Z = \frac{X - min(X)}{max(X) - min(X)} \tag{4.8}$$

Finally, in the case of missing data, among the possible methods of imputation, that of the "nearest neighbors" was used, which consists in introducing a concept of similarity between the units, based on a distance function.

Table 4.1: LVs and MVs of the Multidimensional Poverty CI

LVs (CIs)	MVs	Source
Health	Health expenditure per capita	Worldbank 2007
	Infant Mortality Rate	Worldbank 2007
	Life expectancy at birth	Worldbank 2007
	Hospital beds	Eurostat yearbook 2011
	Rate of Maternal Mortality	Worldbank 2007
	Number of doctors	Eurostat yearbook 2011
Education	Internet	Worldbank 2007
	Graduates	Unesco 2007
	Education expenditure per capita	Eurostat yearbook 2011
	Illiteracy rate	UNDP 2007
	Average School Attendance in years	UNDP 2007
	Book reading	Eurobarometro 2007
Employment	Participation rate	Worldbank 2007
	Unemployment rate	Worldbank 2007
	Youth Unemployment Rate	OECD 2007
	Rate of Part-Time Employment	Eurostat 2007
	Female Employment rate	Worldbank 2007
Living Standards	Housing overcrowding rate	Eurostat 2007
	Available income	Eurostat 2007
	Owned apartments	Worldbank 2007
	Electricity consumption	Worldbank 2007
	Owned cars	Eurofound 2007

4.4.3 The three Higher-Order Constructs Approaches compared

The latent concept of Multidimensional Poverty is considered as a synthesis of its sub-dimensions, devoid of its own MVs, and therefore it is regarded as hierarchical.
We have considered the following models:

- The Repeated Indicators Approach, for the estimation of the MP-CI as a Second-Order Construct which is formatively related to its First-Order dimensions and reflectively measured by its MVs (which are the entire set of indicators of the First-Order dimensions);

- The Two Step Approach, for the estimation of the MP-CI as a Second-Order Construct which is formatively related to its First-Order dimensions and reflectively measured by its MVs (which are the PCA Components of each First-Order dimension estimated in stage one);
- The Hybrid Approach for the estimation of the MP-CI as a Second-Order Construct. The same links exist between the First-Order dimensions and the Second-Order Construct and between the Second-Order Construct and its indicators. The indicators are randomly split in two orders.

The assessment of a structural model estimated with the PLS-PM approach involves the inner as well as the outer model measures of quality. Since the First-Order Constructs are reflectively related to their indicators, traditional measures of reliability can be used to assess the quality of the measurement model. As has been mentioned above, the internal consistency of each construct, assessed through the Composite Reliability and Cronbach's α indexes, is the most commonly used quality criterion for the measurement model. Furthermore, another widely used index in PLS literature is the communality index, which measures the amount of MV variability explained by the corresponding LV. Table 4.2 reports the Reliability Measures of the First-Order Constructs, while Table 4.3 the Reliability Measures of the Higher-Order MP-CI for each approach.

Table 4.2: Reliability Measures of the First-Order Constructs

	Health	Education	Employment	Living Standards
Cronbach's Alpha	0.880	0.789	0.900	0.905
Composite Reliability	0.914	0.865	0.927	0.931
Communality	0.680	0.619	0.717	0.730

All Cronbach's α indexes are close to the conventional acceptability thresholds of 0.7 for all First-Order Constructs. As concerns the Second-Order Construct, the Repeated Indicators Approach appears to generate a more

Table 4.3: Reliability Measures of the Higher-Order MP-CI for each approach

	Repeated Indicators Approach	Two Step Approach	Hybrid Approach
Cronbach's Alpha	0.945	0.875	0.857
Composite Reliability	0.953	0.915	0.892
Communality	0.525	0.730	0.520

reliable construct than the other two approaches (α of Repeated Indicators Approach = 0.945 against α of Two Step Approach = 0.875 and α of Hybrid Approach = 0.857). However, it is worth emphasizing two aspects of the α coefficient. First, the index at issue is a function of the number of items in the scale: in the first approach, the MP-CI has 19 MVs (that are MVs of the First-Order Construct repeated in the Second-Order Construct), while in the second, the MP-CI has only 4 items (that represent a PCA Component for each block), and in the third, it has 8 MVs (that are randomly split MVs). Secondly, a high level of α does not imply the unidimensionality of the construct, being a measure of the average intercorrelation among the items. Despite the high level of α, the MP-CI is clearly measured by the MVs belonging to several dimensions, which are indeed highly intercorrelated. The composite reliability is higher than 0.7 for all constructs, both First-Order and Second-Order Constructs. The communality of the Two Step Approach is higher than that of the other two approaches (the communality of the Two Step Approach, which is equal to 0.730, against the communality of the Repeated Indicators Approach, which is equal to 0.525 and communality of Hybrid Approach, equal to 0.520). Therefore, the amount of variability of the MVs captured by the MP-CI construct is very small when the Repeated Indicators and Hybrid Approaches are adopted; conversely, the communality is slightly higher in Two Step Approach. It is important to note that the low value for communality obtained with the Repeated Indicators and Hybrid Approaches is due to the fact that the Higher-Order Construct is measured by all heterogeneous items of the lower-order construct, and this affects negatively the construct's internal consistency.

The significance of the structural parameters linking the First-Order and Second-Order Constructs in the model is considered for the evaluation of the hypothesized relationships. PLS performs the estimation of the regression coefficients in the structural equation model; the bootstrap procedure approximates the sampling distribution of the estimator by re-sampling from the original sample, in order to test the parameters' significance. The analysis used 200 replications, with a bootstrap sample equal to 1000. In order to assess the significance of the path coefficients, Table 4.4 reports the value and significance of the structural coefficients linking the First-Order dimensions to the MP-CI.

Table 4.4: Path Coefficients and t-statistics for each approach (non-significant parameters are marked in bold)

		Repeated Indicators Approach	Two Step Approach	Hybrid Approach
Health	path	0.288	0.328	0.332
	t-value	3.28	2.32	2.50
Education	path	0.203	0.274	0.503
	t-value	4.02	3.34	3.19
Employment	path	0.304	0.297	**0.226**
	t-value	4.13	3.09	**0.97**
Living Standards	path	0.341	0.252	**0.062**
	t-value	3.24	2.20	**1.29**

In the Second-Order Hybrid Approach the last two parameters, linking *Employment* and *Living Standards* to the *MP-CI* are not significant. In the Repeated Indicators Approach *Employment* and *Living Standards* are the most important dimensions, while in the Two Step Approach *Health* and *Employment* dimensions prove to be the most influential among all the factors. Not considering the third approach, since it produces no significant estimates, the main difference between the Repeated Indicators and Two Step approaches concerns the path coefficients linking the Second-Order LV, the *MP-CI*, with the First-Order Constructs *Health* and *Living Stan-*

dards: in the case of the Repeated Indicators Approach, the strength of the association of *Living Standards* (β=0.341) is higher than that of *Health* (β=0.288). In the case of Two Step Approach this association changes: the *Health* block is stronger than the *Living Standards* one. It should be noted that in the *Living Standards* block an important role is played by the MV of *available income*, that, in the Repeated Indicators Approach, has a relevance in defining the path coefficients. If we consider the Two Step Approach, this block is resized, and therefore also the relevance of income, considering the *Health* PCA Component, is the best among the four PCA components representing the blocks.
The explained variance with the three approaches is shown in Table 4.5.

Table 4.5: Explained variance of the three approaches

Repeated Indicators Approach	Two Step Approach	Hybrid Approach
0.525	0.729	0.504

As we can see, the highest amount of explained variance is reached with the Two Step Approach (0.729).

4.4.4 The Two Step Approach and its results

The PLS algorithm allows, in addition to determining the value of the weights of each variable and showing the value of the path coefficients, allowed us also to determine a score for all the LVs in the model. In this way we could build a list of all European Community countries, so as to identify those countries with a higher incidence of poverty. The ranking, in addition to revealing the MP-CI score calculated, and also the LV score associated with it, is in such a form as to highlight the aspect that has the greatest impact in determining poverty for each country. The scores are normalized and then carry values ranging from 0 (lowest level of poverty) to 100 (maximum level of poverty) (Table 4.6).

	Countries	Health	Education	Employment	Living Standards	MP-CI
1	Turkey	100	84.7	86.44	77.55	94.27
2	Romania	95.86	70.15	57.89	88.04	83.66
3	Macedonia	74.84	78.1	77.84	80.21	82.84
4	Bulgaria	72.78	75.51	64.98	79.99	76.79
5	Croatia	59.91	73.6	73.53	72.46	73.97
6	Poland	60.45	52.34	70.91	68.03	65.75
7	Hungary	61.1	37.33	73.58	70.62	62.49
8	Lithuania	64.34	50.37	49.94	67.78	59.46
9	Slovakia	58.28	31.25	67.33	68.98	57.88
10	Latvia	77.89	40.97	40.19	64.9	57.59
11	Greece	25.89	73.67	74.89	47.45	55.37
12	Estonia	68.49	33.41	35.93	61.54	50.48
13	Italy	26.09	62.95	72.61	37.64	49.13
14	Slovenia	48.7	57.6	37.79	52.23	49.12
15	Cyprus	45.12	81.76	33.9	38.56	48.76
16	Portugal	37.89	74	43.84	40.67	48.65
17	Spain	32.02	57.58	56.55	34.49	44.37
18	Czech Republic	44.57	32.86	46.19	50.09	41.09
19	Belgium	31.05	42.21	53.85	26.39	38.16
20	France	27.48	43.18	52.19	29.61	37.23
21	United Kingdom	41.69	32.69	26.53	27.72	30.81
22	Ireland	28.74	35.68	25.47	31.24	27.2
23	Germany	29.3	26.57	35.36	23.65	26.46
24	Finland	35.81	18.06	37.58	19.11	25.08
25	Austria	20.09	43.15	24.93	24.74	24.88
26	Denmark	27.48	16.58	8.4	30.79	17.77
27	Sweden	21.43	13.76	24.61	14.14	14.79
28	Netherlands	27.63	12.91	5.73	20.38	12.54
29	Norway	14.04	6.04	0	9.97	2.37

Table 4.6: Ranking of countries according to the MP-CI scores based on the Two Step Approach

In order to interpret the previous results we proceeded with a CI Decision Matrix, in which the critical aspects that have a negative impact on Poverty are highlighted.

In Figure 4.5 the scatter plot for the MP-CI based on Two-Step Approach is reported. According to this analysis, Health proves to be especially critical for the MP-CI. In the area to maintain there is Employment. Living Standards is in the area to increase: the impact of this LV on MP-CI is low compared to its mean value. The CI Education is in the area to be improved.

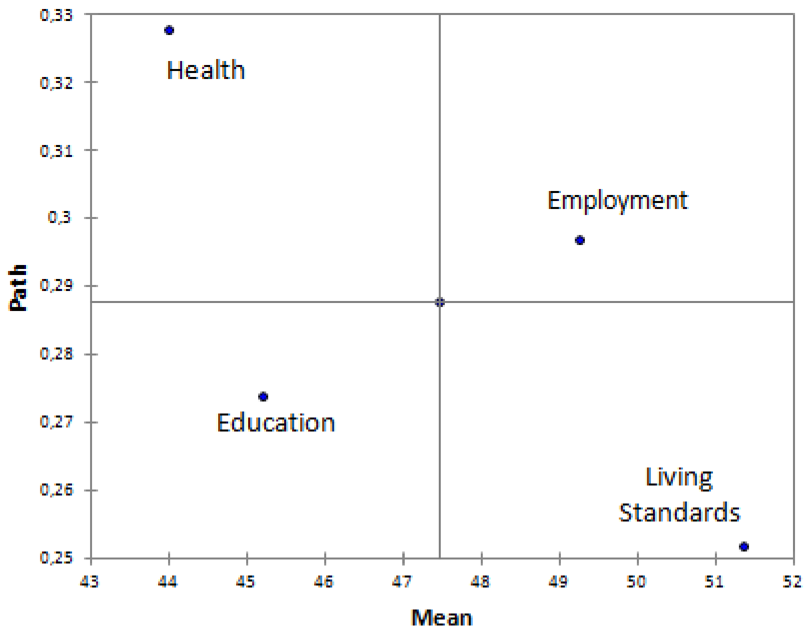


Figure 4.5: The scatter plot of the MP-CI based on the Two Step Approach

4.4.5 Conclusions for Higher-Order MP-CI

The empirical case of a Multidimensional Poverty Composite Indicator was analyzed in order to show and compare three main approaches for the PLS-PM parameter estimation in the presence of Higher-Order Constructs. In particular, this paragraph has focused on the Second-Order Constructs similar to the Type II category reported by Jarvis et al. [71], where the model defines reflective First-Order constructs and a formative Second-Order Construct.

