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Using Machine Learning for Agent Specifications in Agent-Based Models and Simulations: A Critical Review and Guidelines

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Abstract: Agent-based modelling and simulation (ABMS), whether simple toy models or complex data-driven ones, is regularly applied in various domains to study the system-level patterns arising from individual behaviour and interactions. However, ABMS still faces diverse challenges such as modelling more representative agents or improving computational efficiency. Research shows that machine learning (ML) techniques, when used in ABMS can address such challenges. Yet, the ABMS literature is still marginally leveraging the benefits of ML. One reason is the vastness of the ML domain, which makes it difficult to choose the appropriate ML technique to overcome a specific modelling challenge. This paper aims to bring ML more within reach of the ABMS community. We first conduct a structured literature review to investigate how the ABMS process uses ML techniques. We focus specifically on articles where ML is applied for the structural specifications of models such as agent decision-making and behaviour, rather than just for analysing output data. Given that modelling challenges are mainly linked to the purpose a model aims to serve (e.g., behavioural accuracy is required for predictive models), we frame our analysis within different modelling purposes. Our results show that Reinforcement Learning algorithms may increase the accuracy of behavioural modelling. Moreover, Decision Trees, and Bayesian Networks are common techniques for data pre-processing of agent behaviour. Based on the literature review results, we propose guidelines for purposefully integrating ML in ABMS. We conclude that ML techniques are specifically fit for currently underrepresented modelling purposes of social learning and illustration; they can be used in a transparent and interpretable manner.

Keywords: Machine Learning, Agent-Based Modelling, Modelling Purpose, Structured Literature Review, Guidelines

Introduction

1.1 Five decades after Schelling (1971) model of segregation, the embryonic decades of agent-based modelling and simulation (ABMS) have passed, and its role has changed into a more mature method with worldwide and domain diverse applications. As the application of ABMS in different fields of study has increased, the demand for efficient and intelligent tools that enable the development of more advanced models is evident and also highlighted in the literature (An 2012; Kavak et al. 2018; Macal & North 2010; Rand & Rust 2011). In addition, agent-based models (ABMs) also face challenges related to insufficient or incomplete data (Heppenstall et al. 2011), dealing with uncertainty (Galán et al. 2009; Sun & Müller 2013), modelling human irrational behaviour (Sankaranarayanan et al. 2017) and tuning parameters (Zhang et al. 2016). Another, more conceptual, challenge with ABMS is that these models are rule-based (Kocabas & Dragicevic 2013) meaning that the modeller programs predefined rules that the agents behave upon. However, if agents are to learn from their past experiences, they may need to adapt those hard-coded rules (Lorscheid 2014) and parameters (Remondino & Correndo 2006) during simulation runs.

1.2 In order to address many of these challenges, it is beneficial to increase the degree of intelligence and learning in ABMS, which has also been encouraged and highlighted in the literature (An 2012; Kavak et al. 2018; Macal & North 2010; Rand & Rust 2011). Machine Learning (ML) techniques can provide great potential to bring higher degrees of intelligence and learning into the models. ML is a subfield of Artificial Intelligence that aims to enable computers to learn based on input data without explicitly programming all requirements (Samuel 1959). ML allows for developing more precise and reality-based models and provides better means for handling data (Bonabeau 2002).

1.3 In ABMS literature, ML techniques are already used to address various challenges. For example, to represent or enhance decision making, modellers use Bayesian Networks as a learning tool for highly uncertain conditions (Alexandridis & Pijanowski 2007; Lei et al. 2005; Sun & Müller 2013), Neural Networks for building realistic simulations and providing specific behavioural features for each agent (Laite et al. 2016) and Decision Trees to construct rules that agents will act based upon (Chu et al. 2009). The literature provides a wide range of case-specific approaches that either aim to bring learning in the model or to process output data.

1.4 Yet, the ABMS literature is still marginally using ML techniques; we identify two reasons. First, ML is a broad field with numerous techniques, making it difficult to choose the most appropriate ML technique to support a specific modelling challenge, e.g., improving behavioural representativeness and accuracy. Second, depending on what purpose the model is aiming to serve, e.g., prediction or explanation (Edmonds et al. 2019), the usefulness of ML techniques may vary. Determining the modelling purpose is crucial for determining "how one builds, checks, validates and interprets a model" (Edmonds et al. 2019, p.1). Hence, the ABMS purpose also influences the choice of the ML technique that is selected to overcome certain ABMS challenges. Therefore, a literature review that provides an overview of techniques useful to address various challenges in ABMS based on modelling purposes can greatly benefit this flourishing modelling community.

1.5 There are already a handful of literature reviews on using ML in ABMS. Zhang et al. (2021) review literature on ML for the agents' decision-making, distinguishing between micro-agent-level situational awareness learning, micro-agent-level behaviour intervention, macro-ABMS-level emulator, and sequential decision-making. Dahlke et al. (2020) provide a general literature review on using ML for the structural specifications and outputs of ABMS. Their findings constitute an insightful summary of the common advantages and disadvantages of using ML in ABMS. However, it remains unclear which ML techniques can support different ABMS purposes and respective challenges and how. A review of ML and data-driven methods in energy-market models is given by Prasanna et al. (2019). Pereda et al. (2017) provide a brief introduction to the use of ML in the analysis of ABMS outputs. Despite their insightful contributions, none of these reviews considers the specific challenges in ABMS nor the modelling purposes while analysing the use of ML in ABMS. This paper aims to bring ML more within reach of the ABMS community by proposing guidelines to use the most appropriate ML technique that addresses a specific modelling challenge given a modelling purpose. We provide a structured literature review on the application of ML in ABMS with a specific focus on model purpose according to Edmonds et al. (2019). The identified purposes will be linked with ABMS challenges that ML can address, e.g., increasing computational efficiency. Hence, our main research questions (RQs) are also formulated on exploring these two relationships: "*Which ABMS challenges are most relevant for which modelling purpose?*", and "*Which ML techniques can support which ABMS challenges?*". Answering these RQs has these added values: First, it gives a state-of-the-art overview of the use of ML in ABMS. Second, guidelines for purposefully supporting ABMS with ML can be derived. Lastly, research gaps in the use of ML in ABMS can be identified.

1.6 Given the broad range of ML techniques – from statistical regression to deep learning (Jordan & Mitchell 2015) – we narrow down the scope in several ways. First, we divide the overall ABMS process into two parts: structural specification, and output analysis. Techniques used for the analysis of simulation output are usually common data analysis and data mining approaches [1] (Libbrecht & Noble 2015). This step is quite independent of the main purpose of modelling or the actual simulation. Furthermore, there is a grey area in data science research about ML techniques (i.e., is regression a ML technique or statistics?) and leading to a very high number of articles, where the contribution of ML is not necessarily explicit for ABMS purposes but for data analysis in general. Since our goal is to show how ABMS can benefit from ML to address various modelling challenges, we will focus on ML techniques that are integrated into the model for structural specifications: into the decision making of agents, agent logic, or agent interaction rather (and not for the analysis of output data). Finally, to further narrow down the scope of our paper, we will not be looking into agent-oriented software systems that are mainly for control purposes and are installed in real-world applications, e.g., agents in smart grids or traffic systems, usually referred to as multi-agent systems (MAS) (Macal 2016). Because these systems have different objectives such as real-time response or security, the application of ML can be different - see Prasanna et al. (2019) for an overview. Hence, we only focus on agent-based simulation models.

1.7 This paper is organized as follows: Section 2 sets the scene by providing the theoretical foundations on purposeful modelling and a summary of the foundations of ML in ABMS. Section 3 presents the research methodology. Section 4 presents the results. Section 5 includes the discussion as well as the guidelines. Finally, Section 6 summarizes the article, describes the limitations, and proposes future research possibilities.

Theoretical Background

2.1 This section provides the theoretical background both for understanding the modelling purposes and for the application of ML in ABMS.

Modeling purposes

2.2 ABMSs can be developed for multiple purposes. Edmonds et al. (2019) distinguish seven modelling purposes [2], summarized shortly in the following:

- **Prediction**: Prediction is defined as the ability to anticipate ***specified aspects*** of ***currently unknown*** data with a ***valid level of precision*** in a ***reliable*** manner through a computational model. Often, the capacity of a model to make predictions is considered the most robust indicator of a model's "truth". For example, Lee et al. (2018b) use an ABMS to predict the bitcoin price trend by simulating the rational agents' behaviour in the market.

