

The PLS Agent – Agent Behavior Validation by Partial Least Squares

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Abstract—Agent-based modeling is widely applied in the social sciences. However, the validation of agent behavior is challenging and identified as one of the shortcomings in the field. Methods are required to establish empirical links and support the implementation of valid agent models. This paper contributes to this, by introducing the PLS agent concept. This approach shows a way to transfer results about causalities and decision criteria from empirical surveys into an agent-based decision model, through processing the output of a PLS-SEM model. This should simplify and foster the use of empirical results in agent-based simulation and support collaborative studies over the disciplines.

I. INTRODUCTION

Agent-based modeling (ABM) is a promising and increasingly established method in the economics and the social sciences. The basic idea is to model social phenomena based on simplified descriptions of agents and their interactions. The dynamic behavior of these models is investigated based on simulation experiments. This capability of depicting human and societal complexity in a comparatively simple manner makes agent-based modeling very appealing (Macy and Willer 2002). The contribution and relevance of this method is demonstrated by its use in areas such as political science (e.g., policy adoption, voting and demography), technology (e.g., innovation diffusion, technology transfer and healthcare), economics (e.g., public goods, game theory and markets), as well as business. In typical agent-based models in economics and the social sciences, autonomous agents represent humans. Just as human decision maker, agents have attributes and exhibit behavior, which have to be specified during the modeling process. This specification of agents, however, is both challenging and crucial for a good agent-based model. As model behavior is often driven to a large degree by the properties of agents, a valid and credible agent-based model also requires a valid agent description. Recent surveys on the current practice in agent-based modeling, however, have identified exactly validation as a major shortcoming (Heath et al. 2009). Against this backdrop, one can argue that the question of agent validity is one of the major challenges in the scientific endeavor to advance ABM. When agents and their interaction are not validated, the value and credibility of this research method will depreciate for many modeling domains.

The aim of this paper is to discuss how partial least squares (PLS) path models based on empirical data can contribute to agent validation. This will be done both on a conceptual level and at an applied level, i.e. by the means of an illustration in the area of innovation diffusion and acceptance, where agent properties are crucial for subsequently observed characteristics of the diffusion process.

The paper is structured as follows. First, an overview about agent model validation and its challenges is given (see Section II). Next, an introduction to PLS is given, that provide the empirical foundation for agent models (see Section III). In Section IV, the concept of the PLS Agent is introduced. Finally, the paper ends with a discussion and conclusion.

II. AGENT MODEL VALIDATION

For a successful application of agent-based simulation, some challenges have to be met and resolved. One important issue is the validation of the simulation model. Certainly, (simulation) models can only be approximations of the target system and absolute validity is not possible (Law 2007). However, the model has to be close enough, so that valid conclusions can be drawn and do not lead to costly erroneous decisions. On the other hand, models in the social sciences tend to be complex. The “art of modeling” is to find a level of detail that meets the important aspects of the target system in a treatable model (Gilbert 2008). Too complex models include the risk of over-parameterization. Models with too many degrees of freedom can always be adjusted in a way that they fit to the empirical data (Fagiolo et al. 2007). Thus, the model has to be valid in all necessary details, or validation remains a system-inherent problem of agent-based simulation (Klügl 2008).

Windrum et al. (2007) describe the “*problematic relationship between agent-based models and empirical data*”. In agent-based models, the validation process is the assessment of the simulated data with respect to the quality of representation of the observed data, as generated by the empirical process. A methodological basis for the process of empirical validation is clearly needed. However, there is still little consensus on the empirical validation of agent-based simulation models.

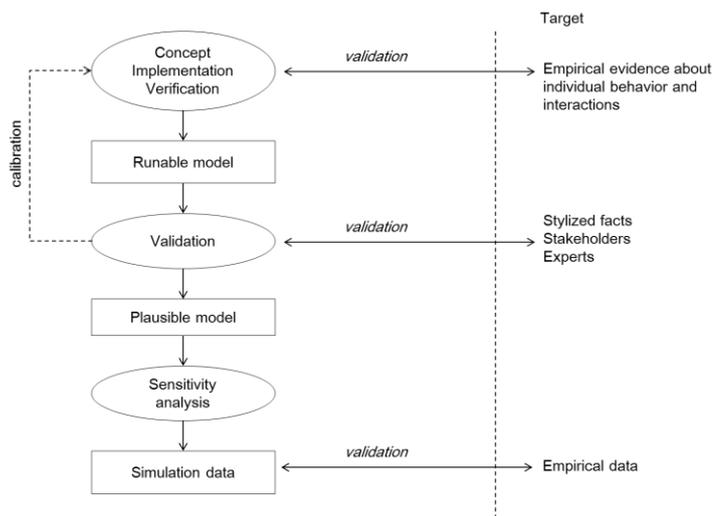


Figure 1: General procedure for validating simulation models (adapted from Klügl, 2008)

Figure 1 illustrates the basic validation process in agent-based simulation research, adapted from the process described in Klügl (2008).