The case study has revealed that the Hybrid Approach has bad performances in terms of measurement indexes and global indexes, and, in addition it produces non-significant parameters. Moreover, in the Repeated Indicators Approach, the path coefficients reported in Table 4.4 (0.288; 0.203; 0.304; 0.341) define the intensity of the causal relationships between the *MP-CI* and its four dimensions, represented by First-Order LVs. This means, for instance, keeping the other parameters constant, if we increase *Health* by a quantity equal to 1, the perception of poverty will increase by 0.288. In the Two Step Approach, the relationships between *Health*, *Education*, *Employment* and *Living Standards* are structural coefficients of a measurement model. The path coefficients (0.328; 0.274; 0.297; 0.252) reflect the composition of the Second-Order *MP-CI*; they do not represent how much the First-Order Dimensions affect the Higher-Order Construct, but, rather, the extent to which the higher level of abstraction is formed by its Lower-Order Constructs.

4.5 Conclusions

Generally, the choice of the best approach clearly depends on the type of design.
In the case where a Second-Order Construct is formatively related to the First-Order Dimensions and each construct is reflectively measured by its MVs, the Two Step Approach works better than the other two approaches. As regards the amount of explained variance, the Two Step Approach produces better explained relationships between the two orders of the model. Additionally, with regard to the parameter estimation, in general, the Two Step Approach is the best.
Next, we can conclude that for the Repeated Indicators Approach, the Second-Order LV, being hierarchically superior, could be seen as a context variable and the focus is on the impact of the First-Order LVs on the Higher-Order LV. In the Two Step Approach, the Second-Order LV is measured by the First-Order LV and the aim is to understand to what extent each First-Order LV reflects (in terms of covariance) the composition of the Second-Order level. Moreover, the Two Step Approach proves suitable for the estimation of formative Second-Order Constructs since it produces estimates that are better than those obtained through the Repeated Indicators Approach. In addition, the Two Step Approach is more theoretically consistent than the Repeated Indicators Approach in the definition of the Second-Order LV measurement model. As a matter of fact, reflectively measured constructs require homogeneous indicators and the Two Step Approach, using an LV component instead of the entire set of MVs, reduces the heterogeneity in the indicators.

Chapter 5

New methods in PLS Path Modeling for the building a System of Composite Indicators

5.1 Introduction

The importance of modeling and estimating Higher-Order Construct, from both a theoretical and an empirical point of view, has been recognized by many researchers since the dawn of factor analysis [67]; [151] and has been emphasized in many studies recently [34];[81];[97]. Unfortunately, the research is almost exclusively conducted in the area of covariance-based SEM. Neverthless, the aim of estimating Higher-Order Constructs can be achieved by means of PLS-PM [95];[186]. Three different approaches that allow you to model and estimate Second (and Higher)-Order Constructs and their relationship with other constructs in a nomological network have been adopted in the literature. In the Chapter 4 these approaches to Higher-Order Constructs have been described in detail and some of their limitations discussed.
Now we will only focus on certain of these limitations, that are typical of Two Step Approach: namely, the meaning of component for each Lower-

Order Construct and the possibility of choosing the number of these components in the analysis of the Higher-Order Construct.
In the classic Two Step Approach, the only first component of the Lower-Order Constructs is estimated without the Higher-Order Construct. This first component is the one that best represents its block of MVs. Next, these first components are included in the analysis as indicators of the Higher-Order Construct.
Therefore, this approach presents two important limitations related to components of each block: only one component is chosen for each block, and this has a strong representative power but a weak predictive power in the analysis of the Higher-Order Construct. For these reasons, in order to overcome these two drawbacks, in this work two alternative methods to estimate the Higher-Order Constructs are proposed. In particular, in order to resolve the issue related to the predictive power of the component for each Lower-Order Construct, the *Mixed Two Step Approach* is proposed and, regarding the choice of the number of components for each block, the *Partial Least Squares Component Regression Approach* is proposed. These approaches will be described in detail in the next section, and for each approach a simulation and an application on real data will be presented.

5.2 The First Alternative Approach: "The Mixed Two Step Approach"

Sanchez [142] suggests an way in order to compute scores for the Lower-Order LVs: you can obtain a score for a First-Order Construct by taking the first principal component of its indicators. Next, the PCA scores of Lower-Order Constructs are subsequently used as indicators for the Higher-Order Construct in a separate PLS path model. This component captures accurately the structure of variability of block so as to maximize the representativeness of the block. Its limitation is that, in a path model where all relationships among the LVs are considered, it is not able to predict the endogenous LV. For this reason, in this work we propose an alternative approach that computes in a different way the scores for the LVs of the

Lower-Order.

5.2.1 The Mixed Two Step Approach implemented in PLS-PM

The Mixed Two Step Approach begins with the implementation of the PLS-PM in the case of the Repeated Indicators Approach. In this way, the algorithm gives the scores of the Lower-Order blocks. Then, the scores of the blocks are used as indicators of the Higher-Order Construct, and at this point the PLS-PM algorithm is performed again.
Schematizing, the Mixed Two Step Approach consists of two steps:

- First, a Higher-Order Construct is formed by all the MVs of the Lower-Order Constructs and the PLS-PM algorithm is performed;

- The scores for each block obtained after the implementation of the algorithm are used as MVs of the Higher-Order Construct and the PLS-PM algorithm is performed again.

In the following sections these steps are described in detail, considering only the Second-Order Construct.
So, initially, because the Second-Order Construct has no MVs of its own, we consider it as formed of all the MVs of the First-Order Constructs, as in Figure 5.1.

Firstly, the outer model of the First-Order Constructs is expressed by the classic equation of PLS-PM:

$$\xi_q^I = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} + \delta_q \tag{5.1}$$

while the structural model, that specifies the relationships between the LVs on the First-Order Construct and the Second-Order Construct, is represented by the following equation:

$$\xi_j^{II} = \sum_{(q:\xi_q^I \rightarrow \xi_j^{II})} \beta_{qj} \xi_q^I + \zeta_j \tag{5.2}$$

where ξ_j^{II} is formed by all the MVs of the First-Order Construct:

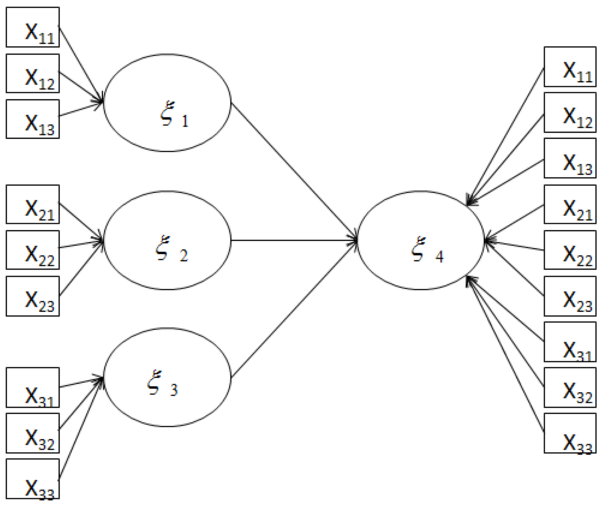


Figure 5.1: Second-Order Construct with all the MVs of the First-Order Construct

$$\xi_j^{II} = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} + \delta_q \tag{5.3}$$

Starting from this structure, a PLS-PM algorithm is performed in such a way as to obtain the scores of each block (Figure 5.2):
Once the scores for the blocks have been obtained, these will be the MVs of the Second-Order Construct (Figure 5.3).
The outer model equation of the First-Order Construct and the structural model equation are the same as before:

$$\xi_q^{I} = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} + \delta_q \tag{5.4}$$

$$\xi_j^{II} = \sum_{(q:\xi_q^I \rightarrow \xi_j^{II})} \beta_{qj} \xi_q^{I} + \zeta_j \tag{5.5}$$

while the outer model equation of the Second-Order Construct becomes a function of the components obtained:

$$\xi_j^{II} = \sum_{q=1}^{Q} \omega_h \hat{\xi}_q^{I} + \delta_j \tag{5.6}$$

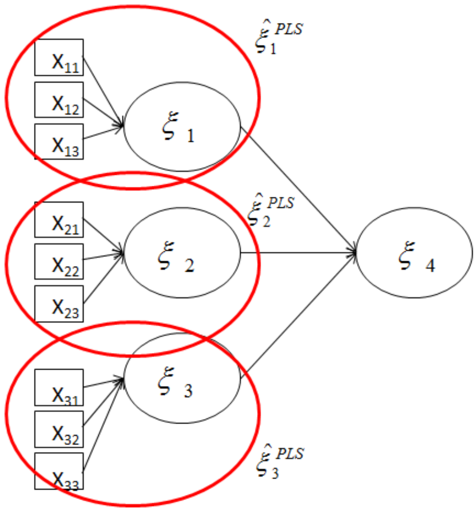


Figure 5.2: The scores of each Lower-Order Construct

At this moment, once that scores of the PLS-PM are assigned as indicators of the Second-Order Construct, the PLS-PM algorithm can be implemented. Therefore, we propose this method in order to use the component that is the best representative of its block and, at the same time, has the best predictive power on the Higher-Order LV.

5.3 The Second Alternative Approach: "Partial Least Squares Component Regression Approach"

In the Two Step Approach only the first component of the block is estimated. As has already been said, according to Sanchez [142], the first principal component is taken into account. The Principal Component Analysis (PCA) is a multivariate statistical method which consists in synthesizing a block of MVs and extracting the most relevant information that describes the systematic variability of the block. Choosing only the first component, it can happen that the remaining portion of the variability of the block is not taken into account. For this reason, the *PLS Component Regression Approach* is proposed in order to overcome the problem related to the number of components of the Lower-Order Constructs, giving the possibility of choosing the number of components to be extracted manually or according

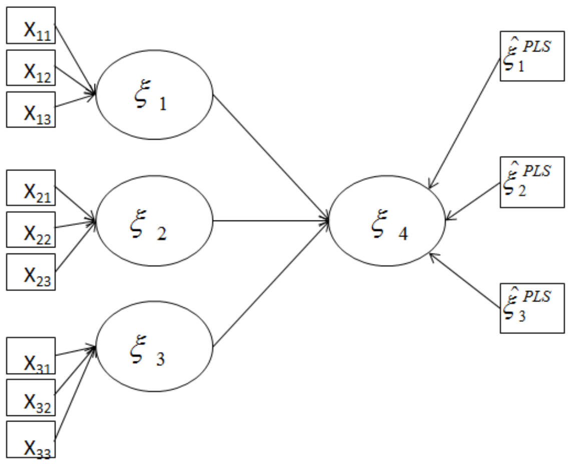


Figure 5.3: Second-Order Construct with the PLS scores of the First-Order Construct

to a criterion. In addition, since the aim of PLS-PM is to estimate the relationships between the LVs, this approach provides components that are at the same time representative of their blocks and predictive of the Higher-Order Construct.

5.3.1 The PLS Regression method

PLS Regression is the method that most people think of when hearing the acronym PLS. Briefly, PLS Regression is just an algorithm for regression analysis in which we want to analyze one block of response variables Y in terms of another block of predictor variables X. When we have more than one response variable, we talk about PLS-R2, the PLS version of multivariate regression.

This technique allows you to relate a set of predictor variables to one or several response variables. At the same time, PLS-R decomposes the predictor matrix by sequentially extracting orthogonal components which at the same time summarize the explanatory variables and allow a modeling and predicting of the response variables. PLS-R can be included among regularized regression methods, as PLS estimators have be proved to be shrinkage estimators [26]. From the algorithmic point of view, PLS Regression can be seen as an extension of the Non Linear Iterative Partial Least

Squares (NIPALS) algorithm to the analysis of a cross-covariance matrix. Moreover, it can be considered as a slightly modified version of the two blocks of the PLS-PM algorithm.
Let $x_1, x_2....x_P$ be a set of P predictor variables and $y_1, y_2, ...y_R$ be a set of R response variables measured on N observations. We suppose that all variables are centred. The PLS-R model assumes that there is a common structure underlying the two blocks of variables, and that this structure can be summarized by a few latent components $t_h(h = 1....H)$, calculated as a linear combination of the predictor variables. The predictor and response matrices **X** and **Y** are decomposed as:

$$X = T_H P_H^{'} + E_H \tag{5.7}$$

$$Y = T_H C_H^{'} + F_H \tag{5.8}$$

where P_H and C_H are the loading matrices, and E_H and F_H the residual matrices representing the part of the variability in the data due to noise. The parameters of the model are calculated by means of the PLS Regression algorithm, also called PLSR2 in the multiple response case and PLSR1 in the single response case [164].
A detailed review of the mathematical properties and the algorithm of PLS-R is given in Tenenhaus [164].
From the computational point of view, the PLS-R algorithm can extract a number of components equal to the rank of **X**. However, the PLS Regression model supposes that the common information carried by the **X** and **Y** matrices can be summarized in a few latent components. So, a crucial issue in the PLS-R model is the definition of the number H of components to retain. In PLS Regression the explicative ability of the model (measured in terms of the R^2 index) increases as long as the number of the components increases. On the contrary, the predictive ability of the model, intended as the explicative ability of the model referred to units that have not been considered in building the model (the validation set), begins to decrease after a certain number of components. This means that the model overfits the data, and the extraction of the components has to stop.

