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Machine-assisted agent-based modeling: Opening the black box

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ABSTRACT

While agent-based modeling (ABM) has become one of the most powerful tools in quantitative social sciences, it remains difficult to explain their structure and performance. We propose to use artificial intelligence both to build the models from data, and to improve the way we communicate models to stakeholders. Although machine learning is actively employed for pre-processing data, here for the first time, we used it to facilitate model development of a simulation model directly from data. Our suggested framework, ML-ABM accounts for causality and feedback loops in a complex nonlinear system and at the same time keeps it transparent for stakeholders. As a result, beside the development of a behavioral ABM, we open the 'blackbox' of purely empirical models. With our approach, artificial intelligence in the simulation field can open a new stream in modeling practices and provide insights for future applications.

1. Introduction

In social and environmental sciences, agent-based modeling (ABM) is the primary method to examine the dynamics and interactions of heterogeneous agent behaviors and understand underlying processes of decision-making [14,47]. It offers a modeling paradigm to simulate agents' interactions within their networks and with the environment, explore their collective actions over time, and develop adaptive systems [38,68]. An ABM can simultaneously simulate individual decisions at the micro-level and the diffusion patterns at the macro-level. For these reasons, it has gained popularity among social scientists, especially for studying coupled human-environmental systems [62].

Modeling has always been a combination of art and science [39,67]. When designing a model, it takes artistic work to choose the right degree of complexity and put together the appropriate assumptions, data, and theories [31,55]. With computer simulations becoming increasingly powerful, there is an interest in how artificial intelligence (AI) can be used to derive the formalism needed for simulation modeling [1]. In one of the early applications, Schmidt and Lipson [54] have used machine learning (ML) to reconstruct equations of motion that govern the kinetics of a double pendulum. They claimed that with no prior knowledge of geometry, physics, and kinematics, they could detect fundamental theoretical insights: nonlinear energy conservation laws, Newtonian force laws, geometric invariants, and system manifolds by processing experimental data about the angles and angular velocities of a chaotic double-pendulum. More recently, using dynamic systems and data-based machine learning algorithms, Chowdhury et al. [12] and Chowdhury et al. [11] developed methods to predict extreme events and identify the mechanism and source of instabilities.

Other applications of ML in physical [10] and material science [63] include automatic classification of structures by crystal symmetry [76], prediction of all possible combinations of material composition and crystal structures ([29], examining properties of liquid crystals directly from their optical images [57] and predicting their physical properties [56].

Deriving rules that describe the agents' behavior is a sophisticated task. Even when detailed data about a particular system is available, the modeler requires proper knowledge of simulation modeling techniques and about the systems themselves to derive agents' rules. Depending on the level of accuracy and completeness in the input data, methods for deriving the behavioral rules of agents vary, ranging from purely theoretical all the way to empirical methods [7]. Modelers can make assumptions to define agent rules heuristically, based on common sense, or knowledge from theory in relevant scientific fields (psychology,

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behavioral economics, neuroscience, etc.).

While theoretical ABM provides insights on possible explanations for general patterns and emergent systems properties, the purpose of developing empirical models is to make predictions of future decisions relying on observations. Data required for parameterizing the agents and deriving decision-making rules (in the case of empirical models only) can be collected by surveys, role-playing games, laboratory experiments, and participatory modeling [50,59,70]. Statistical methods are commonly used to determine model input distribution functions, find the correlations, and deliver the equations.

In both cases, building an ABM can be challenging and time-intensive given the complexity and scale alongside specialized knowledge about systems under study. For complex systems, even when detailed empirical data are available, extracting appropriate functions and equations tends to be complicated. Understanding the decision-making process and agents' rules in ABMs is an ad hoc process that depends significantly on the background, values and expertise of the modeler(s) rather than being driven by what is appropriate for the case study [28,71]. According to Parker et al. [40], "the process of model building can also be a process of knowledge building", which has become the mantra of participatory modeling. Besides, calibration and validation of empirical agents' behaviors can become time-consuming when the number of parameters and model specifications increases.

The limitations of current practices in developing empirical-based ABMs drive modelers' interest in finding ways to automate model development. In this regard, Suleimenova et al. [61] develop an automated simulation modeling tool, FabSim, to facilitate and speed up modeling of refugee movement. This tool incorporates a range of data sources and uses the Flee simulation code and Fabric library to generate simulation workflows. The study of Huang et al. [27] is another example of a framework for automatic model generation using pre-built and validated model components/modules. Coria et al. [13] propose intelligent business process composition based on multi-agent systems to automatically build web services. Vu et al. [72] use multi-objective genetic programming in ABM as a trade-off between empirical fit and theoretical interpretability of complex social science models. Manson [37] adopts a similar approach to model decision-making in the context of human-environment relationships.

There are partial applications of artificial intelligence (AI) and machine learning (ML) algorithms in eliciting the behavioral rules, defining learning and adaptability in agents ([17], and testing the sensitivity and validity of the model outputs [23]. AI is a branch of computer science that has been developed to enable machines to mimic human intelligence. ML, a subdomain of AI, entails the automated ability to learn patterns in data and improve prediction accuracy. Al has multiple applications in the ABM discipline. For example, relying on video data as the data source, Tan et al. [66] combined a support vector machine algorithm with ABM to develop a data-driven pedestrian origin-destination and route choice model. In another study, Cuevas et al. [15] developed a new metaheuristic algorithm based on AI and ABM principles (i.e., generating very complex global search behaviors) that outperforms the existing optimization algorithms.

More specifically, for the challenge of defining agent rules, ML methods can be used to automatically derive predictive models of behavior from available data. This approach can significantly increase the accuracy of predictions, speed up the process of model development and perhaps remove some of the researcher bias in determining the behavioral rules. For instance, Su et al. [60] develop a framework embedding reinforcement learning methods in multi-agent modeling to decide about preventive maintenance policies. Bell and Mgbemena [5] propose a combined ABM-decision tree (DT) method to understand the factors influencing customers' intentions to stay or leave a mobile network operator. Similarly, Sánchez-Maroño et al. [53] and Polhill et al. [42] use this combined method to examine the diffusion of everyday pro-environmental behavior at work. Smajgl and Bohensky [58] simulate the impact of fuel price changes on vulnerable households in Indonesia by developing an ABM based on the results of ML analysis. Gonzalez-Redin et al. [22] integrate geo-spatial data with expert knowledge to build Bayesian Belief Networks to be used as the behavioral rules of an ABM for examining the future impacts of land-use change on the sustainability of the Wet Tropics regions of Australia. Hu et al. [26] empower ABMs with directed information graphs and boosted regression tree algorithms to investigate the impacts of agents' pumping behavior on the underlying groundwater system.

In all these studies, the researchers focus on improving the predictability of behaviors, the accuracy of prediction, and the speed of model development. However, the empirical models produced remain difficult to understand and justify to social scientists and stakeholders. They are often seen as a black box that does not tell us much about the system at stake and remains unclear about the causal relationships and feedback loops in the system. These play critical roles in developing policies to accentuate desired behavior [30] and to communicate the models to stakeholders. Though AI shows state-of-art performance in delivering high prediction accuracy, social scientists are skeptical about its usefulness due to its lack of transparency and failure in explaining the observed phenomena and results [32]. They raise concerns about the deployment of black-box systems and unguided data crunching without clear connections to the social science theories [44], especially when it comes to designing interventions [36,45]. Since interpretability and causality have non-trivial differences from prediction, the main focus of ML algorithms, their findings, particularly for microdata on behavior, are sometimes rejected by social scientists [21].

