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Agent-based Modeling Automated: Data-driven Generation of Innovation Diffusion Models

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Abstract: Simulation modeling is useful to gain insights into driving mechanisms of diffusion of innovations. This study aims to introduce automation to make identification of such mechanisms with agent-based simulation modeling less costly in time and labor. We present a novel automation procedure in which the generation of diffusion models is automated. It comprises three phases: (1) *preprocessing* of empirical data on the diffusion of a specific innovation, taken out by the user; (2) automated *inverse modeling* of decision models from a decision model library for their capability of explaining these data; (3) *policy simulation* automatically assesses user-chosen policy interventions in their potential of influencing the spreading of the innovation. We present a working software implementation of this procedure. We applied this tool to data-analysis on the diffusion of a sustainable innovation, water-saving showerheads. The proposed procedure successfully generated simulation models that explained available diffusion data. This provided a proof of concept. Further, it progresses agent-based modeling by providing *model validation by design* and by enabling detailed bottom-down modeling at the lower complexity of top-down modeling. We believe the proposed approach can widen the circle of persons that can use simulation modeling and better understand and shape innovation.

Keywords: Agent-based modeling; automation; innovation diffusion; data-analysis; policy simulation

1 INTRODUCTION

Understanding the prospects of a new ideas and how they spread is powerful. Persons and organizations are often want to know *"how to speed up the rate of diffusion of an innovation"* (Rogers 2003). Mechanistic understanding of the diffusion of an innovation can help explaining its success. Rogers' theory of Diffusion of Innovations (Rogers 2003) allows understanding diffusions based on mechanisms of inter-personal interactions. From these mechanisms, it is possible to infer general patterns and key actors of diffusion.

Mechanisms that drive the diffusion of an innovation can further be used to project innovation diffusion into the future. Agent-based modeling can simulate these mechanisms, particularly if human decision making is involved. It represents real-world actors with computer agents, whose actions are modeled by explicit decision models. It has for instance been used to simulate the diffusion of environmental-friendly products among consumers (Schwarz2007). Additionally, it allows estimating effects of practical actions regarding an innovation (Delre et al. 2007, Jensen et al. 2016).

However, mechanistic understanding is particularly challenging to gain. It is harder to achieve than statistical inference, which reveals co-occurrence of events in a set of observations. Requirements for gaining it also exceed sole causal understanding, which 'only' requires knowing that one event generally causes another one (Aalen et al. 2007). Instead, mechanistic understanding implies to know if one event *"leads to a specific, deterministic behavior in another"* (Leek 2015).

Agent-based modeling (ABM) can illuminate mechanisms of the diffusion of innovations, but is challenged by time and labor intensive model building (van Dam et al. 2012). Via simulation, it links micro-level actions of actors to 'emergent dynamics', e.g. innovation diffusion (Chappin et al. 2015). Thus, macro-dynamics of innovation diffusion are 'decoded' by being directly explained by micro-behavior of agents (Grimm et al. 2005, Stern et al. 2016). However, ABM is commonly more time-intensive than its alternatives, e.g. system dynamics (Watts & Gilbert 2016) and statistical analysis.

We aim to enable agent-based modeling to overcome these limitations by speeding up model development. We propose to hand over manual tasks to the computer. Several approaches to this exist: (1)

Translating simple specifications into executable models. An examples is the MAIA framework (Ghorbani 2006), which automatically generates simulation models from specifications by domain-experts. (2) *Model building from existing components.* A method to this idea is ‘TAPAS’,¹ via which validated models are reused (Frenken et al. 2006). (3) *Using data for model-building in a structured way.* Grimm et al. (2005) proposed ‘Pattern-oriented Modeling’ to falsify model variants that fail to reproduce a set of patterns in empirical data. This replaces ad-hoc decisions and informed guesses about adequate model structures and parameters with rigid testing against empirical data.

We thus aim to automate model building in ABM for the purposes of: (1) extracting driving mechanisms from empirical observations on innovation diffusion; (2) projecting the innovation diffusions into the future; (3) assessing of effect of real-world actions and policies ex-ante, via simulation. This study aims to answer the questions: “*Can automated generation of agent-based models on the diffusion of innovation be achieved and how could this be useful?*” We propose a procedure by which this task can be undertaken. Proof of concept is provided: an application case on the diffusion of sustainable products among households.