A cross validation procedure is usually performed in order to evaluate if the $h-th$ component increases the predictive ability of the model. The original sample is partitioned into S sub-samples. For S times, a different subsample is retained as validation data and the remaining (S-1) subsamples are used as training data. Each time, for each unit of the validation set, the squared prediction errors $e^2_{(-i)r}$ referred to $\mathbf{y}_r$ are calculated. For each h-component model, the PRediction Error Sum of Squares (PRESS) index is obtained as:

$$PRESS_{rh} = \sum e^2_{(-i)r} \tag{5.9}$$

Model over-fitting is investigated by plotting the PRESS index against the number of components. Typically, PRESS decreases for a certain of components; then, it begins to increase. Obviously, the number of components giving the minimum PRESS is chosen. In order to measure the marginal contribution of the h-th component to the predictive power of the model the Q^2 index [4] is used:

$$Q^2_h = 1 - \frac{\sum_{r=1}^{R} PRESS_{rh}}{\sum_{r=1}^{R} RESS_{r(h-1)}} \tag{5.10}$$

where $RESS_h r$ is the sum of the squared residuals of $\mathbf{y}_r$ in a $h-1$ component model on the whole dataset. There are no *ad hoc* tests to assess the significance of this index; in practice, the h-th component is retained if $Q^2_h \geq 0.0975$.

The regression equation

PLS Regression provides a classic regression equation, in which the response is estimated as a linear combination of the predictor variables. The following equation can be derived from the last step of the PLS-R algorithm:

$$\mathbf{Y} = \mathbf{t}_1\mathbf{c'}_1^{+}\mathbf{t}_2\mathbf{c'}_2 + \mathbf{t}_H\mathbf{c'}_H + \mathbf{F}_H = \mathbf{T}_H\mathbf{C'}_H \tag{5.11}$$

This is the regression equation of a H-component PLS-R model, where the response variables are expressed as a function of the PLS components. In a

PLS-R algorithm each $\mathbf{t}_h$ is calculated as a function of $\mathbf{E}_{h-1}$:

$$t_h = E_{h-1}\omega_h \tag{5.12}$$

In a model with H components, the matrix $\mathbf{T}_H$ of the $\mathbf{X}$-scores factors can be obtained as a function of the original $\mathbf{X}$ variables. After some replacements, we obtain the responses as a linear function of the predictor variables:

$$\mathbf{Y} = \mathbf{T}_H\mathbf{C'}_H + \mathbf{F}_H = \mathbf{X}\mathbf{B}_H^{PLS} + \mathbf{F}_H \tag{5.13}$$

where $\mathbf{B}_H^{PLS}$ is the matrix of the coefficients of an H-component PLS regression model.

5.3.2 The PLS-Regression implemented in Higher-Order PLS-PM

The PLS-R model assumes that there is a common structure underlying the two blocks of variables, and that this structure can be summarized by a few latent components $t_h(h = 1...H)$, calculated as a linear combination of the predictor variables.
In the case of a Higher-Order Construct, Lower-Order Constructs are considered as blocks of predictor variables and the Higher-Order Construct as a block of response variables. In this way, PLS-Regression for each block is performed, so as to obtain h components for each block. Next, these h components will represent MVs of the Higher-Order Construct.
Schematizing, the PLS Component Regression Approach consists of three steps:

- First, a Higher-Order Construct is formed of all the MVs of the Lower-Order Constructs;
- PLS-Regression is applied in order to obtain h components for each block;
- Once h components have been obtained, these will be MVs of the Higher-Order Construct and the PLS-PM algorithm is performed.

This method, at the moment, is applied only for the Higher-Order Construct at the second level. In the following section the steps are described in detail, considering only the Second-Order Construct. So, initially, because the Second-Order Construct has no MVs of its own, we consider it formed of all the MVs of the First-Order Constructs, as in Figure 5.4.

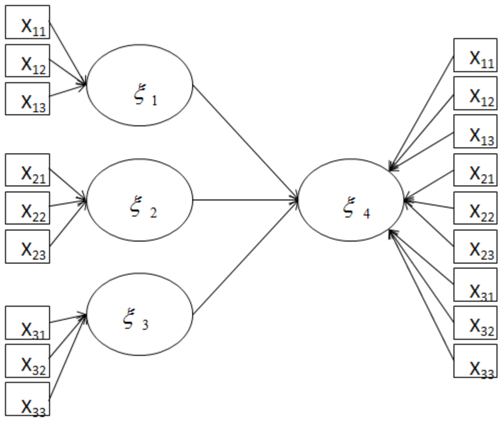


Figure 5.4: Second-Order Construct with all the MVs of the First-Order Construct

First, the outer model of the First-Order Constructs is expressed by the classic PLS-PM equation:

$$\xi_q^I = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} + \delta_q \tag{5.14}$$

while the structural model, which specifies the relationships between the LVs on the First-Order Construct and Second-Order Construct, is represented by the following equation:

$$\xi_j^{II} = \sum_{(q:\xi_q^I \rightarrow \xi_j^{II})} \beta_{qj} \xi_q^I + \zeta_j \tag{5.15}$$

where ξ_j^{II} is formed by all the MVs of the First-Order Construct:

$$\xi_j^{II} = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} + \delta_q \tag{5.16}$$

Starting from this structure, PLS-Regression is applied for each block of the First-Order Construct, where each block of the First-Order represents a set of Predictor Variables and the Second-Order Construct is a set of Response Variables.

Once h components for blocks have been obtained, these will be the MVs of the Second-Order Construct (Figure 5.5):

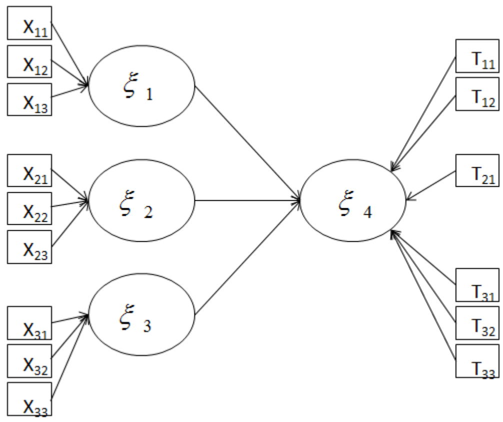


Figure 5.5: Second-Order Construct with the PLS-R Component of the First-Order Construct

The outer model equation of the First-Order Construct and the structural model equation are the same as before:

$$\xi_q^I = \sum_{p=1}^{P_q} \omega_{pq} x_{pq} + \delta_q \tag{5.17}$$

$$\xi_j^{II} = \sum_{(q:\xi_q^I \rightarrow \xi_j^{II})} \beta_{qj} \xi_q^I + \zeta_j \tag{5.18}$$

while the outer model equation of the Second-Order Construct becomes a function of the components obtained:

$$\xi_j^{II} = \sum_{h=1}^{H} \omega_h T_h^I + \delta_j \tag{5.19}$$

At this moment, once the PLS-R Components are assigned as indicators of the Second-Order Construct, the PLS-PM algorithm can be implemented. This approach is proposed in order to overcome the drawback of the Two Step Approach related to the number of components chosen in the First-Order Constructs, and so captures as much of the variability of the block as possible.

5.4 Simulation Study

The aim of this study is to investigate, within the same simulation design, the performance of classic Two Step Approach and the Mixed Two Step and PLS Component Regression Approaches when a block is modeled as reflective and the path structure is modeled as formative. The object of the simulation is to compare these performances using different sample sizes, in order to understand the effect of the sample dimension. The performances are evaluated by means of the prediction accuracy, the estimate bias and the efficiency of the considered approaches. The following paragraphs report the simulation plan and some comments on the results obtained.

5.4.1 Data Generation

The Monte Carlo simulation was conducted by the R language package. The data generation process is consistent with the procedure described by Paxton et al. [117] for a Monte Carlo SEM study. As a first step, we define the structure of the model and the parameters of the population. In the second step, we generate randomly the Second-Order LV and given the parameters and the error terms, we estimate the First-Order LVs. According to the outer parameters and error terms, in the last step, we generate the First and Second-Order MVs. The underlying population model used for the simulation consisted of one Second-Order LV (denoted by ξ^{II}) and four First-Order LVs (denoted by ξ_1^I, ξ_2^I, ξ_3^I, and ξ_4^I), each of them formed by five MVs. Figure 5.6, for simplicity, reports only the LVs.
The relationship between the First and Second-Order LVs is also modeled as formative, so that the construct of the higher level can be seen to be generated by the LVs of the Lower-Order.
The three approach performances have been compared on the basis of the sample size (n = 50, 100, 300, 1000). The study design considers 500 replications for each condition.
Obviously, the Second-Order LV, in terms of the number of items, differs according to the estimation approach used: for the Two Step and Mixed Two Step Approaches, it will correspond to the number of First-Order LVs (which is 4) while for the PLS Component Regression Approach, the nu-

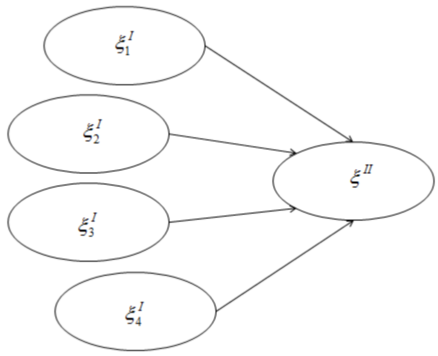


Figure 5.6: Path diagram for the Higher-Order Construct

merosity of block depends on the number of components of the First-Order dimension extracted by the PLS Regression.
The starting point is the generation of the First-Order LVs ξ_i^I as random variables $\xi_q^I \sim N(0,1)$. The data generated are re-scaled in the interval [1, 100]. The Second-Order Construct ξ_j^{II} has been computed as the product of ξ_q^I by the path coefficient vector β_{qj} with the addition of an error component ζ_j according to the following equation:

$$\xi_j^{II} = \sum_{(q:\xi_q^I \rightarrow \xi_j^{II})} \beta_{qj}\xi_q^I + \zeta_j \tag{5.20}$$

where the path coefficient vector (β) of the structural model is assumed to have elements equal to 0.8.
Each vector of the error component ζ_j is drawn from a univariate normal distribution [68] with a mean equal to zero and a standard deviation, $var(\zeta_j)$, chosen to satisfy the j^{th} Second-Order Construct, the equation being:

$$R_j^2 = \frac{var(model_j)}{var(total_j)} = \frac{var(model_j)}{var(model_j) + var(error_j)} \tag{5.21}$$

where $var(total_j)$ is the variance of ξ_j^{II}, given that:

$$\xi_j^{II} = \xi_q^I \beta_{qj} + \zeta_j = model_j + error_j \tag{5.22}$$

and $var(\zeta_j)$ is:

$$var(\zeta_j) = \frac{var(\xi_q^I) * (1 - R_q^2)}{R_q^2} \tag{5.23}$$

The R^2 value for the Second-Order Construct is set at 0.8. MVs are generated starting form the LVs, given the lambda coefficients, following the formula:

$$X_{nq}) = \xi_q^I * (\lambda^I)_k^{-1} + \delta_{nq} \tag{5.24}$$

where the error term is distributed as a continuous uniform: $\delta \sim U(-1, 1)$.
Two commonly reported measures are used to assess how well the methods estimate the parameters: Relative Bias (*RB*) and Standard Deviation (*StD*)
The *RB* is computed as:

$$RB = \frac{1}{n} \sum_{i=1}^{n} \frac{(\hat{\theta}_i - \theta)}{\theta} i = 1, 2, ..., 500 \tag{5.25}$$

where n represents the number of replications in the simulation, $\hat{\theta}_i$ is the parameter estimate for each replication and θ is the corresponding population parameter. The formula is equivalent to the mean *RB* [123]. A positive RB indicates an overestimation of the true parameter, a negative RB an underestimation.
The *StD* is computed as:

$$StD = \sqrt{\frac{1}{n} \sum_{i=1}^{n} (\hat{\theta}_i - E(\hat{\theta}))^2} i = 1, 2, ..., 500 \tag{5.26}$$

where $E(\hat{\theta})$ is the mean of the estimates across the 500 simulated datasets. This index provides information on the efficiency of the estimates.