Bridging theory with computational experimentation could accelerate scientific progress if technical challenges are overcome as explained in the Nature report "Theorists and experimentalists must join forces" [4]. Understanding the rules governing the decision-making process (i.e., theory) and its cumulative impacts (i.e., scenario analyses performed by ABM) is crucial to address many societal challenges, such as behavioral biases and social influences guiding mass behavior in a pandemic or climate change and sustainability transitions. Since many ABMs are about generating exploratory and explanatory knowledge [3], to obtain solid scientific ground outcomes, there is a need to connect the computational experimentations to theories [16,41]. On these grounds, algorithm-driven decisions, and rules, especially in social science, were rejected when ML was considered as a blackbox that cannot be appreciated and communicated to stakeholders. Leveraging the recent advancement in explainable AI [35,52] and the growing availability of micro-data on behavior and social processes [21] can provide an opportunity to endorse transparency of algorithms and facilitate human-computer collaboration.

This paper explores how an ABM can be designed directly from empirical data, while being transparent about the conceptual models involved. Our modeling framework, ML-ABM, aims at facilitating the process of ABM development through deploying ML to automatically identify the causal relationships and derive decision rules for agents from microdata on behavior. At the same time, we generate a conceptual model that links to the appropriate theoretical work and clarifies the feedbacks in the system. Although AI is actively employed for explaining human choices, to the best of our knowledge, this is the first study that extended the scope of modeling beyond the behavior prediction to causality and feedback loop elicitation in a complex nonlinear system. The combined ML-ABM framework enables identification of temporal and dynamic dependencies of the behavior change process, draws individual-level interferences, and uncovers undesired consequences for interventions while adding to the transparency of the model logic open for stakeholders' discussions. We demonstrate the value of the proposed framework in developing an agent-based model related to purchasing behavior. This case study is a suitable experiment for the goal of our study since we have (i) micro-level data on consumer behavior, (ii) a set of behavioral theories – Theory of Planned Behavior, Goal Framing Theory, Alphabet Theory – explaining purchasing behavior, and (iii) a previously built benchmark empirical ABM to compare with.

We discuss how the overall accuracy and reliability of ABM can be improved and maintained, explaining the differences between this modeling approach and the conventional empirical modeling methods, and examining the advantages and limitations. We also go beyond extracting the rules and use ML to generate conceptual models of the system, which can be further discussed, analyzed, and tested for validity and compliance with social theories and common sense. Bayesian Machine Scientist approach follows the same directions in terms of both describing the observed data and predicting new data accurately [24]. Interested readers can find more information about the approach in Reichardt et al. [49] and its application in Vázquez et al. [69].

2. Materials and methods

The empirical data are borrowed from the study of Taghikhah et al. [65], in which a survey provided extensive empirical data about the organic-conventional wine preferences of 1003 Australians living in the City of Sydney. This microdata was used to instantiate the agents' decisions in the data-driven model, ORVin-E [64]. Compared to other topics, modeling human behavior would be more challenging as the agents' decisions are not fully rational. Yet, insufficient information, varying cognitive abilities, emotions and intuitions, and limited time affect the rationality and perceptions of humans about the environment and bias their future evaluations [25].

We next adopt a combination of ML algorithms (in our case, Random Forest (RF) and Decision Trees (DT)) to automatically derive rules to be used in the simulation model ORVin-ML, so that it reproduces patterns by which heterogeneous consumers behave. Behavioral rules can be represented with, for example, a tree of "if-then" statements, fuzzy logic, or other forms of equations.

The ML-ABM approach consists of four phases (Fig. 1). In the first phase, the aim is to obtain structured data allowing the application of supervised ML algorithms. We pre-process the collected data to a format that algorithms can process and interpret. In the second phase, supervised ML algorithms are used to detect important factors influencing behavior decisions. In the third phase, for every explanatory factor of behavior, stand-alone predictive functions are derived, which are then used to formulate the ABM. Further analysis is then conducted to reveal the feedback loops and find the causal links in the system. In a way, a conceptual model of the system is built based on the data available; it can be further analyzed to check against existing social theories as well as the ideas that were originally used when developing the survey. Finally, the synthesis of predictive functions and the theoretically verified conceptual model generated can provide the empirical microfoundation of an ABM.

2.1. Phase 1: survey design and data collection

Both in physical and social sciences, we are trying to provide scientific descriptions of observable phenomena. Nevertheless, the approaches taken in this pursuit and the notions of observable reality are different. Physical sciences rely on repeated laboratory tests and experiments to derive laws about the way the world operates in their concrete reality and predict natural phenomena until the hypothesis can be tested. Social sciences can only describe social phenomena within a cultural context based on experimental data collected in interviews and/or surveys and limited to specific places and times. We cannot be sure that the same surveys will produce similar results when repeated in other locations or with other responders. Moreover, different survey designs can produce different explanations for social phenomena.

For example, in the particular case of purchasing organic wine, Taghikhah et al. [65] designed a survey based on the potential explanatory factors driven from various social theories, such as the Theory of Planned Behavior (TPB) [2], which explains the influence of cognitive (e.g., attitudes, perceived behavioral control (PBC), and norms) on driving planned purchasing behavior, in combination with Alphabet Theory [75], and Goal Framing Theory [34] that consider how the repetition of behavioral patterns and environmental and atmospheric cues (e.g., packaging, posters, and retail environment design) can prompt habitual and unplanned behavior, respectively. One thousand and three (1003) consumers living in the City of Sydney, Australia, have responded to this online survey carried out in Sep-November 2019. Data are related to socio-demographics, shopping-drinking patterns, and behavioral factors [65]. Generally, consumers have positive attitudes (83%) and intentions (80%) towards organic wine. However, there is a significant gap between intention and behavior, as only about 5% of respondents reported purchasing all organic wine. This gap implies that the TPB is not sufficient to explain what stands behind various consumption decisions. Our further analysis explores whether alphabet theory and goal framing theory can justify why consumers act against their intentions.

2.2. Phase 2: A data-driven function for consumer behavior

In this phase, the collected data are transformed into standard formats that ML algorithms can work with. There are several methods for dealing with discrete and categorical variables. In this study, for the variables containing discrete sequences of values, we use the min-max normalization method. For the categorical variables, we use a one-hot encoding method [9] to transform categorical variables to numerical and scale the differences in the range of variables. We also balance the dataset by increasing the size of rare samples using oversampling methods. We then label consumers as organics (i.e., those whose wine purchases were at least 75% organic-class 1) and conventionals (the rest

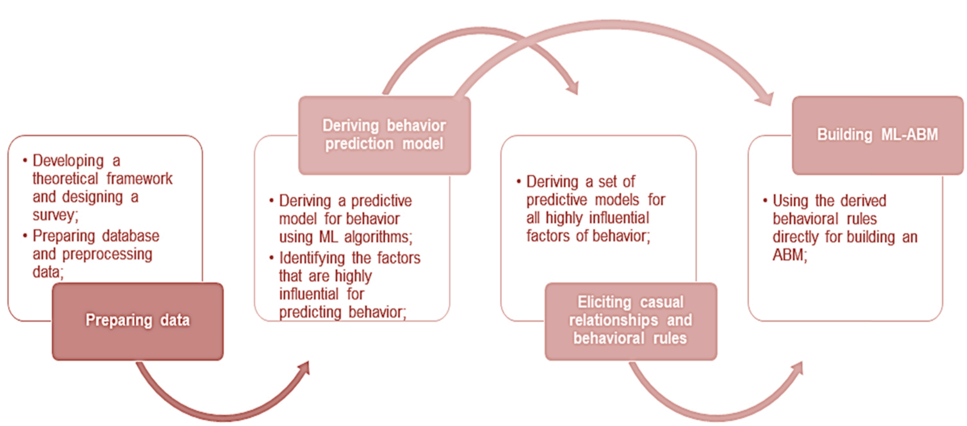

Fig. 1. A brief description of the ML-ABM framework. Initially, the survey is designed, and responses are collected, formatted, and preprocessed to ensure and to enhance the performance of ML algorithms. Next the algorithms drive the data-driven predictive models (i.e., decision rules) related to the variable of interest and elicit the influential factors. Afterwards, data-predictive rules drive the causal relationships among the extracted factors to build a conceptual model with feedback loops. Finally, the derived rules are directly implemented in an ABM.