- **Explanation**: Explanation is defined as the creation of a ***possible causal chain*** from an event to its ***consequences*** based on the structure of a simulation model. Particularly with complex social phenomena, there is a special interest in understanding why something happens. This understanding is essential for managing complex systems. As an example, Xanthopoulou et al. (2022) use an ABMS to explain the casual architectures of bullying.

- **Description**: Simulation models can be used to ***partially*** represent the ***important aspects*** of a particular system. This however does not mean that description aims at entirely replicating the system – but rather focusses on documenting what is important. For example, Pagani (2022) applies an ABMS to describe the importance factors in the process of relocations of tenants.

- **Theoretical exposition**: Theoretical exposition means a systematic mapping and establishment of consequences of mechanisms. It includes formulating and ***subsequently*** evaluating or testing ***hypotheses*** on the ***general behaviour*** of a mechanism. For example, Dehkordi et al. (2021) use an ABMS to support theory development and test hypotheses about the underlying reasons why some specific historical patters emerged in hundreds of years.

- **Illustration**: Illustration focusses on ***clearly*** communicating an idea in often a ***simplified*** and ***exemplary*** manner. It is important that illustrations do not impose assertions but rather focus on highlighting complexities in systems. For example, Delay & Piou (2019) illustrate the impact of resource scarcity on group cooperation by using an ABMS.

- **Analogy**: We speak of an analogy when ***processes*** in a simulation are used as a ***tool*** to ***informally think about something***. It often includes using ideas or concepts from other domains and hence can be useful in reflecting about something with a different perspective. The computational game proposed by Axelrod (1984) is one example of Analogy type of ABMS, which shows a new way of thinking about the process of cooperation.

- **Social learning**: Social learning "encapsulates a ***shared understanding*** (or set of understandings) of a ***group of people***" (p.16). For social learning, the participatory factor is of overriding importance. The model helps people, often from different domains and with different world views, capture a unified understanding. For example, Dumrongrojwatthana et al. (2011) use an ABMS to manage the conflicts between herders and foresters on land-use in northern Thailand. This social learning model helps them to come up with a mutual understanding on the land-use dynamics.

2.3 According to Edmonds et al. (2019, p.1) the modelling purpose determines "how one builds, checks, validates and interprets a model". Hence, if an existing model is used for a different purpose, the modelling processes needs to be reiterated for the new purpose (Edmonds et al. 2019). This means that the modelling purpose also influences the choice of the ML technique, which is selected to overcome the modelling challenges.

ML in ABMS

2.4 This sub-section summarizes the various ML categories and techniques and provides an overview of the reasons for applying ML in ABMS.

Categorization of ML techniques

2.5 ML techniques refer to algorithms that can find patterns and predict outcomes by learning from input data and without programming all requirements explicitly (Murphy 2012; Samuel 1959). Many different techniques and algorithms are labelled as ML. Yet, all ML algorithms have three common components (Domingos 2012): *representation*, *optimization*, and *evaluation*. The *representation* of the ML algorithm must be in a formal way that can be interpreted by a computer. The *optimization* aims to find the minimum or maximum of a goal function under given constraints. In fact, each ML technique can be assumed as an optimization problem in the sense that it learns to optimize solutions for a specific goal function. Finally, the *evaluation* component determines whether an ML algorithm performs according to expectations. In general, ML techniques can be divided into three main learning categories (Alpaydin 2009):

- **Supervised learning (SL)**: In SL, the output variables are known (labelled) and the algorithm learns to map inputs to outputs (Cunningham et al. 2008). This mapping can then be applied to unknown input data to predict the desired output (Cunningham et al. 2008). For example, spam detection is a SL problem that a set of labelled examples (spam or regular emails) is provided for the model. The algorithms learns to find the pattern to distinguish between these two categories and predict if a new email is spam or not. SL includes classification and regression problems – see Alpaydin (2009).

- **Unsupervised learning (UL)**: In contrast, there are no output variables to learn from in UL algorithms (Mohri et al. 2012). Instead, the algorithm learns to identify the distribution, or the structure of input variables. For example, customer segmentation is a UL problem, which finds the clusters of customers based on common characteristics. UL algorithms include clustering, and association problems - see Dutta et al. (2018) and Hastie et al. (2009).

- **Reinforcement learning (RL)**: In comparison to the other categories, RL agents [3] receive information by interacting with the dynamic environment and learn through trial-and-error by receiving rewards for good behaviour (Mohri et al. 2012). The goal of the RL agent is to maximize its rewards (Kaelbling et al. 1996). RL is similar to training a dog - the dog learns what to do or not to do through rewards.

2.6 In Table 1, the main characteristics of the three categories of ML techniques are highlighted.

Table 1: Overview of ML categories.

ML category	Data	Objective	Learning
Supervised	Labelled	Prediction	By mapping inputs to desired outputs
Unsupervised	Unlabelled	Identification of structures or patterns	By identifying the distribution or the structure of input
Reinforcement	Interaction with environment	Optimization	By rewarding good behaviour

ML techniques in ABMS

2.7 In the following, we provide a brief explanation for the four most common [4] ML techniques in ABMS:

- **Bayesian Network (BN)**: A BN is a probabilistic dependency graph including a set of interconnected nodes, where each node represents a variable, and the connecting links represent the causal relationships between these variables (Niedermayer 2008). Each variable has its probability in the dependency graph. BNs aim to model conditional dependencies and causations in the form of directed graphs. Hence, BNs are useful for predicting the occurrence of an event considering all possible causes. BNs can be trained both in a supervised manner via expert knowledge, or in an unsupervised manner based on large datasets (Flores et al. 2011; Horný 2014). Overall, BN is a good white-box method to deal with small and incomplete datasets, uncertainty, and different sources of knowledge (Jensen 1996; Uusitalo 2007). However, converting the expert knowledge into probability distributions can be difficult (Uusitalo 2007).

- **Neural Network (NN)**: NNs are artificial networks, which attempt to simulate the biological nerve cell network. They include many interconnected processing elements working in parallel to solve a certain problem, which can be both supervised and unsupervised. Moreover, as NNs are nonparametric algorithms (Fogel et al. 1990), which do not need a bounded set of parameters (Russell & Norvig 2016), they can be used for a large diversity of problems. Although NNs are strong in adaptation, learning, and approximation, the convergence speed is low. Also, since it is a black box, the interpretation can be a challenge (Shapiro 2002). Additionally, data gathering, and parameterization can be difficult.
- **Decision Tree (DT)**: DTs are predictive algorithms in the form of trees, which have branches that represent observations and leaves that outline conclusions. There are two ways of applying DT: classification and regression (Olkin 2002). For the classification DT (discrete values), leaves are class labels and branches are the links between class labels. In contrary, in a regression DT (continuous values) the leaves can have ranges for the regression. DTs are mostly used in a supervised approach. The advantage of using DTs is the clear knowledge representation, easing interpretation even by non-experts (Jadhav & Channe 2016). Moreover, DTs can map non-linear relationships quite well and can handle missing values (Wu et al. 2008). The disadvantages of these algorithms are the long training time (Jadhav & Channe 2016), overfitting, and no support of real-time learning, meaning that the tree needs to be rebuilt for new data (Brijain et al. 2014).
- **Reinforcement Learning (RL)**: RL builds on reinforcement agents that learn by interacting with the environment and receiving rewards for correct answers. This implies that the correct answer or labelled data is not required for the training phase (Mohri et al. 2012). The reinforcement agents determine their own performance according to the received reward as a feedback from the environment (Sutton & Barto 2018). One of the most popular RL algorithms is Q-learning. Q-learning enables reinforcement agents to act optimally in Markovian domains by experiencing the consequences of actions, without requiring them to build maps of the domains. At each specific state, the reinforcement agent tries an action and evaluates its consequences in terms of the immediate reward or penalty it receives from the environment and estimates the value of the state that is taken. By trying all actions in all states repeatedly, the reinforcement agent learns the best overall solutions (Watkins & Dayan 1992). As RL is basically a search algorithm, the time for finding a good solution increases in relation to the size of the data (Marsland 2011).

Addressing challenges in ABMS using ML

2.8 To explain how modellers can benefit from these ML techniques, we divide the overall ABMS process into two main parts: (1) structural specifications, and (2) model output analysis. The structural specifications can be further represented as a cycle: agents observing the world, agents updating their internal model, and agents taking action (Rand 2006). For each of the two main parts we identify key ABMS challenges from literature, which can be addressed with the help of ML as depicted in Figure 1.