5.4.2 Simulation Results: The path coefficients

Table 5.1 reports the simulation results relating to the coefficients β (computed as the average of the 500 replications), the bias and the standard errors. The results are grouped according to the estimation approach used and sample size. For each combination, the path coefficients, bias and standard error of the four parameters (β_1, β_2, β_3, β_4) are reported.

Table 5.1: Path coefficients, bias and standard error for the inner model

Approach	Sample Size	Value	β_1	β_2	β_3	β_4
Two Step	50	Path	0.7510	0.7631	0.7249	0.7042
		Bias	0.1150	0.0021	0.0132	0.0572
		SE	0.2798	0.1853	0.1583	0.1937
	100	Path	0.7769	0.7857	0.7727	0.7711
		Bias	0.0096	0.0044	0.0084	0.0047
		SE	0.1744	0.1022	0.0872	0.0726
	300	Path	0.7211	0.7754	0.6922	0.7635
		Bias	0.0009	0.0002	0.0003	0.0011
		SE	0.0725	0.1214	0.1173	0.0612
	1000	Path	0.7171	0.6543	0.7731	0.7673
		Bias	0.0005	0.0000	0.0004	0.0003
		SE	0.0245	0.0231	0.0232	0.0226
Mixed Two Step	50	Path	0.7969	0.7957	0.8027	0.8111
		Bias	0.0968	0.0554	0.0125	0.1191
		SE	0.2768	0.1557	0.0414	0.1939
	100	Path	0.8043	0.8128	0.8176	0.8204
		Bias	0.0807	0.00179	0.0176	0.1693
		SE	0.1079	0.0987	0.0940	0.0336
	300	Path	0.8175	0.8226	0.8243	0.8044
		Bias	0.0073	0.0004	0.0012	0.0082
		SE	0.0500	0.0934	0.0071	0.0563
	1000	Path	0.8174	0.8219	0.8159	0.8212
		Bias	0.0042	0.0003	0.0010	0.0051
		SE	0.0171	0.0162	0.0165	0.0160
PLS-R	50	Path	0.8276	0.8121	0.7928	0.8142
		Bias	0.0943	0.0611	0.0213	0.1065
		SE	0.2532	0.1229	0.0328	0.1532
	100	Path	0.8075	0.8164	0.7879	0.7923
		Bias	0.0091	0.0168	0.0198	0.1526
		SE	0.0976	0.0867	0.1010	0.0276
	300	Path	0.7987	0.7876	0.8179	0.8074
		Bias	0.0051	0.0008	0.0018	0.0075
		SE	0.0042	0.0761	0.0068	0.0042
	1000	Path	0.8165	0.7981	0.8134	0.8197
		Bias	0.0047	0.0002	0.0010	0.0043
		SE	0.0162	0.0152	0.0158	0.0090

The estimated path coefficients are all significant, as we expected according to the hypotheses made when defining the simulation plan. Some considerations can be made concerning the standard error. The standard error of each estimation β is shown in Figure 5.7. In all cases of the sample size, variability in the estimations is lower when using the Mixed Two Step and PLS-R Approaches.

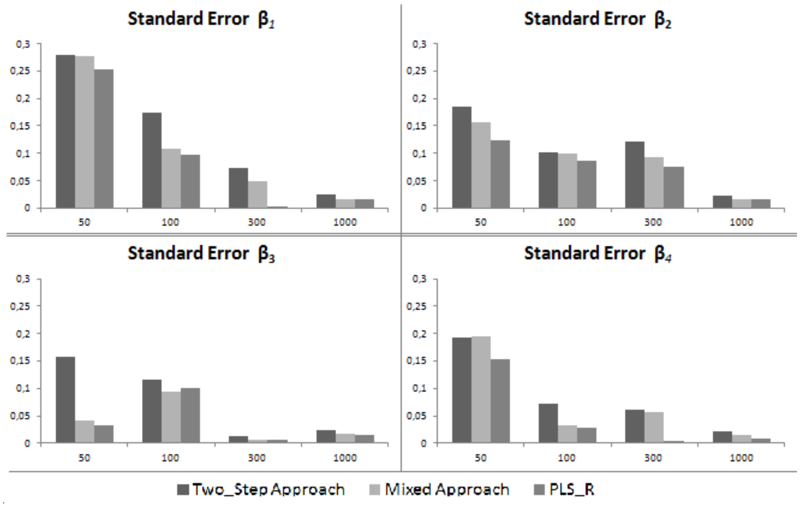


Figure 5.7: Standard errors of the path coefficients

5.4.3 Simulation Results: Bias and efficiency of the parameters

In order to evaluate the estimation accuracy, the relative bias (RB) is calculated according to the formula (5.25). The RB values of the path coefficients are reported in detail in Table 5.2.

Two Step Approach heavily underestimates all the path coefficients linking the First-Order Construct with the Second-Order LV in all sample sizes.

Looking at the new methods proposed, we can see that for small samples (n=50; n=100) the Mixed Approach works best, producing estimates near to zero, while the methods have the same performance for large samples (n=300; n=1000), giving an equivalent accuracy.

Table 5.2: RB of the path coefficients for each approach

	Approach	Sample Size			
		50	100	300	1000
	Two Step	-0.061	-0.029	-0.099	-0.104
β_1	Mixed Two Step	-0.004	-0.004	-0.004	-0.004
	PLS-R	0.034	0.009	-0.002	0.021
	Two Step	-0.046	-0.018	-0.031	-0.182
β_2	Mixed Two Step	-0.005	0.016	0.028	0.027
	PLS-R	0.015	0.021	-0.016	-0.002
	Two Step	-0.094	-0.034	-0.135	-0.034
β_3	Mixed Two Step	0.003	0.022	0.030	0.020
	PLS-R	-0.009	-0.015	0.022	0.017
	Two Step	-0.120	-0.036	-0.046	-0.041
β_4	Mixed Two Step	0.014	0.026	0.005	0.027
	PLS-R	0.018	-0.010	0.009	0.025

5.4.4 Simulation Results: The LV Prediction Accuracy

The prediction accuracy of both new methods is computed according to the Redundancy Index (Table 5.3).

Table 5.3: Redundancy for the Second-Order LV

	Approach	Sample Size			
		50	100	300	1000
	Two Step	0.2404	0.2994	0.3469	0.4725
ξ^{II}	Mixed	0.6502	0.6049	0.6484	0.7731
	PLS-R	0.6873	0.7091	0.7218	0.7371

The Mixed Two Step and PLS-R Approaches demonstrate a greater accuracy in predicting the higher level construct, since the Redundancy Index is higher than that for the Two Step Approach. The difference is remarkable for all sample size. So, these approaches are also the best option for predicting the Second-Order LV.

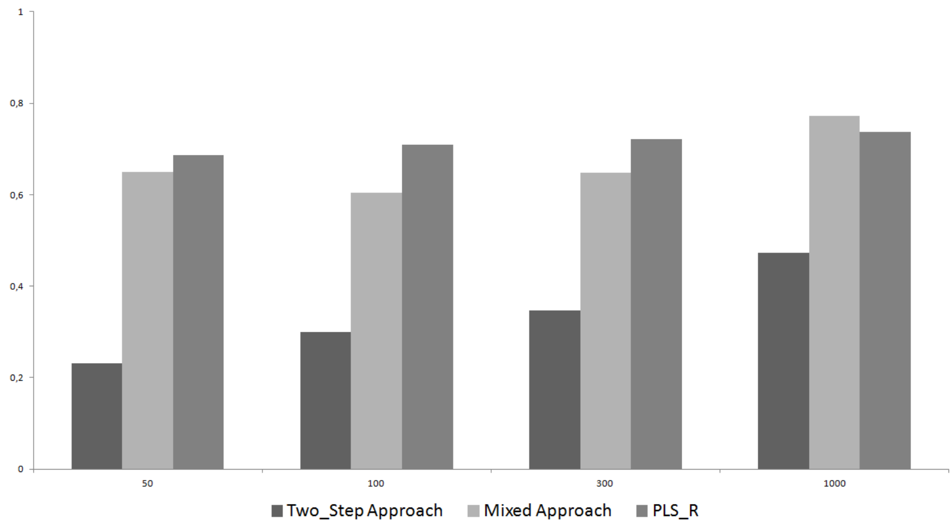


Figure 5.8: Redundancy for the Second-Order LV

5.4.5 Simulation Results: Choosing the Best Method

The performances of the new approaches proposed have been analyzed through a simulation study. The new methods proposed produce less biased and more stable parameter estimates than the Two Step Approach. In terms of the Relative Bias, the Two Step Approach significantly underestimates all the path coefficients linking the First-Order Construct with the Second-Order LV in all sample sizes. Instead, the new methods proposed produce less biased and more stable parameter estimates than the Two Step Approach.They are almost equivalent in terms of bias and MSE, giving an equivalent accuracy for large samples (n=300; n=1000), while in a small sample (n=50; n=100) the Mixed Two Step Approach works better than the PLS-R, producing estimates near to zero. As regards the variability of the estimates, we have found that the Standard Error of all the compared methods decreases when the sample size increases, even if the performances of the new path coefficients proposed are better than in the Two Step Approach. These two methods are always the best choice, in terms of the bias and MSE of the estimates, when the researcher aims at studying the relationships of the model with the formative relationships of the First-Order Constructs and the Second-Order LV.

The advantage of choosing the Mixed Two Step Approach to estimate these models is significant only with the smallest number of items for each construct; with a greater number of items the two approaches are equivalent.

5.5 Application to Real Data: Comparison of Methods

In this section, a case study concerning the Multidimensional Poverty Composite Indicator, already discussed in detail in Chapter 4, Higher-Order Construct in PLS-PM, is proposed in order to show the implementation of the new methods, and to give some comparative empirical results with respect o the Two Step Approach.
The estimation of the MP-CI as a Second-Order Construct is formatively related to the First-Order dimensions and reflectively measured by its MVs. We have considered the following models:

- The Two Step Approach: the PCA Component of each First-Order dimension is estimated at stage one;

- The Mixed Two Step Approach: the indicators of the Second-Order Construct are the PLS scores for each block obtained by the implementation of the PLS-PM algorithm;

- The PLS Component Regression Approach: the indicators of the Second-Order Construct are the Components of each block obtained from the PLS Regression; the number of components for each blocks is different according to their marginal contribution to the predictive power of the model.

5.5.1 Application Results: the Mixed Two Step and the PLS-Component Regression Approaches Performances

Table 5.4 reports the main quality measurements of the three models.
The assessment of a structural model estimated with the PLS-PM approach involves the inner as well as the outer model measurements of quality.
The results of the Two Step Approach are the same as in the previous chapter.

Table 5.4: Reliability Measures of the Higher-Order MP-CI for each approach

	Two Step Approach	Mixed Two Step Approach	PLS-R Approach
Cronbach's Alpha	0.875	0.895	0.852
Composite Reliability	0.915	0.927	0.904
Communality	0.730	0.762	0.727

Let's focus on the performances of the Mixed Two Step and PLS-Component Regression Approaches. The Cronbach's α and Composite Reliability indexes for both models are close to the conventional acceptability thresholds of 0.7 for the MP-CI. The Communality of the Mixed Two Step Approach is higher than that of the Two Step Approach (the communality of the Mixed Two Step Approach = 0.762 against the Communality of the Two Step Approach = 0.730). So, the amount of variability of the MVs captured by the MP-CI construct using this method is higher than when the classic Two Step Approach is adopted. It is important to note that there is a difference in the use of the scores of the First-Order dimensions.

In order to assess the significance of the path coefficients, Table 5.5 reports the value and significance of the structural coefficients linking the First-Order dimensions to the MP-CI.

In the Two Step Approach the Health dimension proves to be most influential among all the factors; in the Mixed Two Step and PLS Component Regression Approaches, the component that is most representative and at the same time most predictive on MP-CI is the Employment, with a path respectively of 0.308 and 0.521.

This means that if we consider the first approach, the component which is derived from the PCA is able to synthesize the more of its block than the most representative block in our case, namely Health.