– class 0). Pre-processing provides us with a structured database to derive the rules. In the first step, the model is developed based on a training set which in our case is 70% of the dataset. In the second step, the rest of the dataset (30%) is used to validate the model built. Thus, we use the training data to fit the model and testing data to test it. All ML analyses are run in Python.

Supervised learning, the most common ML approach for building predictive functions, is a two-step process consisting of learning and then testing expected prediction ability. We use the RF algorithm to set behavior as the target variable (i.e., output to be predicted) and all the other factors in the database as the model inputs. Random Forest (RF) algorithm [8] is a powerful non-parametric ML method, addressing this issue by determining the importance level of factors while enhancing the predictive functions accuracy and reducing the computational complexity. It guides the node splitting process by minimizing the within-node variance to automatically detect the most important predictive factors of the purchasing behavior. Nodes in a tree are the points where the path splits into 'Yes' (observations meet the criteria) and 'No' branches (observations do not meet the criteria). We followed the suggestion of Dong and Rudin [18] to assure that the selected features are consistently highly important across algorithms delivering equally accurate predictions.

We then use Decision Tree (DT) learning algorithms to build a predictive model considering a set of highly explanatory factors identified by RF. DTs are one of the easiest and most popular classification/ regression algorithms to understand and interpret. These algorithms sort data into discrete classes and adopt a top-down recursive strategy to reveal patterns in datasets to produce predictive functions [6]. It has a tree-like structure, where branches denote the classification rules and leaves are the class labels. DTs can handle non-linear relationships between variables and are ideal for understanding, interpreting, and visualizing predictive functions. That is to say, their transparent characteristics allow us to identify thresholds and reconstruct the functions as the behavioral rules for defining the decision-making process of heterogeneous agents. Since each node in the tree separates a single explanatory variable, effectively creating a hyperplane in explanatory variable space orthogonal to that variable's axis, pre-processing is essential to avoid 'bushy' trees that fit classification regions, which do not neatly fit in a hypercube.

As our database has many variables, using the RF method before applying DT algorithms helps us prune the tree without overfitting and reduce the size of the obtained model (i.e., the number of nodes in the tree). Overfitting happens when the learner algorithm tightly fits the given training data so that it fails in making accurate predictions of the untrained data.

2.3. Phase 3: eliciting causal relations and feedback loops for behavior

This phase addresses the core principle of systems thinking and makes our understanding of the system structure explicit by establishing the causal relationships between the explanatory factors using ML. We use a combination of classification and regression tree (CART) [48] to build data-driven functions for all the explanatory factors identified in phase 2. By extending the analysis from building a stand-alone function predicting people's behavior to functions predicting the explanatory factors of behavior, we pursue two objectives: firstly, we automatically extract the causal relationships and understand to what extent changing one factor can cause changes in other interrelated factors as well as resulting behavior; secondly, we prune DTs to facilitate the interpretation of the predictive functions and increase their accuracy. Appendix A presents DTs for all the explanatory factors, and Appendix B lists the applied algorithms and the accuracy results of predictive functions. The highest accuracy rate belongs to the predictive function of wine for special occasions (86%), whereas the social media influence model has the lowest accuracy (57%).

To get an indication of how well the data-driven models can be generalized to an independent/ unseen data set and perhaps avoid the problems of underfitting or overfitting, we use the cross-validation approach. Two popular methods, Stratified *K*-Fold and Leave-*P*- Out [46,73], are used to assure the robustness of results. The former is a non-exhaustive validation method, which is useful for databases with a large imbalance in the response variables. In contrast, the latter computes all possible ways the database can be split into training and test sets. Stratified *K*-Fold is similar to the *K*-Fold method, with the only difference that each fold/database section contains nearly the same percentage of samples of each target class as the full dataset. We set K equal to 10, meaning that the data is divided into 10 subsets, and every time, one subset is used for testing and the rest of subsets are used for training the predictive functions.

Leave-*P*-Out method leaves P data points out of training data, i.e., if there are n data points in the original sample, then $n - p$ samples are used to train the model, and p points are used as the validation set. This process is repeated for all combinations in which the original sample can be separated. Then, the error is averaged for all trials to calculate the overall effectiveness of the model. We use a particular case of this method when $P = 1$ to assess the effectiveness of the models and avoid overfitting. This method, known as Leave-one-out cross-validation, is useful when the amount of training data is small. The number of possible combinations equals the number of data points in the original sample or n. Result of validation tests is available in Appendix B. As the differences between the accuracy rates and the cross-validations of models are negligible (less than 5%), we can claim that the resulting models are valid and do not have the overfitting issue. Conducting validation analysis is particularly critical in our case since the ratio of data points to the number of factors is relatively low. At the end of this phase, we can infer the causal relationships describing the agents' behavior in the ABM.

2.4. Phase 4: data-driven agent-based modeling

The derived predictive functions from phase 2 (a function for predicting behavior) and phase 3 (functions for predicting the explanatory factor of behavior) reveal the relative importance of different variables – similar to the feature selection process in ML – in instigating or influencing the responses at different process-response ranges. DTs can be a bit brittle (i.e., their structure changes a lot for small gains/losses in a fit), and unexpected improvements can be achieved just by leaving out unimportant variables. These functions (DTs) are directly implemented in the agents of ABM to serve as behavioral rules. This integration offers opportunities to understand the relative performance of model structures and parameter settings, from which we may deduce hypotheses about decision-making mechanisms and governing states. The suggested approach does not require data from multiple timepoints; rather, the ABM can be built from single time point measurements. A similar concept has been used in the study of Sachs et al. [51] for building dynamic models from a snapshot in time.

In our case study, ORVin-ML is designed to explore organic wine purchasing decisions. It is a spatially explicit model in which a population of 1003 consumers is distributed over 30 suburbs in the City of Sydney, based on the postal codes of survey participants. The city of Sydney is approximately 26.15 square kilometers and is home to over 103,844 estimated households with an average size of 2.2 in 2016. We locate one wine retailer for each of the five major suburbs of this area, according to Google Maps. Consumers make purchasing decisions between organic and conventional wines based on their attitude, willingness to pay, social norms, personal goals, and norms as well as habits. Every time they go shopping for wine, they consider the available wine retailers and visit the closest one. The shops are assumed to sell similar wines for the same prices, i.e., there are no differences between the shops in the model. Empirical data collected from the survey in phase 1 inform all the parameters of ORVin-ML. The model is programmed in AnyLogic Software, and the code is available (here). Since more than

70% of households report shopping for wine at least once per week, the time step in the model is set to one week, and it runs for 600 weeks.