First, an agent model is specified for the given target system. Based on empirical evidence about individual behavior and interactions, the agent concept is specified, implemented and verified in the first step. This determines the micro level of the simulation model. The resulting simulation behavior is assessed for plausibility on the (macro) system level for behavioral validity (input-output behavior). If necessary, the model is calibrated in this stage to fit the stylized facts. The plausible model is analyzed systematically in a sensitivity analysis. The results from this analysis can be verified by empirical data.

The described verification process of calibrating the micro model based on stylized facts on the macro level, is called the *indirect calibration approach* (Fagiolo et al. 2007). This approach is also useful for the reason, that data on the aggregate level are easier to gather than on the individual level (Klügl 2008). It is problematic to achieve data about the internal structure on the individual level. However, such data is necessary for modeling causalities within the agents' reasoning process, and, thus, for achieving a structural validity on the agent level. Overall, the main problem is the missing availability of empirical data (Klügl 2008).

This paper addresses this by introducing the partial least squares (PLS) method as empirical basis for defining the structure and causalities of agent reasoning. By using PLS, an empirically derived model about the internal structure of reasoning on the individual level as well as about the causalities between the variables of the agents' reasoning provides the basis for the agent architecture. This paper shows, how PLS can build a bridge between empirical data on the one hand and the agent architecture on the other.

III. PARTIAL LEAST SQUARES (PLS)

A. PLS-SEM

Structural equation models (SEM) appeared in the 1970's (Jöreskog, 1973) and have become a quasi-standard statistical method in the social sciences (Hair et al., 2011). The desire to test complete theories and concepts is a key reason for using the SEM method (Bollen, 1989). Variance-based partial least squares (PLS-SEM; Lohmöller, 1989; Wold, 1982) and covariance-based SEM (CB-SEM; Jöreskog, 1978, 1982) represent two alternative but distinctive methods to estimate structural equation models. In short, CB-SEM and PLS-SEM are different but complementary statistical methods for SEM whereby the advantages of the one method are the disadvantages of the other and vice versa (Jöreskog & Wold, 1982).

In general, a structural equation model with latent variables consists of measurement models describing the relationships between latent variables and their observed indicators, and a structural model of the relationships between the latent variables. In the PLS-SEM context, measurement and structural models are frequently called outer and inner models. Measurement models can comprise formative or reflective indicators (Diamantopoulos & Winklhofer, 2001; Jarvis et al., 2003), whereby only one type of relationship is possible per latent variable, although different latent variables in the SEM may use different types of measurement models. Reflective indicators are seen as functions of the latent variable. Changes in the latent variable are reflected by changes in the associated indicator variables. In contrast, formative indicators are assumed to cause a latent variable, i.e. changes in the indicators imply changes in the latent variable's value.

Figure 2 shows an example of a simple PLS path model, which includes one endogenous latent variable (y_3) and two exogenous latent variables (y_1 and y_2). The term "exogenous" is used to characterize latent variables with no preceding ones in the structural model. In contrast, the term "endogenous" characterizes latent variables that are explained by others in the structural model.

PLS-SEM requires the structural model to be recursive, which excludes the use of causal loops in the relationships between the latent variables (there would be a causal loop in the model in Figure 2 if there were relationships between y_1 and y_2 , y_2 and y_3 , and y_3 and y_1). The latent variables y_1 and y_2 are measured by means of formative indicators and y_3 by reflective indicators. It is important to note that PLS measurement models consist of one or more indicators. Each indicator can only be assigned once within a measurement model.