- **Structural specifications**:
  - In ABMS, we are dealing with non-linear multi-parametric models where noise is an intrinsic part of input data. According to Heppenstall et al. (2011), ML techniques can be used to minimize the impact of these noises, which include missing or insufficient data. When data is sufficiently available for modelling purposes, ML techniques can be applied on raw data for pre-processing and calibration – see Zhang et al. (2016) and Lamperti et al. (2018). Alternatively, ML techniques can be applied to find meaningful patterns or trends based on real-world data (e.g., extracting a DT from real-world data). Finally, in cases where real-world data is not used in the model, ML techniques can be used to generate synthetic data (Ratner et al. 2016). All in all, ML can be helpful to ***improve the data pre-processing for the ABMS input***.
  - With regards to the internal specifications of the model such as defining agent behaviour, decision making, and interaction, we determine multiple ABMS challenges which can be addressed by ML:

Dealing with uncertainty (Galán et al. 2009; Sun & Müller 2013), modelling human irrational behaviour (Sankaranarayanan et al. 2017), as well as rule definition and adaption (Lorscheid 2014). Macal (2016, p.152) refers to this as the "behavioural modelling challenge" and hence, we summarize these challenges in one ABMS challenge: ***improving the accuracy of behavioural modelling***.

  - Another considerable hurdle during the model executing stems from the increasing scale of ABMS and the resulting computational challenges such as long simulation time (Macal 2016). ML can be helpful in **improving the computational efficiency** of ABMSs– for instance via surrogate models (van der Hoog 2019). A surrogate ML model can be seen as a computational approximation or emulator of an ABMS, which learns the relationship between ABMS in- and output to achieve reliable results in a more efficient and timely manner (van der Hoog 2019).
  - Moreover, ML ***can improve the ease of implementation*** of ABMSs, e.g., easier model-adjustment to new geographic locations (Drchal et al. 2019).
  - Lastly, Macal (2016) mentions a lack of transparency of ABMS, which can lead to low credibility of results. Some ML techniques can help overcome this hurdle by making the structural specifications more transparent – see Sun & Müller (2013). We call this ABMS challenge ***increasing model understanding***.

- **Model output**: With the increasing complexity of large-scale ABMS, it becomes more and more difficult to extract meaningful information from the simulation output (Macal 2016). ML techniques can be used to analyse the output of the simulation and to extract patterns. Additionally, these intelligent techniques can be applied for validating ABMSs (Parry et al. 2013) and checking the robustness of results (Filatova et al. 2013). Overall, ML can ***increase the understanding of model outputs***.

2.9 These reasons for using ML are not mutually exclusive, as two modelling challenges might reinforce each other, nor are they collectively exhaustive, as other ABMS challenges and hence ML reasons might exist.

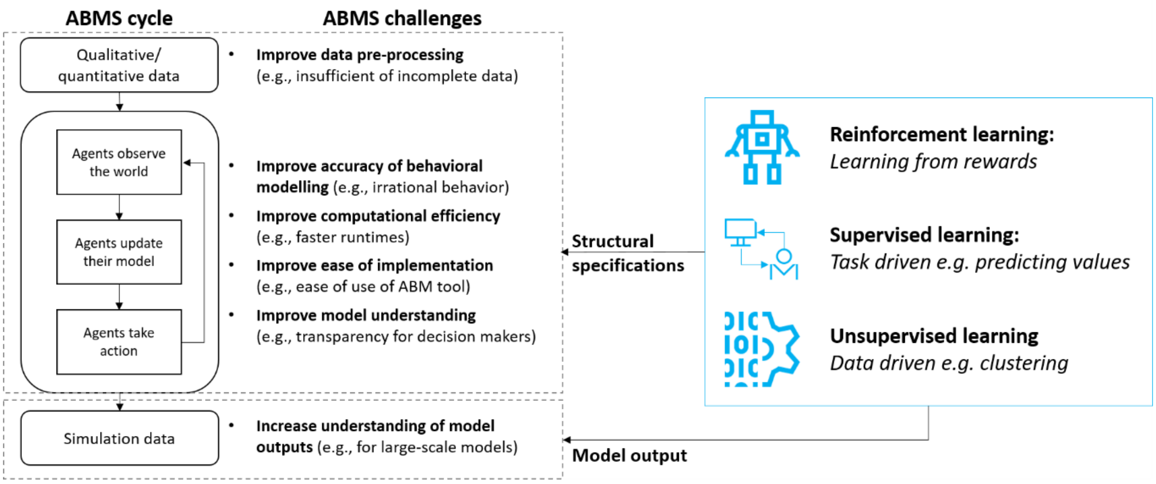

Figure 1: ML in the ABMS process – ABMS cycle adapted from Rand (2006).

2.10 As it appears in the literature, intelligent techniques are extensively used for the analysis of simulation outputs (Remondino & Correndo 2006). These techniques, however, are mostly for advanced data analysis and data mining, which are not necessarily specific to ABMS. Another issue related to output usage of ML techniques in ABMS is that it is a grey area between routine statistics, data mining and machine learning, making it difficult if not impossible to distinguish ML techniques from other techniques such as regression techniques. Given that our aim in this research is to bring ML more within reach of the ABMS community by adding more "intelligence" into simulations, we leave out the output phases of ABMS and only focus on how the actual model (i.e., agents and interactions) can benefit from these techniques.

2.11 To summarize, an ABMS is designed for a specific purpose such as social learning. These models can face a variety of challenges that ML can address e.g., improving the accuracy of behavioural models. Thus, there is a 1 to N relationship between the ABMS purpose and the ABMS challenge. To address these challenges, modellers can choose from different ML techniques such as NN. As the ML techniques can support multiple ABMS challenges, there is a N to M relationship between ABMS challenge and ML technique. The relationship between these three features is summarized in Figure 2.

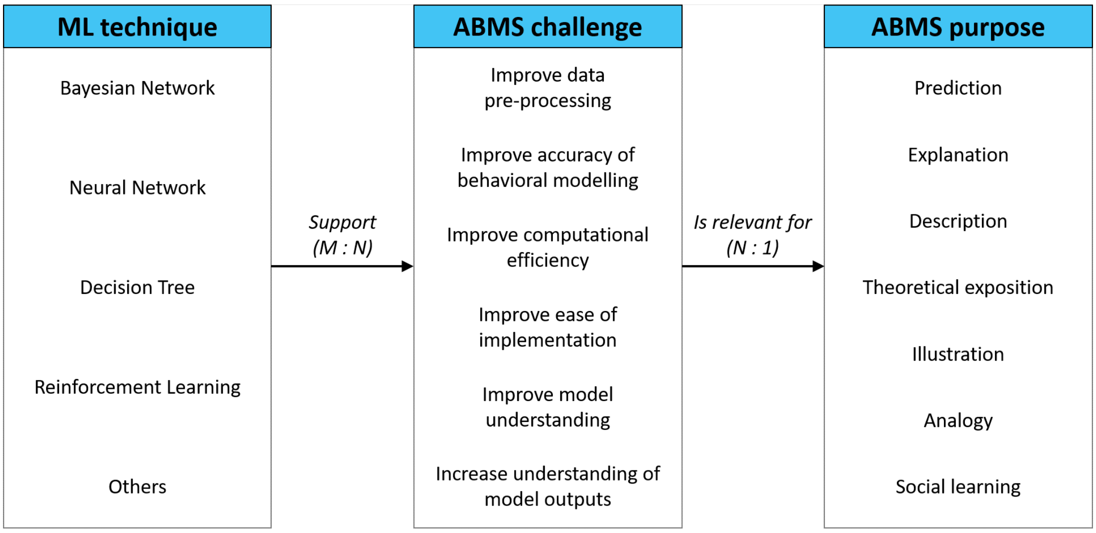

Figure 2: Relationship between ML technique, ABMS challenge, and ABMS purpose

Methodology

3.1 We conduct a structured literature review (SLR) according to the guidelines of Kable et al. (2012). The purpose of this SLR is to identify papers in which ML is applied for the structural specifications of agents. Hence, the research string – see Figure 3– combines three different categories of keywords: ABM, ML, and structural specification. Although there are papers which use the term of ABMS and MAS synonymously (Macal 2016), we exclude MAS from the research string as this would drastically increase the research results. To identify the application of ML in ABMS, we include the ML categories (see Section 'Theoretical Background') in the search string. Lastly, to identify the use of ML for the structural specifications of agents, we search for "decision making", "agent logic", and "agent specification". Additionally, common abbreviations such as "ABM" are included.