3. Results and discussion

3.1. ML for learning feedback loops from data: why do they matter?

A combined Random Forest (RF) / Decision Tree (DT) method derives a set of if-then rules for predicting purchasing behavior and its associated conceptual model as presented in Fig. 2 [3]. Following the recommendation of Li et al. [33], to ensure the validity of predictive models based on their generalizability and reproducibility in different experiments, ML methods should be used to find the complete set of features and relationships influencing the outcome and not only those strong predictive variables contributing to the accuracy. We thus extend the analysis and extract if-then rules and conceptual models for the explanatory factors of behavior – intention, personal norms, perceived behavioral control (PBC), social norm, and hedonism. Appendix A presents the details of rules (in the format of DTs) and related conceptual models for all the explanatory factors.

By linking these conceptual models, we reveal the causal relationships and feedback loops between behavior and explanatory factors that are built with ML algorithms (refer to Fig. 3). The inclusion of data-driven functions of behavior components can develop the causal relationships and make the ABM dynamic. Hence, when one of the factors changes, we observe changes not only in behavior but also in other system factors. For example, changing personal norms (such as purchasing frequencies and shopping size) causes changes in individual purchasing behavior, intention, and PBC. For systems modeling, the feedback concept is an essential component [20] as the outputs of the model come back as inputs to the system, depending on the causal inference. Since ABM is a continuous system, the current actions of an agent change their future decisions. In a way, machine-driven rules/functions should be deployed to support this system property. Thus, ML-ABM drives the analysis beyond the data patterns mined by ML algorithms.

Another interesting observation extracted by the ML-ABM approach (in Fig. 3) is that factors such as attitude and normativism (dotted circles) can indirectly impact consumer choice. These implicit relationships are not captured in Fig. 2, resulting in an incomplete cognitive process of decision-making. A comprehensive conceptual model helps the decision-makers design interventions that target changes in multiple factors, for example, towards more sustainable choices in our case. *Our proposed modeling approach adds the systems thinking perspective to the process of ABM development using ML algorithms and produces qualitative results about how various factors interact in the system.*

This shows how computational models enhanced with ML-preprocessed data on decisions could help testing theoretically-hypothesized relationships. Especially since there could be alternative and competing theories explaining the same phenomenon/behavior. In our case, consistent with the Theory of Planned Behavior, feedback loops exist between behavior and social norm as well as intention and PBC, while intention has a one-way relationship with the behavior. Attitude indirectly influences behavior through impacting intention and social norms. In line with the Goal Framing Theory, hedonism has a two-way relationship with behavior, whereas normativism can only implicitly change behavior. Note PBC entails gain goals as they are highly correlated. We can also see the relevance of these two theories, where attitude, intention, and social norm guide hedonism and vice-versa. Lastly, personal norms, coming from the Alphabet Theory, affect TPB through influencing social norms along with the behavior. Besides, purchasing size and frequency are driven by the pursuit of hedonistic.

While the proposed ML-ABM approach has similarities with the previous applications of ML in extracting agents' rules from data, there is a difference in the inclusion of feedback loops. Our approach focuses on using ML to reveal causal relationships between explanatory factors of behavior, whereas previous studies exclude the causalities and only focus on the predictive function of behavior. We observe a similar line of thinking in a recent study of Xie et al. [74], in which they used unsupervised ML algorithms to cluster the data generated from an ABM for better explaining and understanding of the behaviors of complex systems.

Functions derived by ML algorithms are static, representing a snapshot of relationships captured in data. However, human systems are dynamic, and behavior of agents can change. To use ML for analyzing complex systems, every exploratory factor should be treated as an adaptive subsystem in its own right, interacting with other systems. This gives the factors a dynamic characteristic, enabling them to change, adapt and reorganize in response to their environment. Additionally, interactions and feedback mechanisms may reveal the emergent properties of the overall system that the study of individual system elements cannot capture [19].

In line with Li et al. [33], our results support the importance of using domain knowledge to identify the potential causes of the outcome before data collection and model building. According to Polhill and Salt [43], "validation by fit-to-data is not, on its own, a sound basis for estimating the ability of a model to make reliable predictions, not least because of issues with path dependency." Since fit-to-data cannot be considered as the sole indicator of ABM suitability, it is vital to closely study and monitor the model structure/ontologies and explore how they relate to known theoretical conceptualizations that show a bigger picture, beyond a single dataset or a particular case-specific ABM. The prediction accuracy and even cross validation tests are not sufficient to ensure the reproducibility and validity of the ML outputs.

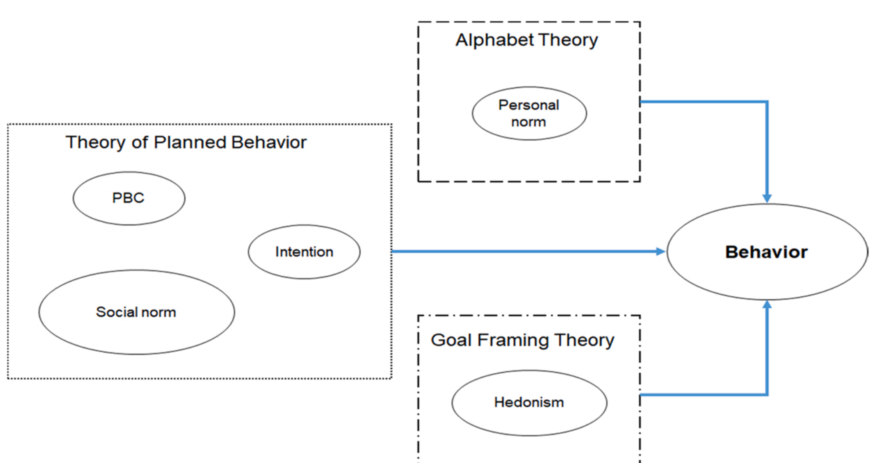

Fig. 2. Conceptual model of factors influencing behavior extracted from the data on purchasing behavior using the machine learning methods. PBC, social norm, and intentions are elements of Theory of Planned Behavior. Hedonism is an element of Goal Framing Theory, while personal norm is the element of Alphabet Theory. The size of circles indicates their importance in predicting behavior. For example, social norm and hedonism have the highest importance. Complementary information is available in Appendix A.

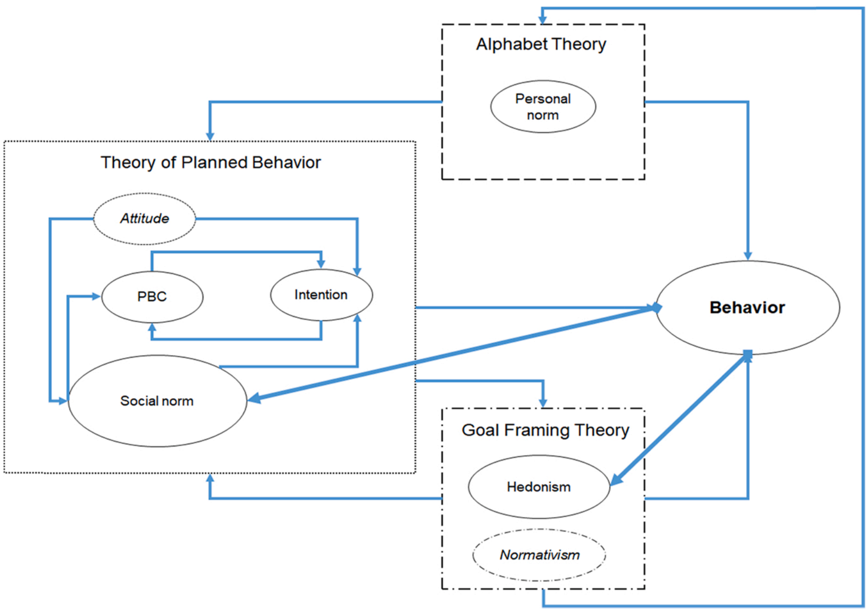

Fig. 3. Conceptual model of ORVin-ML extracted directly from data using ML-ABM. We combined the conceptual models of all explanatory factors. Notably, these factors mirror the Theory of Planned Behavior (PBC, social norm, intention explicitly, whereas attitude implicitly), Goal Framing Theory (hedonism explicitly, whereas normativism implicitly) and Alphabet Theory (personal norm explicitly). Here, there are feedbacks/causalities, between PBC-Intention, social norm-behavior, and hedonism-behavior, which were not present in Fig. 2. We can also observe the co-influence among the behavioral theories. Dotted circles indicate the elements that do not have any direct relationship with behavior. Complementary information is available in Appendix A.