Employment in PCA analysis is not very representative. With the Mixed Two Step Approach, which also considers the extent to which the block is able to predict the endogenous block, this dimension is revalued being the

Table 5.5: Path Coefficients and t-statistics for each approach (the most significant blocks for each method are marked in bold)

		Two Step Approach	Mixed Two Step Approach	PLS-R Approach
Health	path	**0.328**	0.284	0.233
	T-value	2.32	4.06	8.81
Education	path	0.274	0.268	0.284
	T-value	3.34	3.67	5.56
Employment	path	0.297	**0.308**	**0.521**
	T-value	3.09	4.54	2.44
Living Standards	path	0.252	0.284	0.258
	T-value	2.20	3.68	3.64

one with the highest coefficient.
If we consider, in the PLS Component Regression Approach, not just a single component but several components for each block, this dimension becomes even more important in terms of prediction. Table 5.6 reports the global measurement of goodness of fit.

Table 5.6: Global Measure of Goodness of Fit

Two Step Approach	Mixed Two Step Approach	PLS-R Approach
0.669	0.762	0.725

The goodness of fit of model is measured by the Redundancy. The Redundancy measures the percentage of variance explained by the LVs.
Taking into account all the LVs the Communality is never under 60%. The quality of the model is high in all three models, but slightly higher if we estimate the components with the Mixed Two Step Approach and PLS Component Regression Approach.
As was performed for the Two Step approach in the Chapter 4, also for these two methods we have compiled rankings of all European Community countries (Table 5.7; Table 5.8).
Also here, the scores have been normalized so that the values range from 0

(the lowest level of poverty) to 100 (the maximum level of poverty).

	Countries	Health	Education	Employment	Living Standards	MP-CI
1	Turkey	100	84.63	86.64	77.66	92.87
2	Romania	95.95	70.59	58.13	88.26	83.11
3	Macedonia	75.11	78.23	78.02	80.35	82.46
4	Bulgaria	73.22	75.9	65.35	80.26	77.67
5	Croatia	60.13	73.81	73.73	72.72	73.44
6	Poland	60.69	52.55	71.07	68.3	65.76
7	Hungary	61.46	37.61	73.91	70.85	63.58
8	Lithuania	64.86	50.68	50.24	68.13	60.46
9	Slovakia	58.63	31.47	67.56	69.18	58.8
10	Latvia	78.2	41.1	40.54	65.12	58.01
11	Greece	26.3	74.08	75.15	47.67	56.62
12	Estonia	68.82	33.66	36.27	61.79	51.08
13	Italy	26.33	63.16	72.79	37.91	49.98
14	Cyprus	45.26	82.11	34.26	38.77	49.76
15	Slovenia	48.77	57.66	38.11	52.54	49.51
16	Portugal	38.19	74.11	44.02	40.86	49.05
17	Spain	32.2	57.84	56.7	34.67	44.62
18	Czech Republic	44.96	33.26	46.58	50.29	43.68
19	Belgium	30.98	42.4	53.82	26.5	36.8
20	France	27.47	43.29	52.22	29.77	36.6
21	United Kingdom	41.62	32.56	26.51	27.82	29.81
22	Ireland	28.78	35.95	25.63	31.35	28
23	Germany	29.39	26.79	35.26	23.75	26.06
24	Austria	20.31	43.16	25.02	24.86	25.31
25	Finland	35.74	17.99	37.71	19.2	24.84
26	Denmark	27.47	16.47	8.44	30.81	17.31
27	Sweden	21.5	13.81	24.52	14.16	14.4
28	Netherlands	27.68	12.88	5.73	20.4	12.4
29	Norway	13.91	6.17	0	9.97	1.95

Table 5.7: Ranking of countries according to the MP-CI scores based on the Mixed Approach

	Countries	Health	Education	Employment	Living Standards	MP-CI
1	Turkey	100	84.21	87.09	77.93	86.08
2	Romania	96.19	71.88	58.82	88.86	82.78
3	Macedonia	75.75	78.49	78.48	80.7	80.93
4	Bulgaria	74.44	77.02	66.42	81.01	80.59
5	Croatia	60.69	74.33	74.27	73.46	73.72
6	Poland	61.19	53.19	71.49	69.06	66.56
7	Hungary	62.47	38.41	74.82	71.47	66.37
8	Lithuania	66.39	51.61	51.09	69.11	65.1
9	Slovakia	59.53	32.08	68.27	69.72	61.52
10	Latvia	79.16	41.45	41.55	65.85	60.25
11	Greece	27.43	75.26	75.82	48.23	58.78
12	Estonia	69.84	34.37	37.28	62.5	54.78
13	Slovenia	48.88	57.75	39.05	53.37	51.15
14	Cyprus	45.54	83.06	35.35	39.27	50.46
15	Italy	26.96	63.79	73.2	38.64	50.27
16	Portugal	38.98	74.48	44.61	41.39	49.71
17	Czech Republic	45.98	34.43	47.7	50.85	48.12
18	Spain	32.61	58.64	57.08	35.11	44.53
19	France	27.46	43.57	52.29	30.17	35.09
20	Belgium	30.79	42.96	53.66	26.8	33.91
21	Ireland	28.89	36.79	26.05	31.61	29.2
22	United Kingdom	41.41	32.14	26.42	28.06	27.13
23	Austria	21.03	43.08	25.21	25.19	26.29
24	Germany	29.65	27.37	34.92	24.03	25.07
25	Finland	35.48	17.82	38.12	19.5	22.77
26	Denmark	27.56	16.15	8.59	30.89	18.09
27	Sweden	21.68	13.94	24.3	14.3	13.32
28	Netherlands	27.86	12.78	5.69	20.49	12.7
29	Norway	13.78	6.58	0	10.06	2.34

Table 5.8: Ranking of countries according to the MP-CI scores based on the PLS Component Regression Approach

In the Figure 5.9 the scatter for the MP-CI based on two methods are reported.

According to this analysis, all the LVs are in the same location in the Two Step Approach. Only Health changes position considerably; if we estimate the model with the two new methods, the block of Health, which, in the

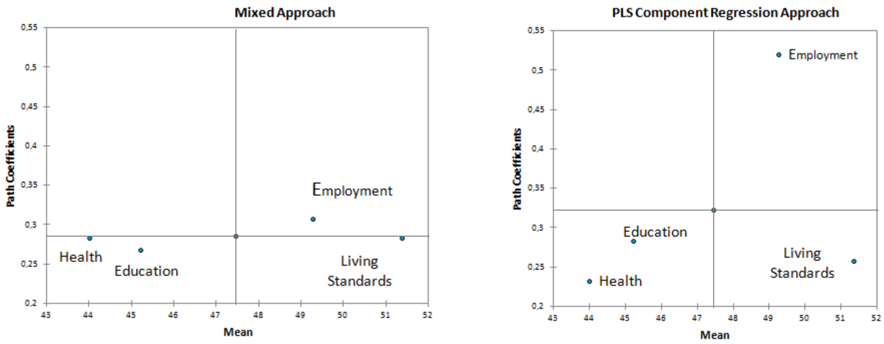


Figure 5.9: The scatter plot of the MP-CI based on the two methods

above analysis, was in the critical area, is now in the area to be monitored, with no LV being critical for the estimation of the MP-CI.

5.5.2 Application Results: Conclusions

The empirical case concerning a Multidimensional Poverty Composite Indicator has been analyzed in order to show the implementation of the new methods for the Higher-Order PLS-PM parameter estimation and to give some comparative results with respect to the classic Two Step Approach.
In all the methods used, unidimensionality is required: the Second-Order MP-CI is measured by the First-Order LVs. Next, the path coefficients measure the composition of the Second-Order MP-CI. These considerations have to be taken into account in the interpretation of the Multidimensional Poverty model. It is remarkable to note that the First-Order Employment, which influences weakly Poverty when the estimation approach used is that of the Two Step Indicators (β= 0.297), it proves to have a great importance in shaping Poverty when the approaches used are the Mixed Two Step Approach (β=0.308) and the PLS Component Regression Approach (β=0.521). Instead, Health, which in the previous analysis is the most important block in explaining the MP-CI, now has a revised impact. The countries' scores change very little, and generally the ranking remains unaltered; but it is important to note that the block of Health, which, in the Two Step Approach (Chapter 4) was in the critical area because it had a high impact on the MP-CI but a low mean value, now, calculated using

these two methods, lies in the area to be monitored, with a low value for the mean and the path coefficient.

5.6 Conclusions

The objective of this Chapter has been to introduce a new approaches for the PLS-PM parameter estimation in the presence of Higher-Order Constructs. In particular, we have focused on Second-Order Models similar to the Type II category reported by Jarvis et al. [71], where the model defines the reflective First-Order Constructs and a formative Second-Order Construct.

The classic Two Step Approach suggests the first principal component of the Lower-Order Constructs as an indicator of the Higher-Order Construct. This approach presents two important limitations related to the components of each block: only one component is chosen for each block, and this has a strong representative power but a weak predictive power in the analysis of the Higher-Order Construct. For these reasons, we have proposed two alternative methods to estimate the Higher-Order Constructs. In particular, in order to to solve the issue related to the predictive power of the component for each Lower-Order Construct, the *Mixed Two Step Approach* has been proposed, and, regarding the choice of the number of components for each block, the *Partial Least Squares Component Regression Approach* has been suggested.

The former approach consists of taking as the indicators of the Second-Order Construct the PLS scores for each block obtained by the implementation of the PLS-PM algorithm. The PLS Component Regression Approach, instead, allows us to choose more than one component for each block, obtained from the PLS Regression; the number of components for blocks is different according to their marginal contribution to the predictive power of the model. The performances of these two approaches have been analyzed through a simulation study and applied to a real case study to clarify the implementation The Mixed Two Step and PLS Component Regression Approaches are always the best choice, in terms of the bias and MSE of the estimates, when the researcher aims at studying the formative relationships of the structural model with constructs measured reflectively by their indicators. Moreover, they slightly outperform, in terms of prediction accuracy, the Two Step Approach. The empirical case on a Multidimensional Poverty Composite Indicators, working on a small sample, the Mixed Two Step Approach is the most powerful method, in terms of quality of the model. If we work on large samples the two method have the same performance or, to be more accurate, the PLS Component Regression Approach would be the best, because, as shown in the simulation, it would work better than the Mixed Two Step Approach.

Conclusions and Future Research

In this dissertation we have addressed the issue of estimating of a complex concept formed of different dimensions, each representing different aspects of the concept, aspect which interact with each other. Many phenomena require, in order to be measured, the 'combination' of different dimensions, which must be considered together as the proxy of the phenomenon. This combination can be obtained by applying methodologies known as Composite Indicator. The existing literature offers different alternative approaches in order to obtain a Composite Indicator. We have focused on the Structural Equation Modeling Methodology, in particular on Partial Least Squares-Path Modeling Approach.
The Partial Least Squares-Path Modeling Approach allows you to estimate causal relationships, defined according to a theoretical model linking two or more latent complex concepts, each measured through a number of observable indicators. The basic idea is that the complexity inside a system can be studied by taking into account the entirety of the causal relationships among the Latent Variables, each measured by several Manifest Variables.
In the third Chapter we have discussed some improvements in the Partial Least Squares-Path Modeling Approach for the estimation of a system of Composite Indicators, especially using tools that have been developed in order to extend the classic algorithm of Partial Least Squares-Path Modeling to the treatment of non-metric data. Such tools allow you to include and test mediator and moderator effects, and to deal with heterogeneous data. By means of an application on these tools to the Italian Social Cohe-

sion Composite Indicator, we have presented three estimated models (an estimated model without the use of mediating Latent Variables and quantification, an estimated model with the use of mediating Latent Variables but no quantification and, finally, an estimated model with the use of mediating Latent Variables and quantification). We have demonstrated how, by using a suitable quantification and entering the effect of the mediation into the model, the estimation of the system of Composite Indicators significantly improves. Moreover, we have seen how a unique model for the construction of Composite Indicators is not always well suited to the entire population that we are studying, but we have noted that there are local models for each population according to its own characteristics; as a matter of fact, in modeling the real world, it is reasonable to expect that different classes showing heterogeneous behaviors may exist in the observed set of units. In the fourth chapter of this work we have focused on another aspect of Partial Least Squares-Path Modeling concerning the construction of a hierarchical component model. As a matter of fact, in a Composite Indicator framework, researchers have recently been focusing their attention on a particular aspect linked to multidimensionality and a high level of abstraction, when a Composite Indicator is manifold, lacks its own Manifest Variables and is described by various underlying blocks, and many approaches have been proposed for treating these particular Composite Indicator aspects.