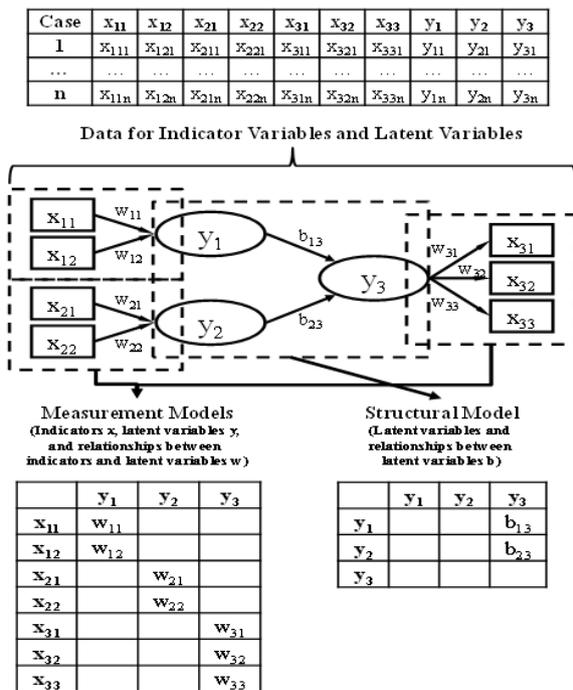


Figure 2: PLS-SEM example: initial set-up

The basic PLS-SEM algorithm - originally developed by Wold (1975) as NIPALS (nonlinear iterative partial least squares) and later extended by Lohmöller (1989) - follows a two-stage approach. This approach consists of the estimation of latent variable scores via the iteration of four steps in the first stage, and the final estimation of outer weights/loadings and path coefficients in the second stage (Figure 3).

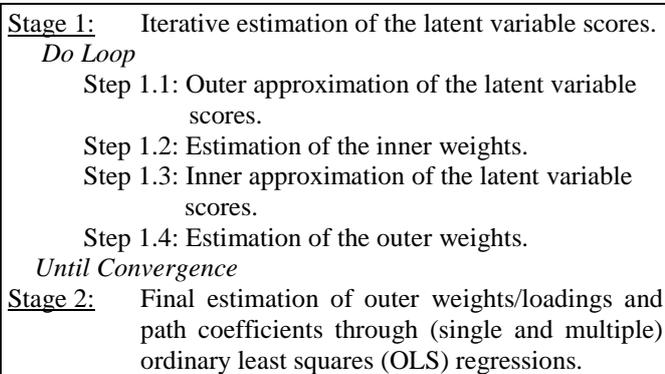


Figure 3: Key steps of the basic PLS-SEM algorithm

The goal of Stage 1 of the PLS-SEM algorithm is determining the latent variable scores. After convergence (Henseler, 2010), in Stage 2 of the PLS-SEM algorithm, the final latent variable scores are used to run OLS regressions that determine the final estimates for all relationships in the PLS path model.

B. Important Characteristics of PLS-SEM to Extend Simulation Methods

The statistical properties of the PLS-SEM method substantiate its use to extend simulation methods. Primarily, PLS-SEM is a non-parametric regression-based estimation method. Its use focuses on the prediction of a specific set of hypothesized relationships that maximizes explained variance in more or less the way as ordinary least squares (OLS) regressions do. Therefore, the focus is much more on prediction rather than explanation, which makes PLS-SEM results particularly beneficial for simulation methods.

PLS-SEM is also very flexible regarding the modeling properties. The only premise is connected to “predictor specification” (i.e., the systematic portion of all OLS regressions is equal to the dependent variables’ conditional expectations; Haenlein & Kaplan, 2004). In accordance, the inner model must be a causal chain system with uncorrelated residuals and an endogenous latent variable’s residual being uncorrelated with the corresponding predictor latent variables. PLS-SEM is also considered as the primary approach when the hypothesized model incorporates formative measures (Diamantopoulos & Winklhofer, 2001). Moreover, PLS-SEM is also a sensible choice in research situations where few observations are used to estimate complex models with many manifest variables. This holds especially true when formative measures are involved (besides the potential identification issues discussed above). Formative measurement models are often more capacious, as formative constructs should be represented by all relevant indicators that forms it to ensure content validity (Diamantopoulos et al., 2008). Thus, PLS-SEM can be a useful way of quickly exploring a large number of variables to identify sets of latent variables that can predict some outcome variable, underlining the approach’s exploratory character. Hence, PLS-SEM can be used for relatively complex models and has only very few requirements to be met. These features make PLS-SEM particularly suitable in combination with simulation methods.