Feature selection and result validation should be guided by domain experts, as well said by Li et al. [33] "data-driven discovery needs a collaboration between domain experts and ML practitioners". Schmidt and Lipson [54] proposed a similar approach to automatically derive equations describing the natural laws without prior field knowledge. The authors discussed that the selection of variables to feed the algorithm determines the data-driven laws. For example, if they have only provided position coordinates, the algorithm would converge on a manifold equation of the system's state space. In our case, indeed, if we additionally supply data about other behavioral traits, the algorithms tend to find new rules for behavior prediction.

We also conducted a simple experiment to test this statement and included data about the feelings and emotions of consumers during their shopping to the existing dataset. As expected, we observed changes in the structure and accuracy of behavior functions and spotted those emotions and habits are new explanatory factors of organic wine purchasing decisions (refer to Appendix A6).

3.2. *Empirical vs. machine driven ABMs: what does the comparison tell us?*

Addressing some of the knowledge gaps and questions regarding replacing empirical rules with machine-driven rules, we conduct a comparative study between ORganic Vine- Empirical model (ORVin-E) [64] and ORganic Vine- ML model (ORVin-ML). Our objective is to assess the quality and performance of the ML-ABM approach and test the validity of results generated by the algorithms. We follow the structure of ORVin-E for setting up the environment, agent types, and networks, but the outputs of ML algorithms are used to define the rules. Survey data are used to parameterize heterogeneous consumer agents of ORVin-E and ORVin-ML. We implement all predictive functions as in ORVin-ML. In ORVin-E, however, data-driven parameters are updated by the changes in the shopping experience and habits of agents, observations, and social learning (e.g., the wine choice of others at shops), the exchange of information about organic products within agents' social networks (e.g., interactions with family and friends), which eventually determine the wine preference of consumers. Much effort is required to deliver a calibrated model with accuracy and precision. Nevertheless, the ML-ABM framework does not require any further calibration, and the model is ready to use as is. In the case of ORVin-ML, in contrast to the long calibration process of ORVin-E, we can skip calibration tests so that the model development process becomes agile.

We empirically conduct a validation test by fixing the parameters across the models and then assessing the intention and behavior outputs against the survey data at the individual (person) level. Fig. 4 compares the performance of models when estimating the number of organic wine consumers and consumers intending to purchase organic wine. The ORVin-E and ML results can estimate the organic-conventional preferences of consumers with high accuracy, translating to an error of 8% and 15%, respectively. This result indicates that our suggested approach is robust enough to deal with heterogeneity in behavior, and its performance is comparable to the empirical methods. Regarding the shopping intention, the estimation errors for ORVin-E and ML are 40% and 49%, respectively, implying that the predictions of ORVin-E is slightly (9%) better than ORVin-ML and the outputs of our approach are still within the acceptable range. Note that the accuracy of intention prediction with the ML algorithm standalone is 67% (see Appendix B, Table B1), which is 16% higher than the accuracy of predicted intention in ORVin-ML (51% as shown in Fig. 4). The prediction power of machine-driven ABMs can be improved when more data points become available, and the accuracy of functions are improved.

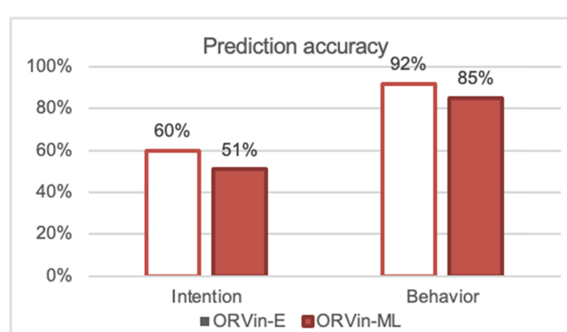

Fig. 4. Comparing the validation results of the hand-calibrated computational agent-based model (ORVin-E) vs. a model enhanced with ML- with pre-processed data on decisions (ORVin-ML) for intention and behavior. The outputs of the latter ML-ABM are within the acceptable range. Overall, the prediction accuracies of ORVin-E with regards to shopping intention and behavior are slightly (9% and 7%, respectively) better than ORVin-ML.

3.3. ML-ABM goes dynamic: what do feedbacks bring to the table when developing ABMs?

It is important to test causality in using ML for developing ABMs. To investigate the performance of casualties in the ML-ABM approach, a straightforward way is to conduct comparative experiments with ORVin-ML.

which has the casual relationships of behavior, and with an otherwise identical model, named ORVin-ML-N, which only has the predictive function of behavior, with no built-in casualties. These experiments are related to changing implicit (e.g., attitude) and explicit (e.g., PBC) factors of behavior. For example, the values of attitude and PBC for all the agents are maximized (set to 1). By comparing the results between the two models in two distinct experiments, it is possible to quantitatively measure the importance of the casualties and isolate their effects.

Fig. 5 highlights how such conceptual modeling differences can affect the simulation results. There are noticeable distinctions between the influence of attitude on shifting consumer preferences toward organic products (0% using the predictive function of behavior only (ORVin-ML-N), compared to 80% using ML-ABM approach (ORVin-ML)). Regarding the PBC, we observe 4% difference between the outputs of two models (57% using predictive function of behavior only (ORVin-ML-N) compared to 61% using ML-ABM approach (ORVin-ML)). This analysis gives rise to the significance of embedding the causal relationships in the machine-driven ABMs.

The findings indicate that a combination of detailed behavioral data and classification and regression tree (CART) algorithms reduces biases, assumptions, and errors, expands simulation capabilities, but not necessarily enhances the accuracy of results. We also observed that in certain instances as in our case study, a well-developed theory-driven model that is parameterized with quality data can outperform the machine-driven ABM with regard to accuracy of prediction. But we should keep in mind that theoretical model development is way more time-consuming and requires a comprehensive and detailed knowledge of conceptual models and theories related to the topic under investigation. We showed that the deployment of machine intelligence speeds up analyzing and interpreting data to be used for the ABM development.

4. Conclusions

When designing policies and practices for behavior change across multiple domains, it is essential to examine the mechanisms underlying human decision making. Most often, linear statistical techniques are used to find the determinants of the behaviors and their impacts on the outcomes, which are assumed to be constant and additive. These limitations related to interrelationship between factors can impede or mislead our understanding of the behavior change process and the consequences of interventions. Applying systems science, however, one can consider the complexity, non-linearity, and dynamics of the human system. The science of complex adaptive systems provides a set of theories and methods for identifying the causality and feedback complexity.