In this perspective, in Chapter five of this dissertation, we have proposed new methods to estimate a system of Higher-Order Composite Indicators, to improve, at a conceptual level, the significance of the model: the Mixed Two Step Approach and the Partial Least Squares Component Regression Approach.

We have compared these two methods and the classical Two Step Approach, in the framework of the same simulation design, investigating the effects of the measurement model and their predictiveness. The model considered for this simulation is a simple pattern, consisting of four First-Order Constructs that impact on a Second-Order Latent Variable. The decision to consider this model has resulted from the need to begin to understand how these methods work. We have encountered several difficulties in studying their performances, difficulties related to the lack of appropriate comprehensive global evaluation indexes, a problem that is still open. Until now, we have no way to compare globally models built with different methods. For this reason, further studies on the global assessment indexes of Partial Least Squares-Path Modeling are needed. We are already working on finding a way to evaluate a Partial Least Squares-Path Modeling in order to construct a system of Composite Indicators.

Moreover, we think that it would also be interesting to look further into the issue of considering different methods of estimation in place of the Ordinary Least Squares, inside the Partial Least Squares-Path Modeling algorithm. Further research will be undertaken to find out if we can use a Weighted Least Squares method, namely a variant of the Ordinary Least Squares method, optimizing the weighted fitting criterion to find the parameter estimates that allow the weights to determine the contribution of each indicator to the final Composite Indicator estimates. We aim to find an internal optimization in the Partial Least Squares-Path Modeling algorithm, which allows us to have indicators weighted according to their importance and their predictive power within the model.

In short, this work represents only a first step in this direction of comprehension. Different levels of complexity of the structural model, with different levels of abstraction and with mediator and moderator effects, will be considered in further studies.

Bibliography

[1] Addinsoft. XLSTAT - Statistics Package for Excel. `http://www.xlstat.com/` (2011).

[2] Agarwal, R. and Karahanna, E. Time flies when you're having fun: Cognitive absorption and beliefs about information technology usage. *MIS Quarterly* (2000).

[3] Anderson, J. C. and Gerbing, D. W. Structural equation modeling in practice: A review and recommended two-step approach. *Psychological Bulletiny, 103, 411 - 423* (1988).

[4] Ball, R. J. The significance of simultaneous methods of parameter estimation in econometric models. *Applied Statistics, 12, 14 - 25* (1963).

[5] Baron, R. M. and Kenny, D. A. The Moderator Mediator Variable Distinction in Social Psychological Research: Conceptual, Strategic, and Statistical Considerations. *Journal of Personality and Social Psychology, 51 (6), 1173 - 1182* (1986).

[6] Becker, J. M., Klein, K., and Wetzels, M. Hierarchical Latent Variable Models in PLS-SEM: Guidelines for Using Reflective-Formative Type Models. *Long Range Planning, 45 (5-6), 363 - 365* (2012).

[7] Becker, J. M., Rai, A., Ringle, C. M., and Vólckner, F. Discovering unobserved heterogeneity in structural equation models to avert validity threats. *MIS Quarterly, 37 (3), 665 - 694* (2013).

[8] Benzécri, J. P. Pratique de L'Analyse des Données, Analyse Des Correspondances. *Exposé Élementaire, Dunod, Bordas, Paris* (1980).

[9] Burt, R. S. Confimatory Factor-Analytic Structures and the Theory Construction Process. *Sociological Methods and Research, 45, 131 - 190* (1973).

[10] Carte, T. A. and Russell, C. J. In pursuit of moderation: Nine common errors and their solution. *MIS Quarterly, 27, 479 - 501* (2003).

[11] Cherchye, L., Knox Lovell, C. A., Moesen, W., and Van Puyenbroeck, T. One Market, One Number? A Composite Indicator Assessment of EU Internal Market Dynamics. *European Economic Review* (2006).

[12] Chin, W. W. Issues and opinion on structural equation modeling. *MIS Quarterly, 22 (1), vii - xvi* (1998).

[13] Chin, W. W. *The Partial Least Squares Approach to Structural Equation Modeling*. Marcoulides G. A. (Ed): Modern Business Research Methods, Mahwah, NJ: Lawrence Erlbaum Associates, 295 - 336, 1998.

[14] Chin, W. W. *Frequently Asked Questions-Partial Least Squares and PLS-Graph*. `http://discnt.cba.uh.edu/chin/plsfac.htm`, 2000.

[15] Chin, W. W. *Bootstrap cross-validation indices for pls path model assessment*. Esposito, Vinzi, V., Chin, W. W., Henseler, J., and Wang, H. (Eds): Handbook of Partial Least Squares (PLS): Concepts, Methods and Applications, Springer, Berlin, 83 - 97, 2010.

[16] Chin, W. W. *How to write up and report PLS analyses*. Esposito, Vinzi, V., et al., 2010.

[17] Chin, W. W. and Dibbern, J. *The partial least squares approach for structural equation modeling*. Marcoulides, G. A. (Ed): Modern methods for business research, London: Lawrence Erlbaum Associates, 2007.

[18] Chin, W. W. and Dibbern, J. *An Introduction to a Permutation Based Procedure for Multi-Group PLS Analysis: Results of Tests of Differences on Simulated Data and a Cross Cultural Analysis of the Sourcing of Information System Services between Germany and the USA*. Esposito, Vinzi, V., et al., 2010.

[19] Chin, W. W. and Gopal, A. Adoption intention in GSS: Relative importance of beliefs. *The Data Base for Advances in Information Systems, 26 (2&3), 42 - 64* (1995).

[20] Chin, W. W., Marcolin, B. L., and Newsted, P. N. A partial least squares approach for measuring interaction effects: results from a Monte Carlo simulation study and an electronic mail emotion/adoption study. *Information Systems Research, 14 (2), 189 - 217* (2003).

[21] Chow, G. C. Tests of Equality between Sets of Coefficients in Two Linear Regressions. *Econometrica, 28 (3), 591 - 605* (1960).

[22] Cohen, J. *Statistical power analysis for the behavioral sciences*. Mahwah, NJ: Lawrence Erlbaum, 1988.

[23] de Leeuw, J. and Van Rijckevorsel, J. *HOMALS and PRINCALS. Some generalizations of principal components analysis*. Diday, E. et al. (Eds): Data Analysis and Informatics, Amsterdam: North-Holland, 1980.

[24] de Leeuw, J., Young, F. W ., and Takane, Y. Additive structure in qualitative data: an alternating least squares method with optimal scaling features. *Psychometrika, 41, 471 - 503* (1976).

[25] De, Muro P., Mazziotta, M., and Pareto, A. Composite indices of development and poverty: An application to MDG Indicators. *Social indicators research, 104 (1), 1 - 18* (2011).

[26] De Jong, S. PLS shrinks. *Journal of Chemometrics, 9 (4), 323 - 326* (1995).

[27] De Lemus, S., Castillo, M., Moya Morales, M. C., Padilla Garcia, J. L., and Ryan, E. Elaboraciòn y validaciòn del Inventario de Sexismo Ambivalente para Adolescentes. *International Journal of Clinical and Health Psychology* (2008).

[28] Diamantopoulos, A. and Winklhofer, H. M. Index construction with formative indicators: An alternative to scale development. *Journal of Marketing Research, 38 (2), 269 - 277* (2001).

[29] Dickens, P., Valentova, M., and Borsenberger, M. A multidimensional assessment of social cohesion in 47 European countries. *CEP/INSTEAD, Luxembourg* (2011).

[30] Dolce, P. *Component-based Path Modeling: Open Issues and Methodological Contributions*. PhD thesis. University of Naples Federico II, 2015.

[31] Dolce, P., Esposito Vinzi, V., and Lauro, N. C. *Non-symmetrical component-based path modeling*. Abdi, H., et al., 2015.

[32] Ebert, U. and Welsch, H. Meaningful environmental indices: a social choice approach. *Journal of Environmental Economics and Management, 47, 270 - 283* (2004).

[33] Edwards, J. R. Multidimensional constructs in organizational behavior research: an integrative analytical framework. *Organizational Research Methods, 4 (2), 144 - 192* (2001).

[34] Edwards, J. R. and Bagozzi, R. P. On the Nature and Direction of the Relationship between Constructs and Measures. *Psychological Methods, 5 (2), 155 - 174* (2000).

[35] Esposito Vinzi, V., Fahmy, T., Chatelin, Y. M., and Tenenhaus, M. PLS Path Modeling: Some Recent Methodological Developments, a Software Integrated in XLSTAT and Its Application to Customer Satisfaction Studies. *Proceedings of the Academy of Marketing Science Conference Marketing Theory and Practice in an Inter-Functional World*. Verona, Italy, 2007.

[36] Esposito Vinzi, V. and Lauro, C. N. PLS regression and classification. *Proceedings of the PLS'03 International Symposium, 45 - 56*. France, 2003.

[37] Esposito Vinzi, V. and Russolillo, G. *Partial least squares path modeling and regression*. Wegman, Y, Scott, D. (Eds): Wiley Interdisciplinary Reviews: Computational Statistics, John Wiley and Sons, 2010.

[38] Esposito Vinzi, V., Trinchera, L., and Amato, S. *PLS path modeling: From Foundations to Recent developments and open issues for model assessment and improvement*. Esposito, Vinzi, V., et al., 2010.

[39] Esposito Vinzi, V., Trinchera, L., Squillacciotti, S., and Tenenhaus, M. REBUS-PLS: A response-based procedure for detecting unit segments in PLS path modeling. *Applied Stochastic Models in Business and Industry, 24 (5), 439 - 458* (2008).

[40] Fornell, C. and Bookstein, F. L. Two structural equation models: LISREL and PLS applied to consumer exit-voice theory. *Journal of Marketing Reseach, 19 (4), 440 - 452* (1982).

[41] Fornell, C. and Larcker, D. F. Evaluating structural equation models with unobservable variables and measurement error. *Journal of Marketing Reseach, 18, 39 - 50* (1981).

[42] Freudenberg, M. Composite indicators of country performance: a critical assessment. *OECD, Paris* (2003).

[43] Funtowicz, S. O. and Ravetz, J. R. Uncertainty and Quality in Science for Policy. *Kluwer Academic Publishers, Dordrecht, Nederland* (1990).

[44] Funtowicz, S. O. and Ravetz, J. R. *Uncertainty and Quality in Science for Policy*. Kluwer Academic Publishers, Dordrecht, NL, 1990.

[45] Garaigordobil, M. and Aliri, J. Sexismo hostil y benevolente: relaciones con el autoconcepto, el racismo y la sensibilidad intercultural. *Revista de psicodidactica* (2011).

[46] Garcia Leiva, P., Palacios, M. S., Torrico, E., and Navarro, Y. El sexismo ambivalente, un predictor de maltrato? *Psicologia Juridica y Forense* (2009).

[47] Geisser, S. The predictive sample reuse method with applications. *Journal of the American Statistical Association, 70, 320 - 328* (1975).

[48] Gifi, A. *Nonlinear Multivariate Analysis*. Wiley, Chichester, UK, 1990.

[49] Glick P., Fiske S. T. The Ambivalent Sexism Inventory: Differentiating hostile and benevolent sexism. *Journal of Personality and Social Psychology* (1996).

[50] Gonzalez Ortega, I., Echeburua, E., and De Corral, P. Variables significativas en las relaciones violentas en parejas jovenes: una revision. *Behavioral Psychology, 16 (2), 207 - 225* (2008).

[51] Gorsuch, R. L. *Factor Analysis*. Hillsdale, NJ: Lawrence Erlbaum Associates, 1983.

[52] Grassia M. G., Lauro N. C. Marino M. and Pandolfo, M. Indicatori Compositi da modello per lo studio della povertà e l'esclusione sociale. *Espanet Italia*. Torino, Italy, 2014.

[53] Guinot, C., Latreille, J., and Tenenhaus, M. PLS path modelling and multiple table analysis. Application to the cosmetic habits of women in Ile-de-France. *Chemometrics and Intelligent Laboratory Systems, 58 (2), 247 - 259* (2001).

[54] Hahn, C., Johnson, M., Herrmann, A., and Huber, F. Capturing customer heterogeneity using a finite mixture PLS approach. *Schmalenbach Business Review, 54, 243 - 269* (2002).

[55] Hair, J. F., Hult T., Ringle C. M., and Sarstedt, M. *A Primer on Partial Least Squares Structural Equation Modeling (PLS-SEM)*. Thousand Oaks, CA: Sage, 2014.

[56] Hair, J. F., Mena, J. A., Ringle, C. M., and Sarstedt, M. An assessment of the use of partial least squares structural equation modeling in marketing research. *Journal of the Academy of Marketing Science, 40, 414 - 433* (2011).