2 AGENT-BASED MODELING OF INNOVATION DIFFUSION

This section will provide details on agent-based modeling of innovation diffusion, which is the application domain of the proposed automation procedure. We argue that increased automation can be aided by increased standardization of input and content of modeled systems.

Dynamic simulation models are useful to understand innovation diffusion. Because innovation itself is process of change, it should be analyzed as a dynamic process (Kiesling et al. 2012). Consequently, simulation of innovation should use models that are dynamic. According to Geels and Johnson (2015), there are four general types of innovation diffusion models. (1) *Adoption models* capture spreading of an innovation among potential adopters, e.g. how user base of a new product increases via word-of-mouth. (2) *Models of up-scaling and system buildings* describe a small system expanding to a larger one, e.g. an electricity system expanding from a decentralized one to a single centralized system. (3) *Replication and circulation models* emphasize the *replication* of an adoption during its *circulation* to other location. Considering replication emphasizes adapting an innovation to other local conditions. (4) *Societal embedding model* considers the embedding of an innovation in business, societal, policy, and user environments.

This study focuses on ‘adoption’ type models. This is because their modeling of “*independent adopters making (adoption) decisions*” (Geels 2015, p.12) fits well with the approach of actor-centric perspective of agent-based modeling. Such models are represented by ‘aggregated’ and ‘individual level’ models (Kiesling et al. 2012). Aggregated models directly model the overall adoption dynamics in a population. This approach is represented by the Bass model and commonly modeled with system dynamics (Kiesling et al. 2012). Conversely, ‘individual level’ models model the adoption decisions of individuals in a population, from which overall adoption dynamics ‘emerges’.

In this study, we will focus on the individual level models, because of their capability to incorporate more aspects of reality. According to Kiesling et al. (2012), ‘individual level’ models are superior to ‘aggregated’ ones (such as system dynamics) for several reasons: (1) *Explanatory power* is greater for ‘individual level’ models, because they explicitly connect behavior and decisions of agents with aggregated diffusion dynamics. (2) *Population heterogeneity* can be captured more detailed in ‘individual level’ models. (3) *Social processes* (e.g. interaction between consumers) are modeled explicitly. This is a process that can have great impact on diffusion success (Delre 2007). Among ‘individual level’ models, ABM is particularly suited to model social interactions. In contrast to discrete-event simulation, it is capable of modeling detailed social interaction topologies in a computationally efficient way (Watts & Gilbert 2014). Thus, this study will focus on innovation diffusion models that are agent-based.

Automating the building of agent-based innovation diffusion models is facilitated by their similarity. This simplifies automated model generation, because there is less variation in input data and less structure variation that an automation procedure needs to tackle. According to a review by Kiesling et al. (2012, Fig. 2), most ‘individual level’ diffusion models have a common structure. They comprise of

¹ ‘TAPAS’ abbreviates “*Take A Previous model and Add Something*”.

the following elements: (1) *Consumer agents* define the individual entities that can adopt an innovation. This can be individual persons, households, or groups of households. (2) *Social structure* is the heterogeneity of consumer agents, e.g. dividing them in different consumer groups. (3) *Decision making processes* are the key actions of consumer agents to model the adoption of an innovation. (4) *Social influence* between agents often affects decision making processes and is commonly modeled as a social network graph. Models vary in the range at which social influence is exceeded. This can be influence from direct peers, from the respective social group or the entire population of agents. All these ranges of influence can be modeled as a social network graph.

3 METHODS

In this section, we will present the automation procedure to building agent-based innovation diffusion models. This procedure will be presented by first describing it conceptually and by giving details on how it was implemented.² Further is presented the application case that provides a proof of concept.

3.1 Automation procedure

We coin a method as specified in Fig. 1, comprising the three phases *preprocessing*, *inverse modeling*, and *policy simulation*. For reasons of brevity, additional details will be given in Section 3.2.