Finally, in situations when it is difficult or impossible to meet more traditional multivariate techniques’ strict assumptions (e.g. distributional assumptions), PLS-SEM’s greater flexibility with modeling problems is emphasized by the label “soft modeling” coined by Wold (1982). Within this context, “soft” is only attributed to distributional assumptions and not the concepts, models or estimation techniques (Lohmöller, 1989). PLS-SEM’s statistical properties provide very robust model estimations both with data that have normal and extremely non-normal distributional properties (Reinartz et al., 2009; Ringle et al., 2009). Thus, PLS-SEM can also be used when distributions are highly skewed (e.g., Beebe et al., 1998; Cassel et al., 1999; Tenenhaus et al., 2010), especially when formative measurement models are included (Ringle et al., 2009). Moreover, the PLS-SEM algorithm principally requires metric data for the indicators in the measurement models. However, the method also generally works with ordinal

scales with equidistant data points - i.e., quasi metric scales (Mooi & Sarstedt, 2011) - and with binary coded data. In the latter case, when using both metric and dummy variables, one must account for the role of dummy coded variables in regressions (Hair et al., 2011b), or the specific considerations provided by Lohmöller (1989) for PLS path model estimations that solely draw on dummy coded variables. This kind of flexibility regarding the data used also represents a beneficial feature when combining the PLS-SEM method with other techniques such as simulation methods.

One of PLS-SEM's most important features relates to the nature of the latent variable scores. Specifically, scores are estimated as exact linear combinations of their associated manifest variables (Fornell & Bookstein, 1982), and PLS-SEM treats these scores as perfect substitutes for the manifest variables capturing the variance that can explain the endogenous latent variables. PLS-SEM builds on the implicit assumption that all the measured variance in the model's manifest variables is useful and should be explained. Consequently, the "correctness" of the model is partly determined by the strength of the structural model relations between the latent variables.

While the strong reliance on latent variable scores has its drawbacks, it also has certain advantages as researchers may use latent variable scores in subsequent analyses. Other research methods already employ the PLS-SEM latent variable score for further analysis (e.g., latent class segmentation; Sarstedt et al., 2011). Similarly, simulation studies may employ these results for their analyses, as we will show in this paper.

IV. THE PLS AGENT

This section shows how PLS results may be used as basis for modeling agent behavior. Therefore, this section starts with (A) general requirements for agent modeling. Afterwards, it is shown (B) how a PLS path model can be transferred into an agent decision model. Finally, (C) the implemented simulation framework *SimPLS* is described, by which a direct link between PLS output and ABM initialization is established, so that the concept is ready to be applied for various PLS path models.

A. Agent modeling

An agent is specified by its properties and abilities. The basic abilities of an agent are to perceive, decide and act. The agent observes its environment and perceives environmental information. The agent determines its behavior with the information received. Programmed rules relate information sensed by the agent to its decisions and actions (Macal and North 2010). Defined by the rules of decision for the given observation, the agent executes the corresponding action in its artificial environment.

The decision rules may be defined deterministically or stochastically. Furthermore, the complexity of decision rules may vary, so that the implementation of complex decision

process is possible. A basic decision rule structure can be described by condition-action rules (see e.g. Holland et al. (2000)). By this concept, the agent may build up a representation about its environment and respond. The condition describes the causal dependency of an action. All possible actions of the agent are assigned to one (or several) condition part(s). In complex situations, where more than one condition is included, some decision criteria may have a stronger link to actions than other.

The design of the agents' decision rules requires a valid foundation. However, the human decision process is an internal process, which is not easy to observe and determine. Therefore, many cognitive agent architectures rely on decision theory and psychological findings (see Brenner 2006). Still, for many studies a more concrete decision model for the given context and situation is needed. PLS path models result from empirical studies, such as surveys. They can provide a modeling anchor for (1) the set of decision criteria that play a role in the given decision process, (2) the existing relationships between the criteria, and (3) their relative relevance. The concept of the PLS Agent will be shown in the following section.

B. PLS Behavior Model

The starting point is a valid and calculated PLS path model, based on verified data from an empirical study. This PLS path model provides the basis for the agent model. As the model should be used to define agent behavior, the target concept of the PLS path model has to be a *decision*, such as "adoption". The structural model describes a latent variable network of causalities. This provides a set of *criteria*, which influence the agent decision or preference. Thus, the PLS path model informs the ABM about the components of reasoning by the list of latent variables. The identified significant relationships of the PLS path model indicate the existing *causality paths* of agent reasoning. Finally, the coefficients of the significant relationships provide the *order of criteria* with regard to their relevance for the agent.