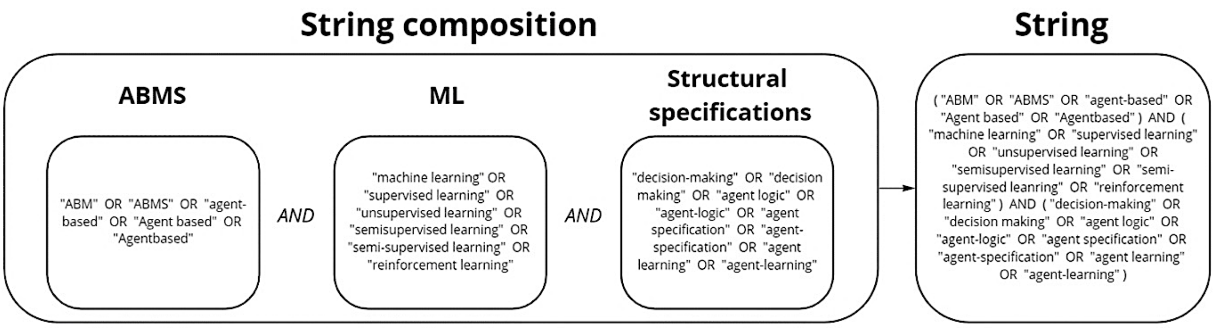

Figure 3: Search String Composition.

3.2 To conduct the search, we use the bibliography search engine Scopus. We search for records within the titles, keywords, and abstract to have a better chance of identifying suitable articles. Furthermore, only English papers are searched for. Moreover, reviews are excluded, as we want to identify specific ABMS applications to be able to identify the modelling purpose. The full search string is shown in the Appendix.

3.3 The review was conducted on the 8th of December 2021 and resulted in 238 hits. A multi-stage screening is applied to the results. First, we exclude 68 records, as they do not discuss ML in ABMS, e.g., books containing separate articles on ML and ABMS. Second, 101 records are removed, as they do not apply ABMS, but MAS instead. The excluded articles focus mostly on traffic, production, financial, and energy control systems focussing on system control and optimization. Third, we remove 16 articles, as they do not focus on specific ABMS applications, which are required to determine the ABMS purpose. Next, three articles are excluded as they focus specifically on analysing output of ABMS using ML without targeting the agent behaviour. Lastly, we remove seven articles, as they are not accessible or in a different language despite applying the English filter. This results in 43 suitable articles, which we directly identified via the SLR. Using snowballing, 28 additional eligible records were identified [5], leading to 71 articles in total.

3.4 These 71 articles are analysed with regards to the modelling purpose, the applied ML techniques, and the ABMS challenge. Despite the fact it is fundamental for determining the usefulness for an ABMS, (as argued for by Edmonds et al. 2019), the modelling purpose is often not explicitly mentioned in the papers. Hence, we classify the purposes based on the author's descriptions of the modelling process and results. When the authors refer to another paper for all the ABMS details, we assume no change in purpose and analyse the purpose based on the original paper. Similarly, we identify the ABMS challenge from the description of the modelling challenges.

3.5 Sometimes the description of the model is associated to more than one specific purpose and most often the purpose is not clearly stated in papers. To minimize bias, this analysis is conducted by a group of interdisciplinary researchers. Two researchers classify the purpose of the model used in each paper, the ML technique, and the ABMS challenge independently. In case of misalignment, the cases are discussed and resolved, sometimes with the help of a third researcher. This 4-eye review in combination with the interdisciplinary backgrounds reduces the potential effect of observer dependency on the classification results.

Results

4.1 The identified articles are summarized in Table 3 in the Appendix together with the classification of the respective ML techniques, the ABMS challenges and the modelling purposes. The articles are distributed between the years 1999 - 2021, whereas more than half were published in the last five years as shown in Figure 4.

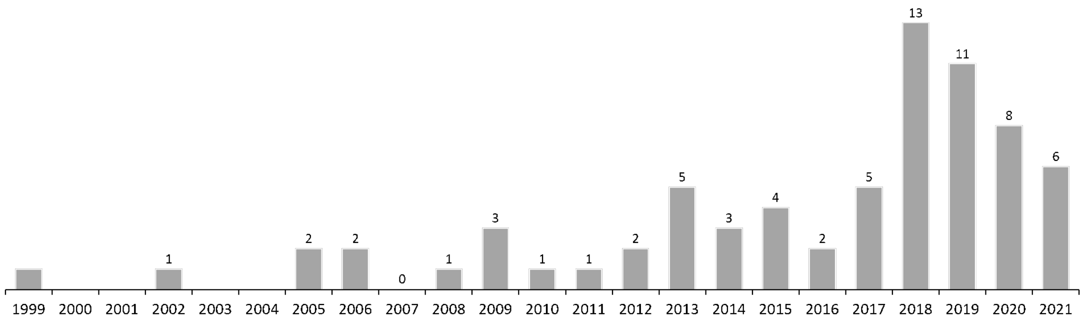

Figure 4: Distribution of included articles over the years.

4.2 First, we analyse the distribution of modelling purposes, ABMS challenges, and ML techniques as depicted in Figure 5. The following observations can be made:

- **ABMS purpose**: In total, there are 73 ABMSs, as two papers include multiple models for which ML is applied. Two third of the ABMSs have prediction, explanation, and description as a purpose. By contrast, illustration, social learning, and analogy are less common, with only five applications each.

- **ABMS challenge**: Improving the accuracy of behavioural modelling is by far the most common ABMS challenge with 65 applications. Moreover, improving data pre-processing is a relatively relevant challenge with 17 applications, followed by computational efficiency with 11 applications. Improving model understanding (6), ease of implementation (5), and understanding of model output (4) are least common. Again, it is important to highlight that we only look at applications of ML for the structural specifications of agents.

- **ML techniques**: Four ML techniques stand out: RL with 38 applications, followed at a greater distance by NNs with 12, DTs with 10 and BNs with 9 applications. The remaining ML techniques are genetic programming, support vector machines, self-organizing maps, and k-nearest neighbour and other algorithms, which in total are applied 10 times.

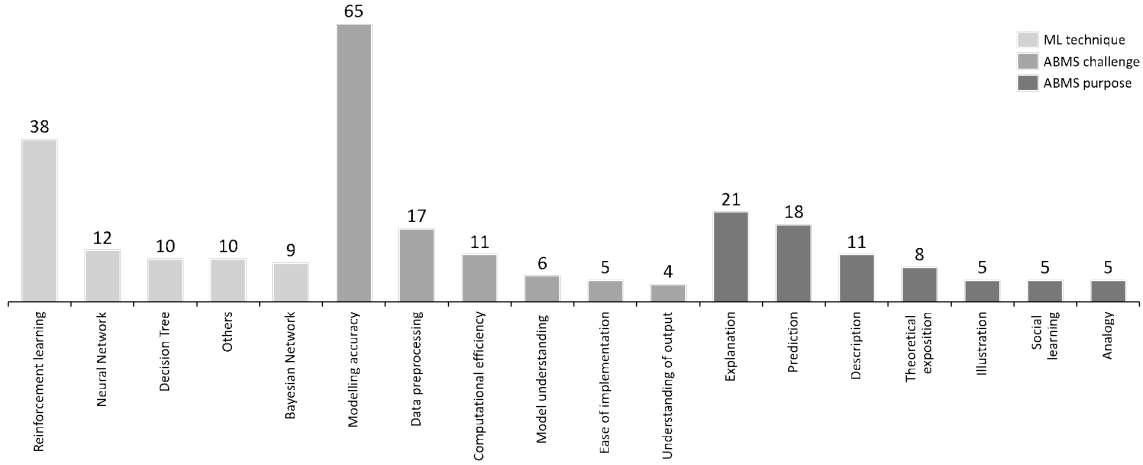

Figure 5: Number of applications of ML techniques, AMBS challenges, and modelling purposes.

4.3 The results are further analysed regarding the relationship between ABMS purpose, ABMS challenge, and ML technique as shown in Figure 6 (and in Figure 7 inthe Appendix). To answer the first RQ, it is important to understand which ML techniques are applied for which ABMS challenge. Our results show that increasing the accuracy of behavioural modelling plays a significant role for all modelling purposes (50% to 80%). However, we cannot identify scientifically significant differences between the modelling purposes. This is partially driven by the fact that the number of observations for certain purposes are too low to derive conclusions e.g., for illustration.