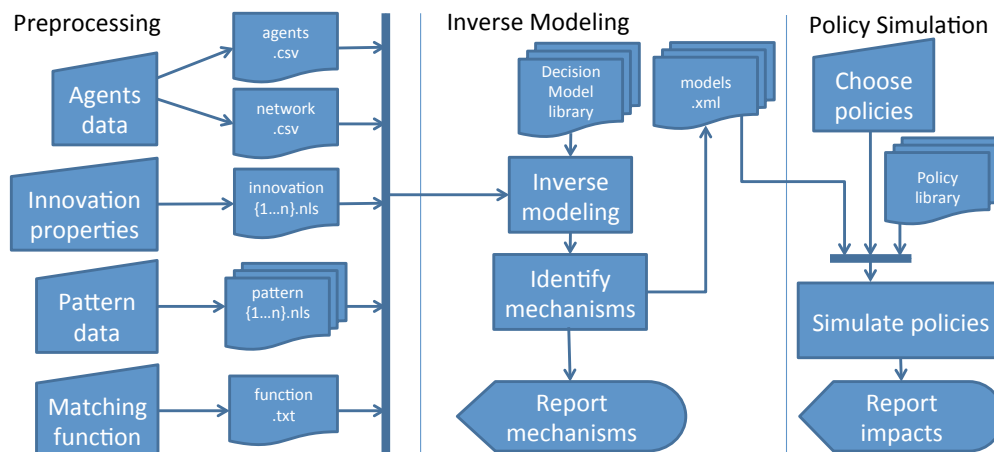


Figure 1. Overview of automation procedure (see text for details).

Preprocessing. The types of input data are the following: (1) Input data is provided on *agents* (i.e. the decision-making entities in an agent-based model). For each agent, a location and a belonging to a social group is defined. This social group serves to enable to capture the heterogeneity of agents. They are defined by a CSV file with the columns ID, X and Y coordinates, and name of the social group they may belong to. *Social influence* is defined by a social network graph. This graph is provided as a CSV file with the column FROM and TO, defining directed links between two agents of given IDs. (2) *Innovation properties* are provided, which represent how an innovation is perceived by households. This idea follows Rogers (2003), according to whom diffusion success of innovations depends on generalizable properties. (3) *Patterns* are provided that characterize the dynamics of the real-world process that shall be modeled. These patterns are “*indicators of essential underlying processes and structures*” (Grimm et al. 2005). Each additional pattern reduces uncertainty about which mechanisms could explain the diffusion of an innovation. An example for a pattern is the exponentially increasing adoption share of a successful innovation during its initial diffusion (Rogers 2003). Adoption decision models from the model library consider these. (4) A ‘*matching function*’ describes the desired behavior of an accepted simulation model in terms of the provided patterns. This function weights and combines patterns to describe model output that would be considered realistic. This function assists at finding simulation runs that represent the empirical patterns best.

² For technical details, please contact the authors. Source code will be published online.

Inverse modeling. In this phase, models that satisfy the matching function are identified. Within a range of plausibility, models are varied structurally and in their parameter values. If a model can generate empirical patterns, then is considered a potential explanation of the input data. Due to the risk of 'overfitting' at increase model complexity (Provost 2013), simple model variants are preferred. For the inverse modeling of potential decision models, we used the NetLogo tool *BehaviorSearch*. It runs each potential model, varies its structure and parameters, and searches for an optimal fit. This optimum is defined by the user-defined matching function. We ran *BehaviorSearch* with a *simulated annealing* optimization. Best fitness value were reported for each structural variation of each model.

Policy simulation. User-defined policies are assessed semi-automatically. This is useful, first, because it prevents redundant manual work. Further, running the same set of policies across all plausible models increases robustness of policy assessment—also referred to as 'bagging' (Breiman et al. 1996). Policies are pre-implemented as NetLogo functions and stored as individual NetLogo source files. Users can choose from a set of policies that support innovation diffusion or define other policy options.³ Each policy simulations executed from an XML file with the 'BehaviorSpace' tool in NetLogo. The used model parameterizations were those that produces the best fit with the empirical data.

3.2 Application case: diffusion of water-saving appliances

We applied the presented automation procedure to the diffusion of water-saving showerheads. This is because there exists rich empirical data on this case. We used the proposed automation procedure to generate models that explain the available data. This provides a proof of concept and illustrates the proposed automation procedure. Also, it informs about the mechanisms with which water-saving showerheads spread.

Empirical data on the diffusion water-saving showerheads was used, as presented by Schwarz (2007): (1) *Agents data.* Data analysis found a significant connection between lifestyle group and adoption behavior regarding water-saving appliances (Schwarz 2007). Accordingly, three social groups are distinguished: 'Leading Lifestyles', which are of relatively high social status, are most interested in adoption of the case innovation. 'Mainstream and Traditional' households have an intermediate interest in them. 'Hedonists' are least interested in the innovation. (2) *Innovation properties.* Properties of water-saving showerheads and conventional showerheads were surveyed. For each lifestyle group, also the relative importance of these properties was surveyed. This assists modeling the attitude of consumer group towards the adoption of water-saving showerheads. (3) *Diffusion patterns.* Two empirical patterns on the diffusion of water-saving showerheads showed in the available data. First, marketing shares in Germany were different for the three consumer groups. Second, the adoption diffusion curve during the first 15 years of innovation diffusion has an exponential shape.