ABM is the favorable method for simulating complex systems. One of the most common applications of ABM in sociology is to test hypotheses about the drivers of behavior and present decision-making theories. As an analytical method in social science, ML has been widely adopted for providing data-driven predictions. The novelty of this research lies in automatically developing ABMs from empirical data by applying ML techniques to derive the rules that define agents' behavior. The ML-ABM framework allows us to understand and simulate causal relationships and feedback loops compatible with common social science theories explaining the fundamentals of behavior and generate models in a timely manner without sacrificing much accuracy (7% drop as shown in Fig. 4).

Although the power of AI for explaining human choices has been acknowledged elsewhere, to the best of our knowledge, this is the first study that extended the scope of modeling beyond the behavior prediction to causality and feedback loop elicitation in a complex nonlinear system. Using AI to extract feedback loops from data to reflect underlying causality and disproportionate influences can greatly add value to the validity and explanatory power of ML-ABMs. The interconnectedness and non-ergodicity characteristics of our framework enables identification of temporal and dynamic dependencies of the behavior change process, draws individual-level interferences, and prevents undesired consequences for interventions. Moreover, it adds to the transparency of the built model, helps to communicate the model to stakeholders, and provides them access to the logic involved in the decision-making process. Opening up the black box to explain and understand the system may reveal new implicit knowledge, potential risks and biases to the stakeholders.

ML-ABM framework offers a basis for broadly applicable analysis methods for complex systems modeling and can be used in different areas including, but not limited to, social science, medicine, physics, and biology, to address theoretical gaps despite abundance in data. When detailed data are available, it provides a generic, flexible approach to

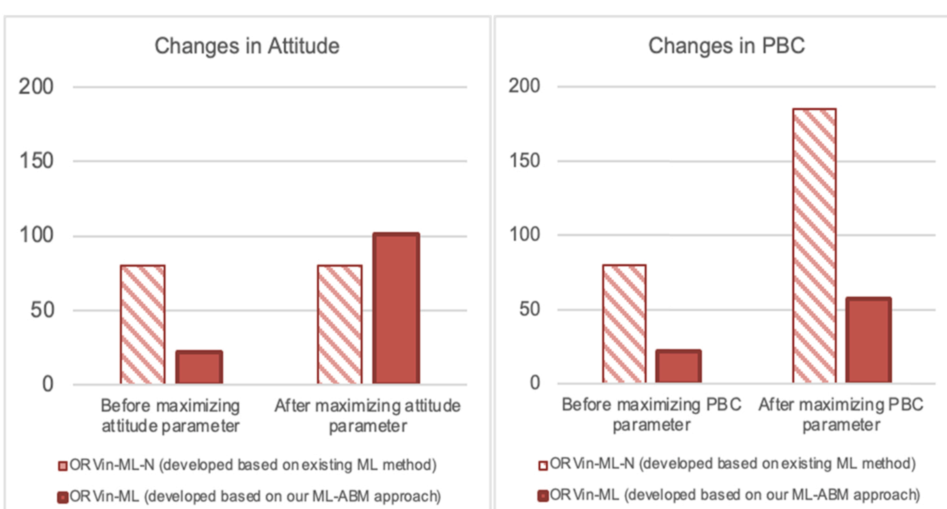

Fig. 5. Comparing the performance of two versions of the model (ORVin-ML developed by ML-ABM approach vs. ORVin-ML-N developed by existing methods) when attitude and perceived behavior control (PBC) values change. There are noticeable distinctions between the outputs of these models when changing the attitude parameter. However, when changing the PBC parameter, we observe a slight difference (4%) between the rate of change in the outputs of the two models.

describe agents and their attributes for further formalization in terms of an ABM experiment, considerably reducing the model development time. This automation allows ABM developers to quickly analyze the data, rapidly develop decision support tools, and explore possible future scenarios or active interventions timely.

Furthermore, it identifies explanatory factors in the decision-making process and therefore provides a direction for future data collection efforts, suggesting what data to include and what data to exclude. When raw data are simply fed into ML algorithms, they are decontextualized, with important information not included. When psychologists collect survey data, the questions asked are carefully designed and typically derived from selected constructs and theories that have been tested and developed over many years by the research community. With just the raw data, this knowledge is not included in the information fed into the algorithms, even though it is relevant and important for understanding the data.

One approach, though limited, to encoding such knowledge is to constrain the set of features acting as explanatory variables for an outcome variable. Another approach is to use expert assessment to evaluate the results of the algorithms. However, this can be time-consuming and may lead to criticism that it would have been better to use knowledge acquisition and engineering to derive the algorithmic formalization of the system and leave out the ML step altogether. This thinking offers insight into why there is skepticism among some social scientists about using ML with big data to derive useful insights into social and psychological phenomena since such data are not collected with appropriate theoretical underpinning to necessarily justify the insights gained.

In the real world, the system environment (e.g., market prices, income, awareness, etc.) unpredictably changes over time and co-evolves with the behavior, and so does the agent behavior (e.g., consumer preference). Under such circumstances, ML-based models, as any data-driven models built based on the initial environmental conditions, are bound to become invalid over time and hence may lose the reliability of their results. Since the ML-ABM does not accommodate these changes, it continues to use the original rules and becomes invalid if there are significant changes in the environment. We can associate this challenge to issues in developing atmospheric prediction models, in which data assimilation methods, such as the Cressman analysis method or the optimal interpolation method, are used to provide an estimate of the system state by combining observations, theory and models. One possible future direction is to complement survey data with real-time market transactions to update the ML-driven rules. This enables the ML-ABMs to be consistently updated in sync with their environment.

A take-home message of this paper is that cautious steps need to be taken to examine the empirical rules and relationships from the perspective of behavioral theories and cross validate the observations with the relationships in theory. Since the models developed based purely on data and over an observed range of explanatory variables are biased, generating the inferences and conceptual models behind the machine-driven models is especially important for further scrutiny and verification. Future research may consider ML-ABM as a tool that can automate the process of theory extraction and matching.

CRediT authorship contribution statement

Firouzeh Taghikhah: Investigation, Conceptualization, Methodology, Software, Formal analysis, Writing – original draft, Validation, Visualization; **Alexey Voinov:** Conceptualization, Methodology, Formal analysis, Writing – original draft, Validation, Review; **Tatiana Filatova:** Conceptualization, Methodology, Writing – original draft; **Gareth Polhill:** Validation, Writing – review & editing.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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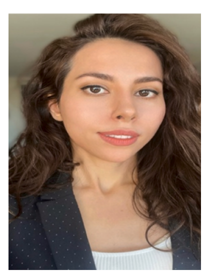
Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.jocs.2022.101854.