For the agent decision process in the simulation model, a representation of the *decision object* is needed. This can be a product or some environmental circumstances. The exogenous variables of the PLS path model can be used as a basis for the set of decision object attributes.

The agent perceives this product type and decides about its adoption. For the agent *decision process*, a probability value for the decision is calculated. Therefore, the implemented causality network provides the basis for a set of linear combinations.

C. Example: TIAM Model

To give a concrete example of the merger of PLS and ABM, we apply the PLS path model "*Technology and Innovation Acceptance Model*" (*TIAM*) to agent based simulation. The *TIAM* describes the causal impact of product innovation attributes and consumption values on the adoption and use of a technological innovation. This model is a further development of the widespread Technology Acceptance

Model (TAM) developed by Davis et al. (1989) and the Unified Theory of Acceptance and Use of Technology (UTAUT) by Venkatesh et al. (2003) - (for further studies see for example: Venkatesh and Bala (2008); Wu et al. (2011); Venkatesh et al. (2012)). While both, the TAM and UTAUT, focus on the technology acceptance in an organizational context, the TIAM furthermore emphasize the adoption of an innovation in a consumer context. The TIAM is built on the Innovation Diffusion Theory (IDT) by Rogers (2003) and the Theory of Consumption Values (TCV) by Sheth et al. (1991). Hence, the TIAM explains consumers' adoption intention of a new technology by the five product attributes introduced by Rogers (1983) and the five consumption values introduced by Sheth et al. (1991).

It is important to note that the TIAM study is work in progress and serves here only as an example to show the concept of the PLS agent. For a content-oriented consideration of the model see Pakur (forthcoming).

The agent architecture based on the TIAM model is included in the simulation model INNOAGE (Iffländer et al. 2012). The purpose of the simulation model INNOAGE is the analysis of the diffusion process of innovations in aging societies. Therefore, the influence of varying age distributions within the population on the adoption rate and speed of diffusion is considered. Also, the interaction effects between individual consumer types, network characteristics, and product attributes are addressed.

a) *Decision Criteria and Relevance*

Figure 4 shows that the TIAM has two main fields, namely product attributes and consumption values. Each field is determined by five constructs, to measure consumers' technology and innovation adoption. Adoption intention is the main construct and target variable. Figure 4 does not show the measurement model, which was used for the calculation of the path loadings. Here, only the significant relationships and their path values are relevant for the agent model.

Given the group analyses of the PLS model, more than one agent type might be initialized in this way. If the PLS results identified groups of individuals with varying causality paths and strengths of causalities, those can be included as different *agent types* in the simulation model. Here, the multi-group analysis identified two consumer groups A and B, which were identified by age. Those will be transferred in the simulation model as agent type A (young consumer) and B (aged consumer).

As one can see, the (preliminary) results of the path model for agent type A have shown, that the criteria *compatibility*