3.2.1 Existing model on showerheads diffusion

An agent-based simulation model that was previously built on some of this empirical data (Schwarz 2007), which we coin the '*Schwarz*' model. This model describes the decision making of agents regarding the adoption of feedback devices. Initially, no household uses water-saving shower heads. At a monthly deliberation rate of 0.004, they decide whether to adopt the water-saving option. There is a probability that agents adopt the technology option that the majority of their peers adopt. This probability is differentiated by the three lifestyle groups (Jensen 2015): (1) Leading Lifestyles always adopt the device. (2) Mainstream agents adopt devices in 50% of the cases. (3) Hedonists always imitate the majority of their peers. Against this model, we compared the automatically generated models.

3.2.2 Evaluated agent-based models for application case

We created a generic *model library* of two models. We coined these models '*Schwarz flexible*' and '*TPB*' (for *Theory of Planned Behavior*, see below). The model '*Schwarz flexible*' is generally similar to the '*Schwarz*' model, but its parameterization is 'flexible' in two ways. First, the monthly deliberation

³ The user is recommended to test policies for all diffusion models that resulted in sufficient fit with the empirical patterns. Of these models, the variants with the least complexity should be chosen.

rate became a flexible parameter between 0.004 and 0.04. Second, the probability of agents from each consumer group to adopt according to the majority of their peers also became a flexible parameter between 0 and 1. The second decision model is based on Ajzen's (1991) *Theory of Planned Behavior* (TPB). Its models adoption based on three factors: the attitude towards the product, the perceived behavioral control over adopting it and the subjective norm towards adoption. For water-saving showerheads, this means that adoption is more likely if first, attitude towards a product is more positive, second, if the adoption is perceived as easy, and third, if more common among peers. We used the formalization shown in Eq. 1 (Schwarz 2007). According to this model, agents calculate utilities for each option and adopt the one with the highest adoption intention, based on the following factors. 'Attitude_i' is the product of two vectors: innovation properties and weights (i.e. importance) that a social group assigns to these characteristics. Example of such a characteristic is environmental-friendliness. 'Perceived_behavioral_control_i' is a product of innovation characteristics (that translate into the ease of adoption) and respective weights. An example is the purchasing cost. 'Social_norm_i' is the ratio of peers of a household that use product 'i'. The parameter 's' is the importance of a household to practice the same behavior as its peers, motivated by need for cohesion or uncertainty about the product.

$$adoption_intention_i = (1 - s) * attitude_i + perceived_behavioral_control_i + s * social_norm_i \quad (1)$$

We extended these two models by an optional word-of-mouth (WOM) mechanism. Without the WOM mechanism, all agents can deliberate on adoption. If the mechanism is active, agents only consider adopting feedback devices if they are 'aware' of them. At adoption, an agent makes the peers that it influences aware of the device. Activation of this mechanism thus becomes an additional degree of freedom in the structure of both models.

3.2.3 Automated policy simulation

The proposed procedure can automatically project the impact of policies on diffusion. This automation phase only uses those models that were found sufficiently plausible in the inverse modeling phase. For innovation diffusion, policies often aim to speed up spreading of an innovation. As a policy to be tested, we chose the strategy of giving away free products: at the beginning of innovation diffusion, 10% of households receive a free water-saving shower head. This has the potential to promote further adoption of this product by social influence and WOM.

4 RESULTS AND DISCUSSION

We conducted two simulation experiments, each representing one of the two automated phases of the procedure. Experiment 1 simulates the simulation models from the model library and compares simulation results to the original 'Schwarz' model. Experiment 2 demonstrates automated policy simulation.

4.1 Experiment 1: Inverse modeling

In this experiment, the models 'Schwarz flexible' and 'TPB' were tested for their ability to explain the diffusion of water-saving showerheads. Each of these two models was modeled in two structural variations: both with and without the WOM mechanism. In the 'inverse modeling' phase of the proposed procedure, simulation results were tested against the two empirical patterns of an exponential takeoff of adoption and the empirical market shares of the three consumer groups after 15 years.