References

[1] M. Agar, My kingdom for a function: Modeling misadventures of the innumerate, J. Artif. Soc. Soc. Simul. 6 (3) (2003).
[2] I. Ajzen, From intentions to actions: A theory of planned behavior. Action Control, Springer, 1985, pp. 11–39, 11-39.
[3] A. Alonso-Betanzos, N. Sánchez-Maroño, O. Fontenla-Romero, J.G. Polhill, T. Craig, J. Bajo, J.M. Corchado, Agent-based modeling of sustainable behaviors, Springer, 2017.
[4] Anonym, Theorists and experimentalists must join forces, Nat. Comput. Sci. 1 (5) (2021), https://doi.org/10.1038/s43588-021-00082-3.
[5] D. Bell, C. Mgbemena, Data-driven agent-based exploration of customer behavior, Simulation 94 (3) (2018) 195–212.
[6] W.A. Belson, Matching and prediction on the principle of biological classification, J. R. Stat. Soc.: Ser. C. Appl. Stat. 8 (2) (1959) 65–75.
[7] R. Boero, F. Squazzoni, Does empirical embeddedness matter? Methodological issues on agent-based models for analytical social science, J. Artif. Soc. Soc. Simul. 8 (4) (2005).
[8] L. Breiman, Random forests, Mach. Learn. 45 (1) (2001) 5–32.
[9] Brownlee, J.2017. Why One-Hot Encode Data in Machine Learning?". *Machinelearningmastery*. Retrieved from ⟨https://machinelearningmastery.com/why-one-hot-encode-data-in-machine-learning/⟩.
[10] G. Carleo, I. Cirac, K. Cranmer, L. Daudet, M. Schuld, N. Tishby, L. Zdeborová, Machine learning and the physical sciences, Rev. Mod. Phys. 91 (4) (2019), 045002.
[11] S.N. Chowdhury, A. Ray, S.K. Dana, D. Ghosh, Extreme events in dynamical systems and random walkers: a review, Phys. Rep. 966 (2022) 1–52.
[12] S.N. Chowdhury, A. Ray, A. Mishra, D. Ghosh, Extreme events in globally coupled chaotic maps, J. Phys.: Complex. 2 (3) (2021), 035021.
[13] J.A.G. Coria, J.A. Castellanos-Garzón, J.M. Corchado, Intelligent business processes composition based on multi-agent systems, Expert Syst. Appl. 41 (4) (2014) 1189–1205.
[14] A.T. Crooks, A.J. Heppenstall, Introduction to agent-based modelling. Agent-based models of geographical systems, Springer,, 2012, pp. 85–105, 85-105.
[15] E. Cuevas, J. Gálvez, K. Avila, M. Toski, V. Rafe, A new metaheuristic approach based on agent systems principles, J. Comput. Sci. 47 (2020), 101244.
[16] R. Dingreville, R.A. Karnesky, G. Puel, J.-H. Schmitt, Review of the synergies between computational modeling and experimental characterization of materials across length scales, J. Mater. Sci. 51 (3) (2016) 1178–1203.
[17] Dogra, I.S., Kobti, Z. , 2013. *I*mproving prediction accuracy in agent based modeling systems under dynamic environment. Paper presented at the 2013 IEEE Congress on Evolutionary Computation.
[18] J. Dong, C. Rudin, Exploring the cloud of variable importance for the set of all good models, Nat. Mach. Intell. 2 (12) (2020) 810–824.
[19] T. Eliassi-Rad, H. Farrell, D. Garcia, S. Lewandowsky, P. Palacios, D. Ross, K. Wiesner, What science can do for democracy: a complexity science approach, Humanit. Soc. Sci. Commun. 7 (1) (2020) 1–4.
[20] J.W. Forrester, System dynamics, systems thinking, and soft OR, Syst. Dyn. Rev. 10 (2–3) (1994) 245–256.
[21] J.L. Furman, F. Teodoridis, Machine learning could improve innovation policy, Nat. Mach. Intell. 2 (2) (2020), 84-84.
[22] J. Gonzalez-Redin, I.J. Gordon, R. Hill, J.G. Polhill, T.P. Dawson, Exploring sustainable land use in forested tropical social-ecological systems: A case-study in the Wet Tropics, J. Environ. Manag. 231 (2019) 940–952.
[23] Granato, B., Li-Jessen, N.Y. , 2020. Sensitivity Analysis for Dimensionality Reduction in Agent-Based Modeling. In *ECAI 2020* (2905–2906pp. 2905–2906): IOS Press.
[24] R. Guimerà, I. Reichardt, A. Aguilar-Mogas, F.A. Massucci, M. Miranda, J. Pallarès, M. Sales-Pardo, A Bayesian machine scientist to aid in the solution of challenging scientific problems, Sci. Adv. 6 (5) (2020) eaav6971.
[25] C.K. Hsee, Y. Zeng, X. Li, A. Imas, Bounded rationality in strategic decisions: undershooting in a resource pool-choice dilemma, Manag. Sci. (2021).
[26] Y. Hu, C.J. Quinn, X. Cai, N.W. Garfinkle, Combining human and machine intelligence to derive agents' behavioral rules for groundwater irrigation, Adv. Water Resour. 109 (2017) 29–40.