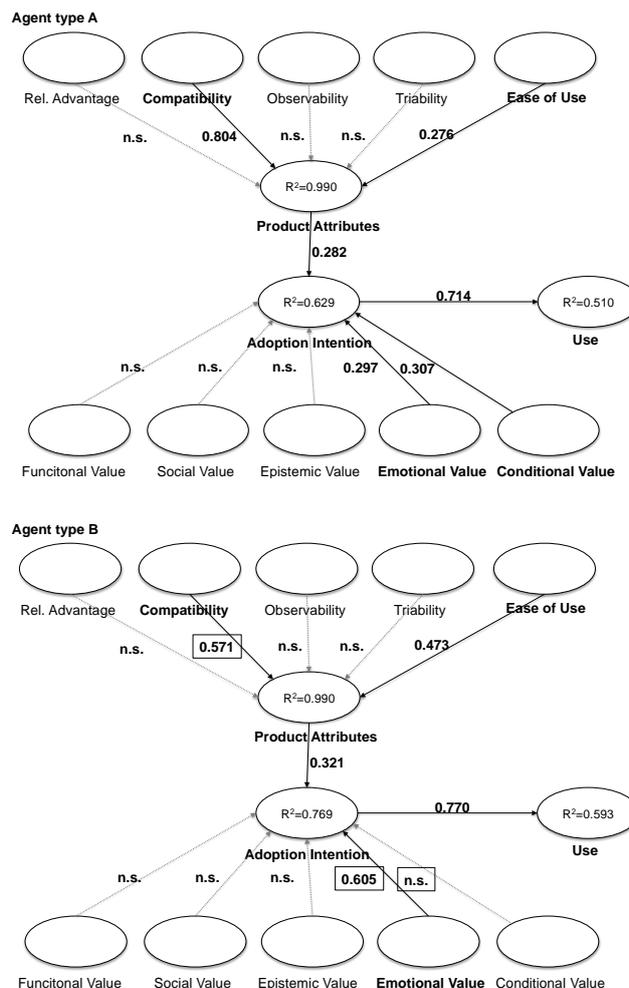


Figure 4 Example: TIAM models as basis for agent type A and B
 (work in progress - preliminary results)

and *ease of use* influence the evaluation of the *product attributes*, whereas *compatibility* has a much greater influence. The *adoption intention* of the consumer is influenced by the perceived *product attributes*, as well as the *emotional* and the *conditional value*. The other potential criteria for the adoption intention are not significant (n.s.). They have no influence, and can be excluded as decision criteria for agent type A. The *use* of the product is explained to 51% by adoption intention.

For agent type B, however, *compatibility* has a much smaller influence, and is only slightly more relevant than *ease of use* on the perceived product attributes. But, the *emotional value* is a stronger driver for the adoption intention than for agent type A, while at the same time the *conditional value* plays no role for agent type B.

This summarizes the results of the PLS path model being important for the agent model and the simulation analysis. In the agent model, all significant paths are included as a link between the criteria, and the path values are included as link

strengths. This implements a network of causality paths in the agent mind.

At this step, the PLS path model results are included in the agent architecture, and the agent initialization is finalized. The subsequent use and calculations happen only in the agent mind within the run of a simulation model. In the following, the agent decision process based on this causality network is described.

b) Decision Object

For the given TIAM model, the consumers decide about a product. The list of product attributes is given by the exogenous variables. Those are the variables *relative advantage*, *compatibility*, *observability*, *trialability*, and *ease of use* on the one hand, and *functional value*, *social value*, *epistemic value*, *emotional value*, and *conditional value* on the other. All these units represent the attributes of the product.

Exogeneous Variables	Endogenous Variable	Scale	Basis Scenario	
Relative Advantage	Product Attributes	[1, 10]	5	medium
Compatibility	Product Attributes	[1, 10]	5	medium
Observability	Product Attributes	[1, 10]	5	medium
Trialability	Product Attributes	[1, 10]	5	medium
Ease of Use	Product Attributes	[1, 10]	5	medium
Functional Value	Adoption Intention	[1, 10]	5	medium
Social Value	Adoption Intention	[1, 10]	5	medium
Epistemic Value	Adoption Intention	[1, 10]	5	medium
Emotional Value	Adoption Intention	[1, 10]	5	medium
Conditional Value	Adoption Intention	[1, 10]	5	medium

Table 1 Product modeling for TIAM

Table 1 shows the description of a *basis scenario*. Within the simulation experiments, the product attributes should vary over simulation runs. Thus, for each exogeneous variable, an input parameter sets the value on a scale between 1 (low) and 10 (high). The combination of these values describes the product type for the respective simulation run. In the basic case, all indicators have the same value (on a medium scale, 5). By holding the product type on the medium level, the effects of various populations and agent interactions may be considered. In further experiments, however, variations of product attributes values allow the analysis of their effects.

c) Decision Process

We know from the PLS path model, that agent type A only considers *compatibility*, *ease of use*, and the *emotional value*

of the product in its decision making process. The agent is ignorant towards variations of other product attributes. The strength of the *adoption intention* value is the result of a linear combination over its relevant criteria and coefficients. Its calculation follows a two-step calculation. First, a *maximum model* provides the basis for the normalized adoption intention strength. This value has only to be calculated once, at the beginning of the simulation run.