[57] Hair, J. F., Ringle, C. M., and Sarstedt, M. PLS-SEM: Indeed a silver bullet. *Journal of Marketing Theory and Practice, 19, 139 - 151* (2011).

[58] Hall, J. Measuring Progress – An Australian Travelogue. *Journal of Official Statistics, 21 (4), 727 - 746* (2005).

[59] Hanafi, M. PLS path modelling: computation of latent variables with the estimation mode B. *Computational Statistics, 22 (2), 275 - 292* (2007).

[60] Helm, S., Eggert, A., and Garnefeld, I. *Modelling the impact of corporate reputation on customer satisfaction and loyalty using PLS*. Esposito, Vinzi, V. et al., 2010.

[61] Henseler, J. On the convergence of the partial least squares path modeling algorithm. *Computational Statistics, 25 (1), 107 - 120* (2010).

[62] Henseler, J. and Chin, W. W. A comparison of approaches for the analysis of interaction effects between latent variables using partial least squares path modeling. *Structural Equation Modeling, (17), 82 - 109* (2010).

[63] Henseler, J. and G., Fassott. *Testing moderating effects in PLS path models: An illustration of available procedures*. Esposito, Vinzi, V. et al., 2010.

[64] Henseler, J., Ringle, C. M., and Sinkovics, R. R. *The use of partial least squares path modeling in international marketing*. Sinkovics, R. R., and Ghauri, P. N. (Eds): Advances in International Marketing, Emerald, Bingley, 277 - 319, 2009.

[65] Henseler, J. and Sarstedt, M. Goodness-of-fit indices for partial least squares path modeling. *Computational Statistics, 28 (2)* (2013).

[66] Hock, C., Ringle, C. M., and Sarstedt, M. Management of multipurpose stadiums: Importance and performance measurement of service interfaces. *International Journal of Services Technology and Management, 14, 188 - 207* (2010).

[67] Holzinger, K. and Swineford, F. The bi-factor method. *Psychometrika, 2 (1), 41 - 54* (1937).

[68] Hulland, J., Ryan, M. J., and Rayner, R. K. *Modeling customer satisfaction: a comparative performance evaluation of covariance structure analysis versus partial least squares*. Esposito, Vinzi, V., Chin, W. W., Henseler, J. and Wang, H. (Eds): Handbook of Partial Least Squares (PLS): Concepts, Methods and Applications, Springer-Verlag, Berlin, 2010.

[69] J., Salzman. Methodological Choices Encountered in the Construction of Composite Indices of Economic and Social Well-Being. *Ottawa Center for the Study of Living Standards* (2003).

[70] Jacobs, R., Smith, P., and Goddard, M. Measuring performance: an examination of composite performance indicators. *Centre for Health Economics, 29* (2004).

[71] Jarvis, D., MacKenzie, S., and Podsakoff, P. A critical review of construct indicators and measurement model misspecification in marketing and consumer research. *Journal of Consumer Research, 30 (3), 199 - 218* (2003).

[72] Jedidi, K., Jagpal, H. S., and De Sarbo, W. S. STEMM: A general finite mixture structural equation model. *Journal of Classification, 14 (1), 23 - 50* (1997).

[73] Johnson, R. E., Rosen, C. C., Chang, C. H., Djurdjevic, E., and Taing, M. U. Recommendations for improving the construct clarity of higher-order multidimensional constructs. *Human Resource Management Review, 22 (2), 67 - 72* (2012).

[74] Jöreskog, K. G. A general method for analysis of covariance structure. *Biometrika, 57, 239 - 251* (1970).

[75] Jöreskog, K. G. Simultaneous factor analysis in several populations. *Psychometrika, 57, 409 - 426* (1971).

[76] Jöreskog, K. G. Structural analysis of covariance and correlation matrices. *Psychometrika, 43, 443 - 477* (1978).

[77] Jöreskog, K. G. *Testing structural equation models*. Bolle, K. A. and Long, J. S. (Eds): Testing Structural Equation Models, Sage Publication, Newbury Park, 1993.

[78] Jöreskog, K. G. and van Thillo, M. LISREL: A general computer program for estimating a linear structural equation system involving multiple indicators of unmeasured variables. *ETS Research Bulletin Series, 2, 1 - 71,* (1972).

[79] Jöreskog, K. G. and Wold, H. *The ML and PLS techniques for modeling with latent variables: historical and comparative aspects*. Joreskog, K. G. and Wold, H. (Eds): Systems Under Indirect Observation, Part 1, North-Holland, Amsterdam, 263 - 270, 1982.

[80] Joseph, F., Hair, J. F., Hult, G. T., Ringle, C. M., and Sarstedt, M. *A Primer on Partial Least Squares Structural Equation Modeling (PLS-SEM)*. SAGE Publications, Inc., 2014.

[81] Kaiser, H. F. The varimax criterion for analytic rotation in factor analysis. *Psychometrika, 23 (3), 187 - 200* (1958).

[82] Keil, M., Saarinen, T., Tan, B., Tuunainen, V., Wassenaar, A., and Wei, K. K. A cross-cultural study on escalation of commitment behavior in software projects. *MIS Quarterly, 24, 299 - 325* (2000).

[83] Kim, G., Shin, B., and Grover, V. Investigating two contradictory views of formative measurement in information systems research. *MIS Quarterly, 34, 345 - 365* (2010).

[84] Kline, R. *Principles and practice of structural equation modeling*. Guilford Press, New York, 1998.

[85] Koka, B. R. and Prescott, J .E. Strategic alliances as social capital: a multidimensional view. *Strategic Management Journal, 23 (9), 795 - 816* (2002).

[86] Kramer, N. *Analysis of high-dimensional data with partial least squares and boosting*. PhD thesis. Technischen Universitat Berlin, Berlin, Germany, 2007.

[87] Kruskal, J. Multidimensional scaling by optimizing goodness of fit to a nonmetric hypothesis. *Psychometrika, 29 (2), 115 - 129* (1964).

[88] Lameiras Fernandez, M., Rodriguez Castro, Y., and Sotelo Torrejòn, M. J. Sexism and racism in a Spanish sample of secondary school students. *Social Indicators Research, 54 (3), 309 - 328* (2001).

[89] Law, K. S. and Wong, C. Multidimensional Constructs In Structural Equation Analysis: An Illustration Using the Job Perception and Job Satisfaction Constructs. *Journal of Management, 25 (2), 143 - 160* (1999).

[90] Law, K. S., Wong, C., and Mobley, W. H. Toward a Taxonomy of Multidimensional Constructs. *Academy of Management Review, 23 (4), 741 - 755* (1998).

[91] Lebart, L., Morineau, A., and P., Fénelon J. *Traitement des données statistiques*. 1979.

[92] Lee, L., Petter, S., Fayard, D., and Robinson, S. On the use of partial least squares path modeling in accounting research. *International of Accounting Information Systems 12, (4) 305 - 328* (2011).

[93] Little, T. D., Bovaird, J. A., and Widaman, K. F. On the merits of orthogonalizing powered and product terms: Implications for modeling latent variable interactions. *Structural Equation Modeling* (2006).

[94] Lohmöller, J. B. *PLS-PC: Latent Variables Path Analysis with Partial Least Squares - Version 1.8 for PCs under MS-Dos*. 1987.

[95] Lohmöller, J. B. *Latent Variable Path Modeling with Partial Least Squares*. Physica, Verlag, Heidelberg, Germany, 1989.

[96] Ludwig von, Bertalanffy. *General System Theory: Foundations, Development, Applications*. 1968.

[97] MacKenzie, S. B., Podsakoff, P. M., and Jarvis, C. B. The Problem of Measurement Model Misspecification in Behavioral and Organizational Research and Some Recommended Solutions. *Journal of Applied Psychology, 90 (4), 710 - 730* (2005).

[98] Mannarini, T., Ciavolino, E., Nitti, M., and Salvatore, S. The role of affects in culture-based interventions: Implications for practice. *Psychology, 3 (8), 569 - 577* (2012).

[99] Martinez Ruiz, A. and Aluja, T. Toward the definition of a structural equation model of patent value: PLS path modelling with formative constructs. *REVSTAT, 7(3), 265 - 290* (2009).

[100] Mazziotta, M. and Pareto, A. Nuove misure del benessere: dal quadro teorico alla sintesi degli indicatori. *SISmagazine, rivista on-line della Società Italiana di Statistica, `http://old.sis-statistica.org/magazine/spip.php?article194`* (2011).

[101] Merino Verdugo, E., Martinez Arias, N. R., and Diaz Aguado Jalòn, M. J. Sexismo, inteligencia emocional y adolescencia. *Psicologia Educativa, 77 - 88* (2010).

[102] Monecke, A. and Leisch, F. semPLS: Structural Equation Modeling UsingPartial Least Squares. *Journal of Statistical Software, 48 (3)* (2012).

[103] Moya Morales, M.C. *Actitudes sexistas y nuevas formas de sexismo*. Berbera, H. E., Benlloch, I. M., and Amparo, B. (Eds): Psicologia y genero, Madrid, Esoala: Pearson Educaciòn, 271 - 294, 2004.

[104] Munda, G. Social multi-criteria evaluation (SMCE): methodological foundations and operational consequences. *European Journal of Operational Research, 158 (3), 662 - 677* (2004).

[105] Munda, G. *Multi-Criteria Decision Analysis and Sustainable Development*. Figueira, J., et al., 2005.

[106] Munda, G. *Social multi-criteria evaluation*. Springer, Verlag, Heidelberg, New York, Economics Series, 2007.

[107] Munda, G. and Nardo, M. Constructing Consistent Composite Indicators: the Issue of Weights. *Joint Research Centre, Ispra* (2005).

[108] Munda, G. and Nardo, M. Non-compensatory/Non-Linear composite indicators for ranking countries: a defensible setting. *Applied Economics* (2007).

[109] Nappo, D. *SEM with ordinal manifest variables An Alternating Least Squares approach*. PhD thesis. University of Naples Federico II, 2009.

[110] Nardo, M., Saisana, M., Saltelli, A., and Tarantola, S. Tools for Composite Indicators Building. *European Commission, Ispra* (2005).

[111] Nardo, M., Saisana, M., Saltelli, A., Tarantola, S., Hoffman, A., and Giovannini, E. *Handbook on Constructing Composite Indicators: Methodology and User Guide*. OECD, 2005.

[112] Nations, United. *Human Development Report*. United Kingdom: Oxford University Press, `http://www.undp.org`, 1992, 1999, 2000, 2001.

[113] Netemeyer, R. G., Bearden, W. O., and Sharma, S. *Scaling Procedures: Issues and Applications*. Thousand Oaks, CA: Sage Publications, 2003.

[114] Noll, H. H. Social indicators and indicators systems: tools for social monitoring and reporting. *OECD, World Forum Statistics, knowledge and policy*. Palermo, Italy, 2004.

[115] Noonan, R. and Wold, H. Evaluating School Systems Using Partial Least Squares. *Evaluation in Education, (7), 219 - 364* (1993).

[116] OECD. *Quality Framework and Guidelines for OECD Statistical Activities*. OECD, `www.oecd.org/statistics`, 2003.

[117] Paxton, P., Curran, P. J., Bollen, K. A., Kirby, J., and Chen, F. Monte carlo experiments: Design and implementation. *A Multidisciplinary Journal, 8 (2), 287 - 312* (2001).

[118] Petter, S., Straub, D., and Rai, A. Specifying Formative Constructs in Information Systems Research. *MIS Quarterly, 31 (1), 623 - 656* (2007).

[119] Preacher, K. J. and Hayes, A. F. SPSS and SAS procedures for estimating indirect effects in simple mediation models. *Behavior Research Methods, Instruments, and Computers, 36, 717 - 731* (2004).

[120] Preacher, K. J. and Hayes, A. F. Asymptotic and resampling strategies for assessing and comparing indirect effects in simple and multiple mediator models. *Behavior Research Methods, 40, 879 - 891* (2008).

[121] R., Nilsson. Confidence Indicators and Composite Indicator. *CIRET conference*. Paris, France, 2000.

[122] Rajala, R. and Westerlund, M. Antecedents to consumers' acceptance of mobile advertisements – a hierarchical construct PLS structural equation model. $XLIII^{th}$ *Hawaii International Conference on Systems Sciences (HICSS)*. Hawaii, 2010.

[123] Reinartz, W., Echambadi, R., and Chin, W. W. Generating non-normal data for simulation of structural equation models using Mattson's method. *Multivariate Behavioural Research, 37 (2), 227 - 244* (2002).