4.4 To answer the second RQ, which considers the use of ML techniques for supporting ABMS challenge, the following two observations can be made. First, improving the accuracy of behaviour modelling has a relatively high proportion for all ML techniques (> 45%), especially RL (84%). RL is applied in 37 cases to improve the modelling accuracy of agent behaviour. Second, DTs and BNs with 6 applications each appear common ML techniques to improve the accuracy of data pre-processing for agent-behaviour. These two observations will be detailed in the following using examples from the SLR.

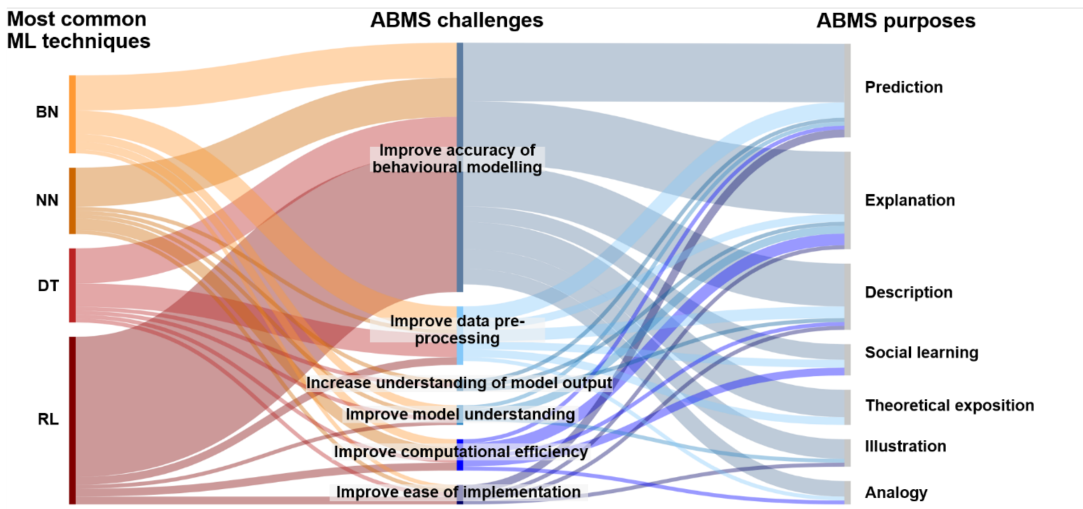

Figure 6: Relationship between applications of ML techniques, ABMS challenge, and ABMS purpose.

Application of RL to improve the accuracy of behavioural modelling

4.5 Our results show that to improve the accuracy of behavioural modelling in ABMS, RL is applied in more than 50% of ABMSs [6]. Therefore, we can assume RL as a relevant technique for improving the accuracy of behavioural modelling. It is applied in a large variety of domains. For instance, Li et al. (2019) apply an extended RL model which takes into account both personal but also other agent's learning for the agent's decision-making in a residential land growth ABMS in Nanjing, China. According to Li et al. (2019, p.10) the extended RL model "contributed to the improvement of the model's simulation power and modelling agent's adaptive decision-making process to a certain extent." Gaines & Pakath (2013) compare two RL systems – a classical and an extended learning classifier – for the decision-making in the Iterated Prisoner's Dilemma. Bone & Dragićević (2010) use RL in an ABMS for multi-stakeholder forest management. Here, RL helps incorporating optimization procedures in ABMS, which enables forest companies to interact with the environment and with each other while learning how to maximize their profits.

4.6 In particular, Q-learning appears to be a popular RL technique in our domain. For example, Chen et al. (2020) use deep recurrent Q-learning to research complex economic systems. Instead of relying on ad-hoc rules for decision-making, this ML technique allows agent interactions with the environment for improving their strategies over time. Using such adaptive decision-making strategies enables the representation of internal feedback and emergence.

4.7 To understand the "popularity" of RL for improving behavioural modelling accuracy, we analyse the author's arguments for applying this ML technique. We identify four main reasons. First, RL appears a suitable technique for the optimization of decision rules that govern the agent behaviour (Froelich et al. 2006; Junges & Klügl 2012). Second, RL can help in modelling adaptive agent behaviour (Gazzola et al. 2016; Li et al. 2019; Ramchandani et al. 2017). Third, RL can be used to model human decision-making more realistically (Al-Khayarin & Halabi 2021; Hassanpour et al. 2021; Li et al. 2020; Pang et al. 2018). For instance, Al-Khayarin & Halabi (2021) apply RL to emulate the behaviour of people in the real-world in the context social distance measures. Lastly, by using RL, agents are able to learn from interacting with each other (Bone & Dragićević 2010; Li et al. 2019) and with the environment (Jamshidnezhad 2015).

Application of DTs and BNs to improve data pre-processing for the agent behaviour

4.8 DTs and BNs appear favoured techniques of the ABMS community to support data pre-processing for agent-behaviour. Hence, it is of interest to see how and why these ML techniques are applied.

Decision trees

4.9 Our results show a large span of DT applications for data pre-processing. For instance, Gaube et al. (2009) apply DTs from survey data and statistics for agent decision-making in the domain of land use change. Sengupta et al. (2018) apply DT to extract rules that govern the movement of monkey groups in Uganda based on GPS movement data. Sánchez-Maroño et al. (2017) derive behavioural rules for an ABMS, which models the low-carbon transition in Europe using a DT learned from questionnaire data. In the ABMS of Rosés et al. (2021, p. 6), agents "decide whether to commit a crime or not by means of a decision tree" based on a large variety of quantitative data (e.g., crime, street, taxi, weather, or land-use data).

4.10 We identify three main reasons from the authors' arguments for applying the DT for data pre-processing: First, DT appears a useful tool for extracting rules from data which then can be implemented in the simulation model for the decision-making (Rosés et al. 2021; Sengupta et al. 2018). Next, DTs can be applied on questionnaires or survey results hence providing an empirical foundation for the agent behaviour (Gaube et al. 2009; Sánchez-Maroño et al. 2017). Lastly, Sánchez-Maroño et al. (2017) highlight the DT's transparent structure and results which can be interpreted and critiqued by non-technical experts.

Bayesian networks

4.11 Our results also highlight a variety of BN applications for the data pre-processing for agent-behaviour. For instance, Abdulkareem et al. (2018) use BNs for a cholera spreading model in Ghana to extract and model the behavioural patterns in an uncertain context. They show that intelligent agents using BN perceive risk in a more realistic way. Pooyandeh & Marceau (2014) use BNs amongst others to deal with incomplete information in their ABMS for simulating the negotiation procedure between agents in land development in Canada. The results show that the agreement can be achieved in fewer simulation runs because of the more human-like and intelligent algorithm. Sun & Müller (2013) use BN in agents' payment decision-making process for ecosystem services in land-use changes. The BN structure is derived from qualitative empirical data, expert knowledge, and quantitative survey data. This structure is then embedded in the agents to enable them to make land-use decisions under uncertainty. Kocabas & Dragicevic (2013) apply BN to derive behavioural rules from census data for simulating the negotiations for the evaluation of land development scenarios. This enables agents to learn based on their historical actions instead of using pre-defined rules.

4.12 To understand why the BN is common for improving data pre-processing to model agent behaviour, we analyse the authors' arguments for applying this technique and identify four main reasons: First, Abdulkareem et al. (2019), Kocabas & Dragicevic (2013), Sun & Müller (2013), Tian et al. (2020) highlight the ability of BN to deal with both qualitative data such as expert knowledge and quantitative data e.g., from surveys, which facilitates better decision-making (Heckerman & Wellman 1995; Uusitalo 2007). Second, Kocabas & Dragicevic (2013) and Pooyandeh & Marceau (2014) emphasise BNs ability to handle incomplete or small data sets. Third, BNs are cable of dealing with uncertainty in decision-making (Abdulkareem et al. 2018; Sun & Müller 2013). Lastly, BNs are capable to model causal relations (Sun & Müller 2013), which better captures the decision-making of the agents (Ma et al. 2007).

Discussion and Guidelines

5.1 In this section, we discuss the results and derive guidelines for the application of ML in ABMS. While the first subsection "*Discussion of results*" focuses on how ML is currently used in ABMS, the second subsection "*Guidelines for purposefully supporting ABMS with ML*" is forward-looking and shows how ML can be used in ABMS.