[27] Huang, Y., Seck, M.D., Verbraeck, A.2011. *From data to simulation models: component-based model generation with a data-driven approach.* Paper presented at the Proceedings of the 2011 Winter Simulation Conference (WSC).
[28] R. Huber, M. Bakker, A. Balmann, T. Berger, M. Bithell, C. Brown, G. Mack, Representation of decision-making in European agricultural agent-based models, Agric. Syst. 167 (2018) 143–160.
[29] D. Jha, L. Ward, A. Paul, W.-k Liao, A. Choudhary, C. Wolverton, A. Agrawal, Elemnet: Deep learning the chemistry of materials from only elemental composition, Sci. Rep. 8 (1) (2018) 1–13.
[30] R. Kaufmann, D. Newberry, C. Xin, S. Gopal, Feedbacks among electric vehicle adoption, charging, and the cost and installation of rooftop solar photovoltaics, Nat. Energy 6 (2) (2021) 143–149.
[31] P.S. Kruger, The art of simulation modelling, South Afr. J. Ind. Eng. 14 (1) (2003) 39–50.
[32] E. Le Merrer, G. Trédan, Remote explainability faces the bouncer problem, Nat. Mach. Intell. 2 (9) (2020) 529–539.
[33] J. Li, L. Liu, T.D. Le, J. Liu, Accurate data-driven prediction does not mean high reproducibility, Nat. Mach. Intell. 2 (1) (2020) 13–15.
[34] S. Lindenberg, L. Steg, Normative, gain and hedonic goal frames guiding environmental behavior, J. Soc. Issues 63 (1) (2007) 117–137, https://doi.org/10.1111/j.1540-4560.2007.00499.x.
[35] S.M. Lundberg, G. Erion, H. Chen, A. DeGrave, J.M. Prutkin, B. Nair, S.-I. Lee, From local explanations to global understanding with explainable AI for trees, Nat. Mach. Intell. 2 (1) (2020) 56–67.
[36] E.E. Maeda, P. Haapasaari, I. Helle, A. Lehikoinen, A. Voinov, S. Kuikka, Black boxes and the role of modeling in environmental policy making, Front. Environ. Sci. 3 (2021) 63.
[37] S.M. Manson, Agent-based modeling and genetic programming for modeling land change in the Southern Yucatan Peninsular Region of Mexico, Agric., Ecosyst. Environ. 111 (1–4) (2005) 47–62.
[38] R.B. Matthews, N.G. Gilbert, A. Roach, J.G. Polhill, N.M. Gotts, Agent-based land-use models: a review of applications, Landsc. Ecol. 22 (10) (2007) 1447–1459.
[39] R.E. Nance, R.G. Sargent, Perspectives on the evolution of simulation, Oper. Res. 50 (1) (2002) 161–172.
[40] D.C. Parker, A. Hessl, S.C. Davis, Complexity, land-use modeling, and the human dimension: fundamental challenges for mapping unknown outcome spaces, Geoforum 39 (2) (2008) 789–804.
[41] A.W. Peters, A.J. Howarth, O.K. Farha, Experimentalists and theorists need to talk, Nature 551 (7681) (2017) 433–435.
[42] Polhill, G., Craig, T., Alonso Betanzos, A., Sanchez Maroño, N., Fontenla Romero, Ó., Dumitru, A.,. Fornara, F. , 2014. *Empirical agent-based modelling of everyday pro-environmental behaviours at work.* Paper presented at the 7th International Congress on Environmental Modelling and Software.
[43] G. Polhill, D. Salt, The importance of ontological structure: why validation by 'fit-to-data'is insufficient. Simulating social complexity, Springer,, 2017, pp. 141–172, 141-172.
[44] L.M. Possati, Algorithmic unconscious: why psychoanalysis helps in understanding AI, Palgrave Commun. 6 (1) (2020) 1–13.
[45] M. Prosperi, Y. Guo, M. Sperrin, J.S. Koopman, J.S. Min, X. He, J. Bian, Causal inference and counterfactual prediction in machine learning for actionable healthcare, Nat. Mach. Intell. 2 (7) (2020) 369–375.
[46] Purushotham, S., Tripathy, B. , 2011). Evaluation of classifier models using stratified tenfold cross validation techniques. Paper presented at the International Conference on Computing and Communication Systems.
[47] A. Pyka, T. Grebel, Agent-based modelling—a methodology for the analysis of qualitative development processes. Agent-based computational modelling, Springer,, 2006, pp. 17–35, 17-35.
[48] M.A. Razi, K. Athappilly, A comparative predictive analysis of neural networks (NNs), nonlinear regression and classification and regression tree (CART) models, Expert Syst. Appl. 29 (1) (2005) 65–74.
[49] I. Reichardt, J. Pallarès, M. Sales-Pardo, R. Guimerà, Bayesian machine scientist to compare data collapses for the Nikuradse dataset, Phys. Rev. Lett. 124 (8) (2020), 084503.
[50] D.T. Robinson, D.G. Brown, D.C. Parker, P. Schreinemachers, M.A. Janssen, M. Huigen, E. Irwin, Comparison of empirical methods for building agent-based models in land use science, J. Land Use Sci. 2 (1) (2007) 31–55.
[51] K. Sachs, S. Itani, J. Fitzgerald, B. Schoeberl, G. Nolan, C. Tomlin, Single timepoint models of dynamic systems, Interface Focus 3 (4) (2013), 20130019.
[52] W. Samek, Learning with explainable trees, Nat. Mach. Intell. 2 (1) (2020) 16–17.
[53] N. Sánchez-Maroño, A. Alonso-Betanzos, O. Fontenla-Romero, J.G. Polhill, T. Craig, Empirically-derived behavioral rules in agent-based models using decision trees learned from questionnaire data, 53-76. Agent-Based Modeling of Sustainable Behaviors, Springer,, 2017, pp. 53–76, 53-76.
[54] M. Schmidt, H. Lipson, Distilling free-form natural laws from experimental data, science 324 (5923) (2009) 81–85.
[55] Shannon, R.E. , 1998. *Introduction to the art and science of simulation.* Paper presented at the 1998 winter simulation conference. proceedings (cat. no. 98ch36274).
[56] H.Y. Sigaki, R. de Souza, R. de Souza, R. Zola, H. Ribeiro,). Estimating physical properties from liquid crystal textures via machine learning and complexity-entropy methods, Phys. Rev. E 99 (1) (2019), 013311.
[57] H.Y. Sigaki, E.K. Lenzi, R.S. Zola, M. Perc, H.V. Ribeiro, Learning physical properties of liquid crystals with deep convolutional neural networks, Sci. Rep. 10 (1) (2020) 1–10.
[58] A. Smajgl, E. Bohensky, Behaviour and space in agent-based modelling: poverty patterns in East Kalimantan, Indonesia, Environ. Model. Softw. 45 (2013) 8–14.
[59] A. Smajgl, D.G. Brown, D. Valbuena, M.G. Huigen, Empirical characterisation of agent behaviours in socio-ecological systems, Environ. Model. Softw. 26 (7) (2011) 837–844.
[60] J. Su, J. Huang, S. Adams, Q. Chang, P.A. Beling, Deep multi-agent reinforcement learning for multi-level preventive maintenance in manufacturing systems, Expert Syst. Appl. 192 (2022), 116323.
[61] D. Suleimenova, D. Bell, D. Groen, A generalized simulation development approach for predicting refugee destinations, Sci. Rep. 7 (1) (2017) 1–13.
[62] Z. Sun, I. Lorscheid, J.D. Millington, S. Lauf, N.R. Magliocca, J. Groeneveld, J. Schulze, Simple or complicated agent-based models? A complicated issue, Environ. Model. Softw. 86 (2016) 56–67.
[63] C. Sutton, M. Boley, L.M. Ghiringhelli, M. Rupp, J. Vreeken, M. Scheffler, Identifying domains of applicability of machine learning models for materials science, Nat. Commun. 11 (1) (2020) 1–9.
[64] F. Taghikhah, T. Filatova, A. Voinov, Where Does Theory Have It Right? A Comparison of Theory-Driven and Empirical Agent Based Models, J. Artif. Soc. Soc. Simul. 24 (2) (2021).
[65] F. Taghikhah, A. Voinov, N. Shukla, T. Filatova, Shifts in consumer behavior towards organic products: Theory-driven data analytics, J. Retail. Consum. Serv. 61 (2021), 102516.
[66] S.K. Tan, N. Hu, W. Cai, A data-driven path planning model for crowd capacity analysis, J. Comput. Sci. 34 (2019) 66–79.
[67] B. Thalheim, The science and art of conceptual modelling, in: Transactions on Large-Scale Data-and Knowledge-Centered Systems, VI, Springer,, 2012, pp. 76–105, 76-105.
[68] O. Thebaud, B. Locatelli, Modelling the emergence of resource-sharing conventions: an agent-based approach, Jasss J. Artif. Soc. Soc. Simul. 4 (2) (2001).
[69] D. Vázquez, R. Guimerà, M. Sales-Pardo, G. Guillén-Gosálbez, Automatic modeling of socioeconomic drivers of energy consumption and pollution using Bayesian symbolic regression, Sustain. Prod. Consum. 30 (2022) 596–607.
[70] A. Voinov, K. Jenni, S. Gray, N. Kolagani, P.D. Glynn, P. Bommel, R. Jordan, Tools and methods in participatory modeling: selecting the right tool for the job, Environ. Model. Softw. 109 (2018) 232–255.
[71] A. Voinov, R. Seppelt, S. Reis, J.E. Nabel, S. Shokravi, Values in socio-environmental modelling: persuasion for action or excuse for inaction, Environ. Model. Softw. 53 (2014) 207–212.
[72] Vu, T.M., Probst, C., Epstein, J.M., Brennan, A., Strong, M., Purshouse, R.C.2019. Toward inverse generative social science using multi-objective genetic programming. Paper presented at the Proceedings of the Genetic and Evolutionary Computation Conference.
[73] T.-T. Wong, Performance evaluation of classification algorithms by k-fold and leave-one-out cross validation, Pattern Recognit. 48 (9) (2015) 2839–2846.
[74] S. Xie, A.T. Lawniczak, C. Gan, Optimal number of clusters in explainable data analysis of agent-based simulation experiments, J. Comput. Sci. 62 (2022), 101685.
[75] L. Zepeda, D. Deal, Organic and local food consumer behaviour: Alphabet theory, Int. J. Consum. Stud. 33 (6) (2009) 697–705, https://doi.org/10.1111/j.1470-6431.2009.00814.x.
[76] A. Ziletti, D. Kumar, M. Scheffler, L.M. Ghiringhelli, Insightful classification of crystal structures using deep learning, Nat. Commun. 9 (1) (2018) 1–10.



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