[124] Reinartz, W., Krafft, M., and Hoyer, W. D. The Customer Relationship Management Process: Its Measurement and Impact on Performance. *Journal of Marketing Research, 41 (3), 293 - 305* (2004).

[125] Rifkin, J. *The European Dream*. Tarcher-Penguin, New York, 2004.

[126] Ringdon, E., Ringle, C. M., and Sarstedt, M. *Structural modeling of heterogeneous data with partial least squares*. Malhotra N. (Ed): Review of Marketing Research (Review of Marketing Research), 7, Emerald Group Publishing Limited, 255 - 296, 2010.

[127] Ringle, C. and Schlittgen, R. A genetic algorithm segmentation approach for uncovering and separating groups of data in PLS path modeling. *PLS'07: V^{th} International Symposium on PLS and Related Methods*. Oslo, Norway, 2007.

[128] Ringle, C. M. Segmentation for path models and unobserved heterogeneity: The finite mixture partial least squares approach. *Research Papers on Marketing and Retailing, 35 (1), University of Hamburg* (2006).

[129] Ringle, C. M., Wende, S., and Will, A. *Customer segmentation with FIMIX-PLS*. Aluja, T., et al., 2005.

[130] Ringle, C. M., Wende, S., and Will, A. *SmartPLS 2.0 (beta)*. University of Hamburg, 2005.

[131] Ringle, C. M., Wende, S., and Will, A. *Finite Mixture Partial Least Squares Analysis: Methodology and Numeric Examples*. Esposito, Vinzi, V., et al., 2010.

[132] Rosen, R. *Life Itself: A Comprehensive Inquiry into Nature, Origin, and Fabrication of Life*. Columbia University Press, 1991.

[133] Russet, B. M. Inequality and instability. *Word politics, 21, 422 - 454* (1964).

[134] Russolillo, G. *Partial Least Squares Methods for Non-Metric Data*. PhD thesis. University of Naples Federico II, 2009.

[135] Russolillo, G. Non-Metric Partial Least Squares. *Electronic Journal of Statistics, 6, 1641 - 1669* (2012).

[136] Ryan, T. and Joiner, B. Normal probability plots and test for normality. *Technical report, Statistic Departement, The Pennsylvania State University, USA* (1976).

[137] Saisana, M., Saltelli, A., and Tarantola, S. Uncertainty and Sensitivity Analysis Techniques as Tools for the Quality Assessment of Composite Indicators. *Journal of the Royal Statistical Society, 168 (2), 1 - 17* (2005).

[138] Saisana, M. and Tarantola, S. State-of-the-art. Report on Current Methodologies and Practices for Composite Indicator Development. *Institute for the Protection and Security of the Citizen Econometrics and Statistical Support to Antifraud Unit* (2002).

[139] Saltelli, A. Composite Indicators between analysis and advocacy. *Social indicators research, 81, 65 - 77* (2007).

[140] Saltelli, A. and Tarantola, S. On the relative importance of input factors in mathematical models: safety assessment for nuclear waste disposal. *Journal of American Statistical Association, 97 (459), 702 - 709* (2002).

[141] Sanchez, G. *PATHMOX Approach: Segmentation Trees in Partial Least Squares Path Modeling*. PhD thesis. Universitat Politecnica de Catalunya, 2009.

[142] Sanchez, G. *PLS Path Modeling with R*. Berkeley: Trowchez Editions, 2010.

[143] Sanchez, G. and Aluja, T. *Pathmox: a PLS-PM segmentation algorithm*. Esposito, Vinzi, V.,and Lauro, N. C., et al., 2006.

[144] Sanchez, G. and Aluja, T. A simulation study of PATHMOX (PLS path modeling segmentation tree) sensitivity. V^{th} *International Symposium - Causality explored by indirect observation*. Oslo, Norway, 2007.

[145] Sanchez, G. and Aluja, T. *Pathmox: Segmentation Trees in Partial Least Squares Path Modeling. R package version 0.1-1*. `http://CRAN.R-project.org/package=pathmox`, 2012.

[146] Sanchez, G. and Trinchera, L. *plspm: Partial Least Squares Data Analysis Methods. R package version 0.2-2*. `http://CRAN.R-project.org/package=plspm`, 2012.

[147] Sarstedt, M. A review of recent approaches for capturing heterogeneity in partial least squares path modelling. Journal of Modelling in Management*, 3 (2), 140 - 161* (2008).

[148] Sarstedt, M., Becker, J. M., Ringle, C. M., and Schwaiger, M. Uncovering and Treating Unobserved Heterogeneity with FIMIX-PLS: Which Model Selection Criterion Provides an Appropriate Number of Segments? *Schmalenbach Business Review, 63 (1), 34 - 62* (2011).

[149] Sarstedt, M. and Ringle, C. M. Treating Unobserved Heterogeneity in PLS Path Modelling: A Comparison of FIMIX-PLS with Different Data Analysis Strategies. *Applied Statistics, 37 (8), 1299 - 1318* (2010).

[150] Sarstedt, M., Ringle, C. M., Henseler, J., and Hair, J. On the emancipation of PLS-SEM: a commentary on rigdon. *Long Range Planning, 47, 154 - 160* (2014).

[151] Schmid, J. J. and Leiman, J. M. The development of hierarchical factor solutions. *Psychometrika, 22 (1), 83 - 90* (1957).

[152] Sen, A. Poverty and Famines: An Essay on Entitlement and Deprivation. *Oxford Clarendon Press* (1981).

[153] Sen, A. Development as capabilities expansion. *Journal of Development Planning, 19, 41 - 58* (1989).

[154] Sen, A. Development as Freedom. *Oxford University Press, Oxford* (1999).

[155] Sharpe, A. Literature Review of Frameworks for Macro-Indicators. *Ottawa Center for the Study of Living Standards* (2004).

[156] Sobel, M .E. Asymptotic confident intervals for indirect effects in structural equation models. *Socialogical Methodology, 13, 290 - 312* (1982).

[157] Sörbom, D. A general method for studying differences in factor means and factor structures between groups. *British Journal of Mathematical and Statistical Psychology, 27, 229 – 239* (1974).

[158] Squillacciotti, S. *Prediction oriented classification in PLS path modelling*. Aluja, T., et al., 2005.

[159] Stone, M. Cross-validatory choice and assessment of statistical predictions. *Journal of the Royal Statistical Society, 36, 111 – 147* (1974).

[160] Tarantola, S., Jesinghaus, J., and Puolamaa, M. *Global sensitivity analysis: a quality assurance tool in environmental policy modelling*. Saltelli, A., Chan, K., and Scott, M. (Eds): Sensitivity Analysis, John Wiley & Sons, New York, 385 - 397, 2000.

[161] Tarantola, S., Liska, R., Saltelli, A., Leapman, N., and Grant, C. The Internal Market Index 2004. *European Commission: JRC-Italy* (2004).

[162] Tarantola, S., Saisana, M., Saltelli, A., Schmiedel, F., and Leapman, N. Statistical techniques and participatory approaches for the composition of the European Internal Market Index 1992 - 2001. *European Commission: JRC-Italy* (2002).

[163] Tenenhaus, A. and Tenenhaus, M. Regularized generalized canonical correlation analysis. *Psychometrika, 76 (2), 257 - 284* (2011).

[164] Tenenhaus, M. *La Régression PLS: thórie et pratique*. Paris: Technip, 1998.

[165] Tenenhaus, M., Amato, S., and Esposito Vinzi, V. A global goodness-of-fit index for PLS structural equation modelling. $XLII^{th}$ *SIS Scientific Meeting*. Contributed paper. Padua, Italy, 2004.

[166] Tenenhaus, M., Esposito Vinzi, V., Chatelin, Y. M., and Lauro, N. C. PLS Path Modeling. *Computational Statistics and Data Analysis, 48 (1), 159 - 205* (2005).

[167] Tenenhaus, M., Mauger, E., and Guinot, C. *Use of ULS-SEM and PLS-SEM to measure a group effect in a regression model relating two blocks of binary variables*. Esposito, Vinzi, V., et al., 2010.

[168] Trinchera, L. *Unobserved heterogeneity in structural equation models: A new approach to latent class detection in PLS path modeling*. PhD thesis. University of Naples Federico II, 2007.

[169] Trinchera, L. and Esposito Vinzi, V. Capturing unobserved heterogeneity in PLS path modeling. *Proceedings of IFCS 2006 Conference*. Contributed paper. Ljubljana, Sloveny, 2006.

[170] Trinchera, L., Russolillo, G., and Lauro, N. C. Using categorical variables in PLS Path Modeling to build system of composite indicators. *Statistica Applicata* (2008).

[171] Trinchera, L., Squillacciotti, S., and Esposito Vinzi, V. *PLS typological path modeling : a model-based approach to classification*. Esposito, Vinzi, V., Lauro, N. C., Braverma, A, Kiers, H. and Schmiek, M. G. (Eds): Proceedings of KNEMO 2006, Tilapia, Ancapri, 87, 2006.

[172] Trufte, E. R. *The Visual Display of Quantitative Information*. Graphic Press, Connecticut, USA, 2001.

[173] Valor Segura, I., Expòsito, F., and Moya Morales, M. C. Victim blaming and exoneration of the perpetrator in domestic violence: the role

of beliefs in a just world and ambivalent sexism. *The Spanish Journal of Psychology* (2011).

[174] Van Rijckevorsel, J. and de Leeuw, J. *An outline of PRINCALS*. Internal Report RB 002, Leiden, Department of Data Theory, University of Leiden, 1979.

[175] Venaik, S. *A Model of Global Marketing in Multinational Firms: An Empirical Investigation*. Unpublished Doctoral Dissertation. The Australian Graduate School of Management, Sydney, 1999.

[176] Wedel, M. and Kamakura, W. A. *Market segmentation – conceptual and methodological foundations*. 2 edn. Boston: Kluwer, 2000.

[177] Wedel, M. and Kamakura, W. A. *Market segmentation: Conceptual and methodological foundations*. Kluwer Academic Publishers, Boston, 2000.

[178] Wetzels, M., Odekerken-Schröder, G., and van Oppen, C. Using PLS path modeling for assessing hierarchical construct models: guidelines and empirical illustration. *MIS Quarterly, 33 (1), 177 - 195* (2009).

[179] Wilson, B. *Using PLS to Investigate Interaction Effects Between Higher Order Brand Constructs*. Esposito, Vinzi, V., et al., 2009.

[180] Wilson, B. and Henseler, J. Modeling reflective higher-order constructs using three approaches with PLS path modeling: A Monte Carlo comparison. *Australian and New Zealand Marketing Academy Conference, 791 - 800*. University of Otago, Dunedin, New Zealand, 2007.

[181] Wold, H. *Principles Estimation of principal components and related models by iterative least squares*. Krishnaiah, P. R. (Ed): Multivariate Analysis, Academic Press, New York, 391 - 420, 1966.

[182] Wold, H. Modelling in complex situations with soft infromation (1975).

[183] Wold, H. *PLS path models with latent variables: the nipals approach*. Blalock, H. M., et al., 1975.

[184] Wold, H. *Soft modeling by latent variables: the nonlinear iterative partial least squares approach*. Gani, J. (Ed): Perspectives in probability and statistic, Academic Press, London, 117 - 142, 1975.

[185] Wold, H. *Model construction and evaluation when theoretical knowledge is scarce*. Kmenta, J., and Rmsey, J. B. (Eds): Evaluation of econometric models, 47- 74, 1980.

[186] Wold, H. *Soft modeling: the basic design and some extensions*. Jöreskog, K. G., and Wold, H. (Eds): Systems under Indirect Observation: Causality, Structure, Prediction, Part 2, North-Holland, Amsterdam, 1 - 54, 1982.

[187] Wold, H. *Partial Least Squares*. Kotz, S., and Johnson, N. L. (Eds): Encyclopedia of Statistical Sciences, 6, Wiley, New York, 581 - 591, 1985.

[188] Wold, H., Martens, H., and Wold, H. *The multivariate calibration problem in chemistry solved by the PLS method*. Ruhe, A., and Kagstrom, B. (Eds): Proceedings of the Conference on Matrix Pencils. Lectures Notes in Mathematics, 1983.

[189] Young, F. W., Takane, Y., and de Leeuw, J. The Principal Components of Mixed Measurement Level Multivariate Data: an Alternating Least Squares Method with Optimal Scaling Features. *Psychometrika, 45, 279 - 281* (1978).

[190] Zhang, P., Li, N., and Sun, H. Affective Quality and Cognitive Absorption: Extending Technology Acceptance Research. $XXIX - th$ *Hawaii International Conference on Systems Sciences, IEEE Computer Society*. Hawaii, 2006.