Discussion of results

5.2 In the following based on Figure 6 and Figure 7 in the Appendix, we discuss the identified patterns of the ABMS purposes, ABMS challenge, and ML techniques.

ABMS purposes

5.3 For each purpose, based on the associated ABMS with, we investigate if the purpose is (un)common between the other purposes or not. We can distinguish two reasons why certain modelling purposes are common or uncommon [7] for ABMS applications that use ML: (a) the modelling purpose is in general (un)common for ABMS, and (b) ML is an (un)favourable tool for the ABMS community to support this purpose. Using this logic, we analyse the results to determine why certain purposes might be particularly (un)common.

- **Explanation**: We conclude that explanation is used in more than a quarter of the papers that use ML in ABMS and hence is a relatively common purpose in this cluster. At the same time, Macal (2016, p. 146) argues that ABMS provides a "framework for explicitly specifying causal mechanisms." Hence, explanation in general appears a common purpose in ABMS, which can explain the high number in our ABMS/ML cluster.

- **Prediction**: We identify prediction as another common purpose in articles that use ML in their models. However, according to Edmonds et al. (2019, p. 5): "Prediction (as we define it) is very hard for any complex social system. For this reason, it is rarely attempted". Hence, based onEdmonds et al. (2019, p. 5), we conclude that it is not a common purpose for ABMS in general. ML is seen by the ABMS community as a suitable tool to increase the reliable anticipation of data, which is one of the key pillars of a prediction model (Edmonds et al. 2019). This is supported by our results showing that *increasing modelling accuracy* is the most relevant ABMS challenge that can be addressed by ML. It means that although prediction is a common purpose based on our analysis, the more than half of the cases (16 out of 27) there are related to *improving the accuracy of behavioural modelling*.

- **Description**: Description is the third most common purpose in articles that use ML in ABMS research. On the one hand, this can be explained by the fact that ABMS provides a good basis for descriptive purposes as actors can be directly described via agents and as it allows the representation of dynamics and interactions in a system (Edmonds et al. 2019). On the other hand, Edmonds et al. (2019, p. 8) highlight that the "simulation has to relate in an explicit and well-documented way to a set of evidence, experiences and data." Our results support this argument by showing that DT or BN are suitable tools to build descriptive models based on a variety of data sources.

- **Illustration**: We only identified a few cases of ABMS with illustrative purposes. We think that ML might not be the right tool to support illustrative purposes. For illustrations, the model clarity is of overriding importance (Edmonds et al. 2019). Rudin (2019, p. 206) points out problems with so-called "black box" ML models, which are mainly models that are "too complicated for any human to comprehend". Hence, adding such an untransparent algorithm can negatively impact the model clarity. This might explain why illustrations are so rarely observed.
- **Social learning**: We only observe five ABMSs with a social learning purpose in our cluster. It appears that ML is not seen as a highly suitable tool to support social learning ABMS. On the one hand, the development of social learning models (for environmental management) can be very time-consuming (Barreteau et al. 2003). Adding ML to the model development process might thus exceed the available timeframes. On the other hand, the lack in transparency of some black box models might counteract a shared understanding.
- **Analogy**: Analogies are also rarely observed. On the one hand, we think that analogies are not common for ABMS in general, as not every idea might be applicable in a bottom-up manner. The ABMS community might view ML as too complicated and resource-intensive to support an informal way of thinking about an idea.

ABMS challenges

5.4 Here we reflect on the main challenges for the structural specifications of agents, which the ABMS community perceives can be overcome with the help of ML. We will discuss in the following why certain ABMS challenge are more common than others.

- **Accuracy of behavioural modelling**: According to van Dam et al. (2012, p. 60) the "overall system (or model) behaviour is an emergent property of the interactions between all of the agents behaviours and the environment." As the agent behaviour drives the system behaviour, we argue that increasing the accuracy of the agent behaviour directly influences the accuracy of the system behaviour. We, therefore, conclude that increasing the accuracy of behavioural modelling plays a crucial role in ABMS. This can explain why this ABMS challenge is mentioned so frequently.
- **Data pre-processing**: As argued before, we specifically look at ML techniques, which process real-world data to model agent-behaviour. Sometimes, the ML technique is applied to find some meaningful patterns or trend based on real-world data, which help to build agents' behaviour. Hence, using ML for data pre-processing might indirectly help improving the accuracy of the agents' behavioural modelling. Moreover, An et al. (2021, p. 9) mention data limitation as "one of the most fundamental reasons" why the progress of Artificial Intelligence in ABMS is slower than expected. This can explain why improving data pre-processing is the second most common ABMS challenge.
- **Computational efficiency**: Only a fraction of authors (11) use ML to improve the computational efficiency. Often, increasing computational efficiency appears a secondary challenge next to improving the accuracy of behavioural modelling. In the remaining cases, ML is often used to create surrogate or meta-models which learn the relationship between ABMS in- and output to achieve reliable results in a more efficient manner, see Vahdati et al. (2019), ten Broeke et al. (2021), or Yousefi et al. (2018). As outlined by van der Hoog (2019, p. 1260) surrogate ML models have the potential to drastically reduce "the complexity and computational load of simulating agent-based models".
- **Model understanding**: Similar to computational efficiency, improving the model understanding is often regarded as a secondary ABMS challenge. Moreover, the use of black box ML techniques might hinder model understanding. Technological advances have led a majority of scientists to the belief that "the most accurate models for any given data science problem must be inherently uninterpretable and complicated." (Rudin & Radin 2019, p. 2). Hence, ML might not be seen by the ABMS community as a tool to improve model understanding, as this may otherwise negatively impact their main ABMS challenge, the ML accuracy. This can explain why model understanding is an uncommon ABMS challenge. To compensate for this lack in transparency, often a "second (post hoc) model is created to explain the first black box model" (Rudin 2019, p. 206). For instance, Cummings & Crooks (2020) use explainable AI for RL in their ABMS. These explanation models are usually not reliable and can easily be manipulated (Lakkaraju & Bastani 2020; Lipton 2018; Rudin 2019). According to Rudin (2019), the trade-off between accuracy and transparency is a myth, as oftentimes there is no significant performance difference between complex black box models and transparent counterparts. Therefore, the conclusion would be to use transparent ML techniques instead (Rudin 2019).

- **Ease of implementation**: Improving the ease of implementation is always combined with other ABMS challenges such as improving the accuracy of behavioural modelling. Hence, we conclude that it is also a secondary challenge. Moreover, if the ABMS community thinks that high performing ML techniques are inherently complicated (Rudin & Radin 2019), it appears counterintuitive to add such a complicated model to improve the ease of implementation. This can explain why this ABMS challenge is scare in our results.
- **Understanding of model output**: ML is only applied for understanding the model output for the creation of surrogate models. The main challenge of surrogate models is however the computational efficiency. This explains their rare appearance in our results.

ML techniques

5.5 Our results show that four techniques particularly stand out in the ABMS literature: RL, NN, DT, and BN. RL is by far the most common technique. Looking at the main reasons why authors apply RL such as the optimization of decision rules, adaptive behaviour, or the ability of reinforcement agents to learn from the environment and from each other (see Section 'Results'), we see lots of similarities to the nature of ABMSs. Similar to ABMS, RL is also built upon agents that interact with the environment and adapt their behaviour based on the interactions. This not only means that the two techniques fit together conceptually, but also that RL can reinforce core concepts of ABMS, such as agent adaptiveness (van Dam et al. 2012). This might further explain the popularity of RL for improving behavioural modelling.

5.6 A currently underrepresented ML technique in our results is Genetic Algorithm (GA). GA is an evolutionary algorithm (Bäck 1996), which is used for optimization and searching problems (Mitchell 1998). The algorithm is inspired by the process of natural selection (Kumar et al. 2010) by making slow changes until the best solution is reached. In this process, the fittest portion of a population is selected for reproducing the next generation in each round based on a fitness or goal function. Mutations in subsequent generations allow the algorithm to search the whole domain area to prevent solutions being trapped in local minimums. This biologically inspired learning can be useful for agent specifications. The behaviour or agents' specification in certain condition can be coded into bit strings as chromosomes of GA (Weidlich & Veit 2008). The most successful ones are consequently transferred to the next generation. Hence, the behaviours which are associated with more benefits that lead to maximize the agents' goal function will be preserved and passed to the next generation by a mutation process. Consequently, the set of agents' behaviour which leads to more fitness can be extracted. For instance, Lorscheid & Troitzsch (2009, p. 7) apply a GA which "extends the behavior rules with new rules by adding mutated copies of existing event-action trees." Therefore, we recommend researchers to take into consideration GAs as potential ML techniques for the application in ABMS.