The provided matching function – used to identify realistic models – is shown in Eq. 2. Mainly, the simulated and empirical market shares for the 3 consumer groups are compared. The inverse modeling phase searches model variants that minimize this mismatching. Further, if the shape of the adoption curve is not exponential, then a significant penalty is added to the matching function. Basis for this is the overall adoption share over all agents and the length of a simulation run of 180 months. Matching results (i.e. best fitness and according parameters) are shown in Table 2.

$$\text{Minimize } \{ 'adoption_shares' + 1000 * 'exponential' \} \quad (2)$$

Results of best matches, shown in Fig. 2, revealed that model versions without WOM were less able to match the patterns: the ‘Schwarz flexible’ model, was not able to generate an exponential pattern; the ‘TPB’ model could generate exponential increase in adoption, but was not able to match the adoption data at the same time. With the WOM mechanism being active, both models were able to match both patterns – with the only limitation being a relatively bad reproduction of the empirical market shares of the ‘Hedonists’ group. Based on these results, we regard both simulated models generally suited to explain the diffusion of water-saving showerheads, but only if the WOM mechanism is included.

Table 2. Results of inverse modeling phase: best fit and parameterizations.

| Model | WOM | Fitness | delta_alpha | s _{LL} | s _{MS} | s _{HD} |
|------------------|-----|---------|-------------|-----------------|-----------------|-----------------|
| Schwarz | No | - | 0.004 | 0 | 0.5 | 1 |
| Schwarz flexible | No | 1008.71 | 0.013 | 0.591 | 1 | 0.839 |
| Schwarz flexible | Yes | 6.79 | 0.015 | 0.085 | 0.673 | 1 |
| TPB | No | 31.18 | 0.005 | 0.607 | 0.277 | 0.006 |
| TPB | Yes | 7.18 | 0.015 | 0.086 | 0.413 | 0.743 |

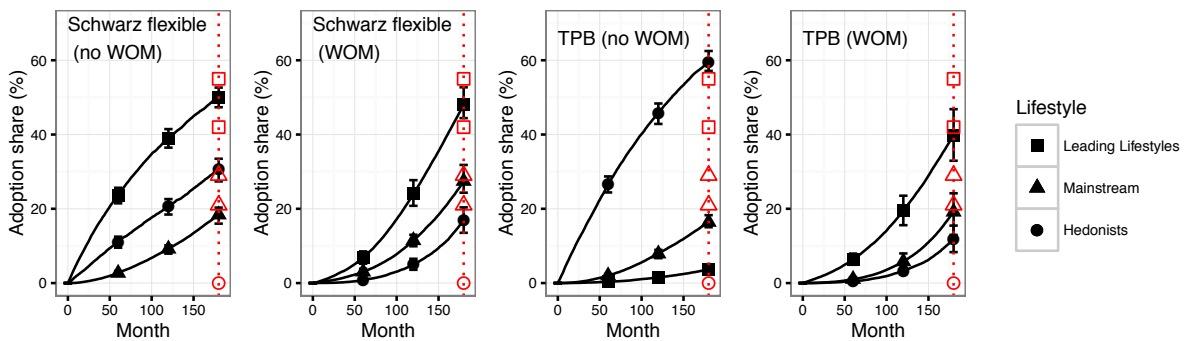


Figure 2. Average adoption of water-saving showerheads, as simulated by the tested models at best matching parameters. Hollow points show empirical market shares after 15 years of diffusion. For the consumer groups ‘Leading Lifestyle’ and ‘Mainstream’, two market share data points were used, each.

4.2 Experiment 2: Policy simulation

In this experiment, we applied the proposed procedure to automatically assess the impact of a policy on innovation diffusion. This assessment only based on those model variants that were found ‘plausible’ in the inverse modeling experiment. The simulated policy is to give away free water-saving showerheads to 10% of agents at the beginning the diffusion of this innovation (see Section 3.2.3).