Maximum model - agent type A

Exogenous variables	Product values	Coefficients	Results	Product Attributes
Compatibility	10	0.804	8.040	10.800
Ease of Use	10	0.276	2.760	
				Adoption Intention
Product Attributes	10.800	0.282	3.046	9.086
Emotional Value	10	0.297	2.970	
Conditional Value	10	0.307	3.070	

Table 2 Calculation of the maximum model for agent type A

The calculation of the maximum model is described in Table 2. Therefore, a scenario with a product type of best quality (value 10) is assumed. The idea is, to weight the relevant attributes with their influence. Hence, the product values are multiplied with the coefficients from the path model and result in a value per criteria. Given this, the value for *product attributes* can be calculated by the sum of all influencing criteria values. Based on this, and the other influencing criteria on adoption intention, a maximum strength for *adoption intention* may be calculated (here: 9.086). In the simulation run, this provides a basis for calculating the normalized intention strength. This will be again shown by an example (see Table 3). The *adoption intention* value for the consumer agent, observing a medium product quality of 5, is 4.543. In the final step of the decision making process, the probability for adoption is determined, based on this calculated value.

Decision model (basis scenario) - agent type A

Exogenous variables	Product values	Coefficients	Results	Product Attributes
Compatibility	5	0.804	4.020	5.400
Ease of Use	5	0.276	1.380	
				Adoption Intention
Product Attributes	5.400	0.282	1.523	4.543
Emotional Value	5	0.297	1.485	
Conditional Value	5	0.307	1.535	

Table 3 Calculation of the decision model - agent type A

The probability for adopting a product is given by dividing the calculated intention strength from the decision model with the maximum model. Here, this results in an intention

probability of 50%. This is in accordance with the assumption, that the product type represents a scenario with an average quality. In the next step of the simulation run, the agent observes another product type, and decides about its adoption by the given calculation.

Given this behavior model, it is recommended to conduct a pre-experiment with varying values for the decision object, to do a micro-validation. The causalities of the PLS path model should be recognized in the simulation results.

This section showed, that the PLS agent provides an agent architecture with a direct empirical link. Depending on the focus of research, the behavior may be embedded in a wider decision context, or a network of different agent types, to consider their interactions.

D. SimPLS Framework

To make use of the PLS-Agent concept, a *SimPLS* simulation framework was developed. It is implemented in JAVA/Repast. The default PLS report is an html-file that provides the input for *SimPLS*. By reading the html-file, the agent types are automatically created.

PLS path model	Agent model
Latent variables	Decision criteria
Exogenous variables	Decision object (product) attributes
Target construct	Decision or preference
Significant coefficients	Relationships between criteria
Strength of (sign.) coefficients	Strength (relevance) of criteria
Groups	Agent types

Table 4 Components of the SimPLS Interface

Table 4 shows how the concepts of the PLS path model are transferred into an agent-based model by *SimPLS*. The latent variables are the decision criteria of the behavior model. The exogenous variables provide a list of attributes for the decision object. By the target variable, the agent decision or preference is defined, depending on the focus of research. All paths with significant coefficients are translated into relationships between the criteria of the agent model. By the path values, the relevance of criteria is indicated. Finally, multi-group analysis may provide different agent types. *SimPLS* creates automatically the agent types according to the output files from PLS. Therewith, flexibility for changing SEM models is given.

V. DISCUSSION AND CONCLUSION

This paper presented a way to link agent models to empirical results, by transferring results from PLS path models into ABM. By this, two elements for the agent decision model are provided: (1) the set of criteria, which are relevant for the decision process, also in comparison to other agent types, and (2) the existing causalities and strengths of causalities between the criteria. Furthermore, attributes about the decision object can be derived by the exogenous variables.

One crucial aspect might be the use of the path values as described. This approach involves the threat of an over-parameterization of the PLS path model in the agent behavior model. To address this, the resulting value of the decision model provides a probability value that is used for a stochastic decision. By this, the result is a tendency in behavior instead of a determination. However, further ways about including the distribution of coefficient values might be valuable.

In some cases, the resulting decision model may result in highly stochastic agent behavior. This may be due to the complexity of the PLS path model, such as a high number of decision criteria. This can be limited by focusing on the most relevant influences.

Next to the empirical link, this study may foster interdisciplinary collaboration. The simulation method may include and compare results from different empirical studies and support their communication. Furthermore, not only PLS can be useful to inform ABM, but also *SimPLS* can be useful to further analyze PLS path models, given the questions that arise from the perspective of the empirical study.

In future research, the applicability of the PLS agent should be tested in more depth by additional analyses of the existing model, as well as by including PLS path models from other empirical studies.

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