Guidelines for purposefully supporting ABMS with ML

5.7 In previous part, we have focused on what articles suggest on using ML in ABMS. In this part, we recommend ML techniques that might be used for each specific purpose of the ABMS. When selecting a ML technique, it needs to be aligned with the purpose of the ABMS. This is also important when integrating ML into an existing model. We put the focus on highlighting selection criteria, which should have a high priority when choosing ML to support a certain purpose. The criteria are determined in a bottom-up manner based on the fundamental goals of each purpose. Table 2 shows the prioritized selection criteria for choosing ML technique, which are associated with each modelling purposes; in addition to the candidate ML technique.

- **Explanation**: Explanatory ABMS help in creating a causal chain from event to consequences. To support identifying these causal relations, we argue that the ML technique should be transparent. For instance, our results show that BNs appear suitable for explanations, as they provide a transparent way of modelling causal relations. DTs are also a transparent ML technique that can support this purpose.
- **Prediction**: If the modelling purpose is prediction, we recommend using ML techniques, which support reliable anticipation of data. Hence, we suggest techniques with a high accuracy. For instance, our results show that RL can achieve a high accuracy for behavioural modelling.
- **Description**: When a descriptive model is to be supported using ML, we suggest using ML techniques which are capable of establishing a "direct and immediate connection with observation, data or experience" (Edmonds et al. 2019, p. 8). This includes the ability of the ML technique to derive information from data. Our results show that DTs and BNs are suitable techniques to support data pre-processing.

- **Theoretical exposition**: According to Edmonds et al. (2019, p. 11) "a near complete understanding of the simulation behaviour is desired" for models focused on theoretical exposition. Therefore, for supporting this purpose, we recommend using transparent ML techniques so that modellers can track the step-by-step process and the output (e.g., DTs or BNs).
- **Illustration**: If the ABMS purpose is illustration, adding a black box ML technique such as NNs (Mas et al. 2004) might counteract with the model clarity. Hence, we suggest using transparent ML techniques instead e.g., DTs or BNs (Singh et al. 2016).
- **Social learning**: For social learning two points need to be considered. On the one hand, the modelling and executing time of the ML technique should not drastically worsen the already time-intensive participatory process. On the other hand, transparent techniques should be used to enable a shared understanding by non-technical experts. Therefore, DTs or BNs seem to be the most suitable techniques.
- **Analogy**: If analogies are to be supported with ML, the ML technique should be easy to implement to be able to experiment with the simulation model without substantial implementation efforts. Hence, ML techniques with good availability of tools and mature libraries such as BNs or NNs are recommended.

5.8 The prioritized selection criteria (Table 2) can give readers an idea of which characteristics play a relevant role for their desired modelling purpose so that they can best align the ABMS purpose with the ML technique. However, setting priorities on certain selection criteria doesn't mean that other factors should not be considered. Furthermore, we would like to emphasise that ML is by no means always the best solution to overcome modelling challenges in ABMS. When selecting ML for agent specification, the pros and cons should be thoroughly considered. In addition, we would like to underline that the performance of a technique regarding a criterion can be considered a snapshot in time and can change in the future. For instance, technological improvements of surrogate models could make NNs more transparent and thus make them more suitable for explanatory purposes.

Table 2: Guidelines for selecting ML techniques to support agent specifications.

Purpose	**Prioritized selection criteria for ML technique**					**Possible ML techniques**
	Accuracy	Transparency	Ability to process data	Time-intensity	Tool availability	
Explanation		✓				BNs and DTs
Prediction	✓					RL
Description			✓			DTs and BNs
Theoretical exposition		✓				DTs and BNs
Illustration		✓				DTs and BNs
Social learning		✓		✓		DTs and BNs
Analogy					✓	BNs or NNs

Conclusion

6.1 Research shows that by bringing more intelligence into models, ML can address various ABMS challenges and thus significantly improve modelling practices. This literature review used ABMS modelling purposes to analyse the applicability of ML techniques in this modelling domain as the purpose influences the entire modelling process and hence also the selection of the ML technique to overcome the ABMS challenges. As the sheer vastness of the ML domain makes it difficult to choose the right ML technique for an ABMS purposes, we explore the following research questions: "**Which ABMS challenge are relevant for which modelling purpose and which ML techniques are applied to support which ABMS challenge?**"

6.2 To answer these research questions, we focused our structured literature review on the use of ML for agent specifications. We analyse the existing body of literature regarding the purpose of the ABMS, the ABMS challenges, and the applied ML techniques. Our results show that explanation, description, and prediction are common modelling purposes in the literature that uses ML in comparison to illustration, social learning, and analogy purposes. Both the commonality of these purposes in ABMS in general, and the suitability of ML to support these purposes can explain this pattern. Improving the accuracy of behavioural modelling is the most relevant ABMS challenge for all modelling purposes followed by improving data pre-processing for agent behaviour. Increasing the computational efficiency, model understanding, ease of implementation, and understanding of model output are secondary ABMS challenges. We identified four main ML techniques in the ABMS literature that are used to address the mentioned improvements: RF, BN, DT, and NNs. RF appears a suitable technique to improve the accuracy of behavioural modelling, partially because it is conceptually similar to ABMS. Moreover, DTs and BNs show favourable characteristics for modelling agent behaviour using real-world data and are hence commonly applied to support this ABMS challenge.

6.3 To make ML more accessible to the ABMS community, we derive guidelines from these results. We highlight for each ABMS purpose which criteria should be prioritized when selecting an ML technique. This can help ABMS researchers better match the ML technique to the purpose of their ABMS. Moreover, we emphasize that ML techniques can be both accurate and transparent and underline the use of transparent ML techniques for the currently underrepresented ABMS purposes of social learning and illustration.

6.4 This work has several limitations. First, we focus on the core part of ABMS, the structural specifications of the agents, and do not include the papers on using ML in output of ABMS. Second, the search string only contains ABMS-related keywords. Hence, we neglect papers that apply ABMS but refer to it as MAS. Third, only one database, Scopus, is used to identify articles. Fourth, we classify ABMSs based on authors' descriptions because authors often do not specify the modelling purpose. Although we perform double-checking, this approach is still observer dependent, which might affect the classification results. Finally, given the diversity of ML techniques, we narrowed our focus on the techniques that have been already applied in the ABMS field to learn from best practices. However, the next step would be to expand our vision to see what other techniques can be useful for this field and how the can be used.

6.5 Based on these limitations, future iterations are recommended, for example by extending the research to other databases such as Web of Science and by including MAS and ML techniques in the search string. This would allow for better article identification and hence improve the statistical significance of the results. Moreover, we recommend author's to explicitly highlight the modelling purpose, as stated in the ODD protocol, as this would allow readers to better understand the model (Grimm et al. 2020). Lastly, despite us focusing only on structural specifications of the agent it would be interesting to see how ML is used for the output of ABMS. Hence, we recommend a literature review on the use of ML for the ABMS output as a next step.

Appenix

Full research string

TITLE-ABS-KEY (("ABM" OR "ABMS" OR "agent-based" OR "Agent based" OR "Agentbased") AND ("machine learning" OR "supervised learning" OR "unsupervised learning" OR "semisupervised learning" OR "semi-supervised learning" OR "reinforcement learning") AND ("decision-making" OR "decision making" OR "agent logic" OR "agent-logic" OR "agent specification" OR "agent-specification" OR "agent learning" OR "agent-learning")) AND (LIMIT-TO (PUBSTAGE , "final")) AND (EXCLUDE (DOCTYPE , "re")) AND (LIMIT-TO (LANGUAGE , "English"))