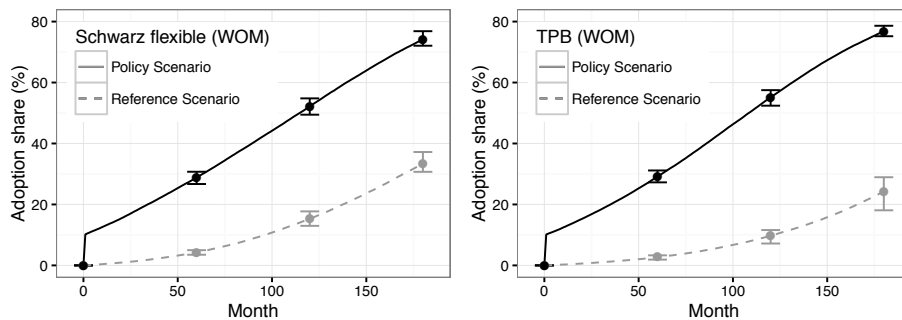


Figure 3. Simulation results of the four tested model structures at best performing parameterizations.

Figure 3 shows the impact of the assessed policy, which revealed the following findings. First, impacts for the two models are relatively similar: giving away free devices at the beginning of product diffusion makes the scenarios with and without policy intervention diverge quickly. Following the interventions, the innovation spreads at a higher rate. Overall, the similar additional impact for the two models underlines the robustness of the proposed procedure.

4.3 Limitations

Discussion of limitations will focus on two aspects of the proposed automation procedure. (1) The proposed automation procedure might not be applicable to very uncertain processes or models. It appears limited to cases where potential explanations are restricted to a bounded space of options. This is e.g. the case for innovation diffusion, where a relatively standardized model structure meets many cases. For innovation diffusion, the proposed procedure has shown able to handle structural uncertainty. But to which limit such uncertainty can be managed is not known yet. (2) The proposed procedure can not easily be applied by every user, because it requires data processing skill in the preprocessing phase. This might limit the circle of potential users. Yet, the procedure still widens this circle of users, compared to prevailing model building 'from scratch'.

5 CONCLUSION

Experiments of this study showed that the automation procedure was applicable to the diffusion of water-saving showerheads. It further increased efficiency of time and labor in the model building process. This serves as a *proof of concept* and adds weight of evidence to its suitability to automate the identification of decision models in agent-based models of innovation diffusion. For the diffusion of water-saving heads, some potential decisions models could be falsified. Conversely, word-of-mouth marketing between consumers was found a potentially crucial process in their diffusion. This supports importance of future marketing efforts to leverage word-of-mouth.

The rigid use of data in the proposed procedure creates *model validation by design*. The procedure is driven by comparing model output to empirical data, which is central to validation (Rand & Rust 2011). Further, comparing multiple mechanisms (or models, theories) enables the good scientific practice of being able to falsify those that can not explain empirical data. Overall, this has the potential to make agent-based modeling more rigorous than in common practice (Grimm et al. 2006).

The presented approach to agent-based modeling further combines the advantages of top-down and bottom-up simulation modeling. In a top-down way, the user only provides key data on a system. This reduces complexity and labor-demand for the user. The advantages of bottom-up modeling are provided by the automated search for decision models that explain these data. Bottom-up modeling further makes the driving mechanisms transparent and thus enables mechanistic understanding. In combination, useful mechanistic understanding is thus provided at low effort and complexity.

We expect the proposed automation structure to help at increasing the circle of persons that can build simulation models on innovation diffusion. We see the classical role of the *modeler* being extended by the role of the *user*. A user could build and execute useful models without requiring highly developed modeling or simulation skills. Such user should be skilled in data processing—to process and provide the required input data. A user would likely also be interested in identifying the best policy actions to shape the fate of an innovation.

We suggest to progress this study in two directions. (1) The central phase of inverse modeling is crucial to the proposed automation procedure and could be improved. We propose to support anticipated users of this automation procedure to make good matching function choices. For this, different design of the inverse modeling phase should be compared. Those designs that are robust in providing good results over several applications case should be preferred. (2) User-friendliness of the procedure can be increased by accepting unstructured input data. The presented application case used structured empirical data. Approaches from data science might allow to execute the procedure with unstructured data could be integrated. Overall, increased user-friendliness further increase the circle of potential users.

Finally, we suggest to expand the application of the proposed automation procedure to more cases of diffusions and to more decision models. This could help establishing *reference models* on the diffusion of innovations, which can further speed up the development of sound innovation diffusion models. We further suggest to explore ways for the automation procedure to be as generally applicable as reasonably possible. Trust in this will likely encourage more non-modelers to apply the proposed automation approach and to exploit the merits of agent-based modeling of innovation diffusion.

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