Literature review

Table 3: Literature review results

Author	ABMS Purpose	ML technique				ABMS Challenges						

		BN	NN	DT	RL	Other	Data pre-prepro.	Modelling accur.	Comp. efficiency	Ease of impl.	Model underst.	Output underst.
Abdulkareem et al. (2018)	Theoretical exposition	✓					✓	✓				
Abdulkareem et al. (2019)	Theoretical exposition	✓					✓	✓				
Abdulkareem et al. (2020)	Explanation	✓						✓				
Aguilar et al. (2019)	Analogy				✓			✓				
Al-Khayarin & Halabi (2021)	Prediction				✓			✓				
Baghcheband et al. (2019)	Illustration				✓			✓				
Batata et al. (2018)	Prediction		✓	✓		✓		✓				
Bennett & Tang (2006)	Explanation		✓			✓		✓				
Bone & Dragićević (2009)	Explanation				✓			✓				
Bone & Dragićević (2010)	Description				✓			✓				
Cenek & Franklin (2017)	Explanation			✓				✓				
Chen et al. (2020)	Theoretical exposition				✓			✓				
Cruz Cortés & Ghosh (2020)	Explanation				✓			✓				
Cummings & Crooks (2020)	Illustration				✓			✓			✓	
Drchal et al. (2019)	Prediction			✓			✓	✓		✓		
Fano & Slanzi (2019)	Illustration				✓			✓				
Froelich et al. (2006)	Description				✓			✓				
Gaines & Pakath (2013)	Analogy				✓			✓				
Gaube et al. (2009)	Social learning			✓			✓	✓				
Gazzola et al. (2016)	Description				✓			✓				
Hassanpour et al. (2021)	Prediction				✓			✓				
Heinrich & Gräbner (2015)	Explanation				✓			✓	✓			
Lee et al. (2018a)	Description				✓			✓				
Jäger (2019)	Analogy		✓				✓	✓				

Jamshidnezhad (2015)	Theoretical exposition				✓			✓				
Junges & Klügl (2012)	Illustration				✓			✓		✓		
Lee et al. (2018b)	Prediction				✓			✓				
Kocabas & Dragicevic (2013)	Prediction	✓					✓	✓		✓	✓	
Laskowski (2011)	Prediction					✓					✓	
Lei et al. (2005)	Description	✓						✓				
Li et al. (2019)	Explanation				✓			✓				
Li et al. (2020)	Prediction				✓			✓				
Ling et al. (2016)	Prediction				✓			✓				
Lorscheid & Troitzsch (2009)	Explanation				✓	✓		✓				
Mei et al. (2014)	Prediction					✓	✓	✓				
Moriyama et al. (2019)	Analogy				✓				✓			
Nawa et al. (2002)	Theoretical exposition				✓			✓				
Nawaz & Hadzikadic (2018)	Prediction			✓		✓	✓	✓				
Norman et al. (2018)	Social learning				✓			✓				
Osoba et al. (2020) [8]	Analogy				✓			✓				
Osoba et al. (2020)	Prediction				✓			✓				
Ozik et al. (2021)	Explanation					✓	✓					
Padilla et al. (2014)	Theoretical exposition		✓					✓				
Pageaud et al. (2017)	Prediction				✓			✓				
Pang et al. (2018)	Explanation				✓			✓				
Pooyandeh & Marceau (2014)	Social learning	✓					✓	✓	✓			
Pope & Gimblett (2015)	Explanation	✓						✓				
Vahdati et al. (2019)	Explanation			✓					✓			✓
Ramchandani et al. (2017)	Description				✓			✓				
Remondino (2008)	Social learning				✓			✓				
Resta (2015)	Theoretical exposition					✓		✓				

Rosés et al. (2021)	Prediction			✓			✓	✓				
Sánchez-Maroño et al. (2017)	Description			✓			✓	✓			✓	
Sankaranarayanan et al. (2017)	Explanation		✓					✓		✓	✓	
Schuster (2012)	Theoretical exposition				✓			✓				
Schwab & Maness (2013)	Description				✓		✓	✓		✓		
Sengupta et al. (2018)	Description			✓			✓	✓				
Shukla et al. (2013)	Prediction		✓	✓				✓				
Songhori & Garcia-Diaz (2018)	Illustration				✓			✓				
Sun & Müller (2013)	Explanation	✓					✓	✓			✓	
Takadama et al. (1999)	Explanation				✓			✓				
ten Broeke et al. (2021)	Explanation					✓			✓			✓
ten Broeke et al. (2021)	Explanation					✓			✓			✓
Tian et al. (2020)	Explanation	✓					✓	✓	✓			
Tkachuk et al. (2018)	Prediction		✓					✓				
Valluri & Croson (2005)	Explanation				✓		✓	✓	✓			
Wolf et al. (2015)	Explanation		✓					✓				
Zhang et al. (2018)	Social learning		✓						✓			
Yao et al. (2020)	Description		✓					✓	✓			
Yousefi et al. (2018)	Prediction		✓						✓			✓
Zangooei & Habibi (2017)	Prediction				✓			✓				
Zhao et al. (2019)	Description		✓					✓				
Zubiria Perez et al. (2021)	Explanation				✓			✓				

Analysis of results

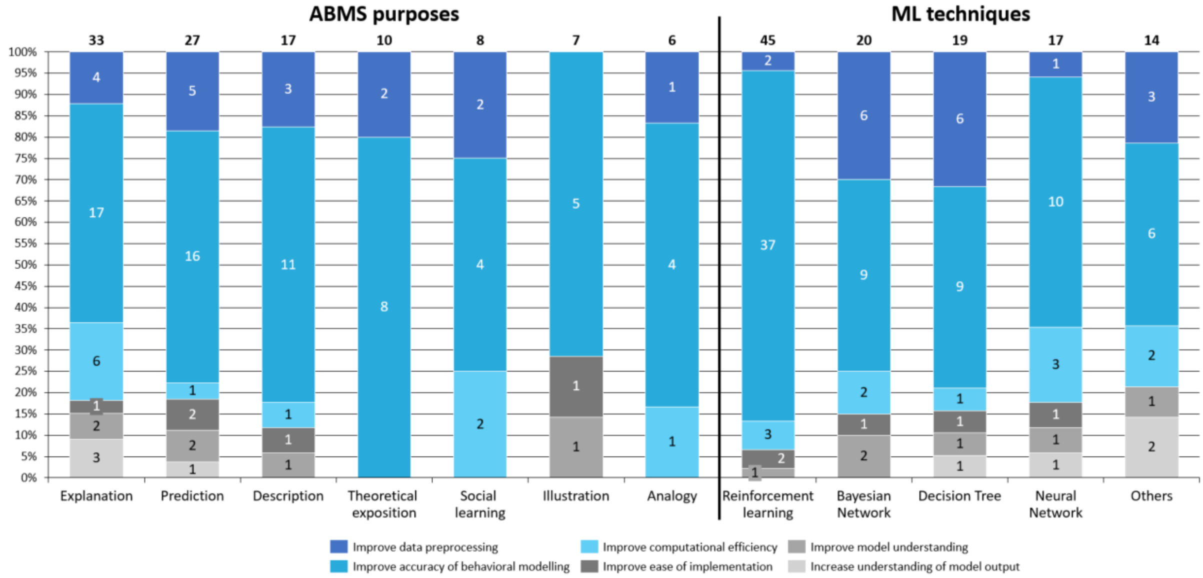

Figure 7: Proportional and absolute distribution of applications of ABMS challenges over ABMS purposes and ML techniques

Notes

[1]It is worth mentioning here that the domain of ML is different from Data Mining (DM), which is the process of finding data patterns from large datasets by using intelligent methods (Han et al. 2011). The main difference here is learning: ML techniques learn based on data while DM techniques find hidden patterns without using learning ability. However, there are some common techniques that can be used with or without learning, meaning that some techniques e.g., clustering can be categorized in DM as well as in ML techniques depending on how users apply them.

[2]Although other modelling purposes can exist, these seven appear most relevant for social simulations (Hauke et al. 2017; Squazzoni et al. 2014)

[3]The term "agent" is both used in RL and ABMS. To avoid confusion, we always refer to agents in RL as RL agents.

[4]Each category of ML includes several techniques. And some techniques can be differently used in more than one category. These four techniques are the most common ML techniques used for the structural specifications of agents, identified from the 71 articles from the structured literature review conducted in the next chapter, see Figure 5.

[5]These articles, which have been found in this round were not necessarily based on the Scopus. For these articles we focused on finding the articles' titles anywhere rather than concentrate on one specific database.

[6]Based on Figure 7, RL is applied in 37 ABMSs to improve accuracy of behavioral modelling. While the summation of using other techniques to improve accuracy of behavioral modelling in total is 34.

[7]There are also 8 ABMS for Theoretical exposition. The reason why we did not mention this purpose was that we aimed to mention the purposes with the highest number of ABMS associated with and simultaneously the purposes with the lowest number of ABMS.

[8]Each row represent an ABMS. As both Osoba et al. (2020) and ten Broeke et al. (2021) describe multiple ABMS applications within their papers, there are multiple rows of the same authors in the table.

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