Using Process Mining for Face Validity Assessment in Agent-based Simulation Models: An Exploratory Case Study

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Abstract. In the field of simulation, the key objective of a system designer is to develop a model that performs a specific task and accurately represents real-world systems or processes. A valid simulation model allows for a better understanding of the system's behavior and improved decision-making in the real world. Face validity is a subjective measure that assesses the extent to which a simulation model and its outcomes appear reasonable to an expert based on a superficial examination of the simulator's realism. Process mining techniques, which are novel data-driven methods for obtaining real-life insights into processes based on event logs, show promise when combined with effective visualization techniques. These techniques can augment the face validity assessment of simulation models in reflecting real-life behavior and play a key role in supporting humans conducting such assessments. In this paper, we present an approach that utilizes process mining techniques to assess the face validity of agent-based simulation models. To illustrate our approach, we use the Schelling model of segregation. We demonstrate how graphical representation, immersive assessment, and sensitivity analysis can be used to assess face validity based on event logs produced by the simulation model. Our study shows that process mining in combination with visualization can strongly support humans in assessing face validity of agent-based simulation models.

Keywords: Face validity · Agent-based simulation · Agent-based modeling · Process mining · Schelling model.

1 Introduction

Simulation provides a powerful tool for researchers and practitioners to model and analyze complex systems and processes [24]. The primary objective for designers of simulation models is to develop models that accurately represent the real-world systems or processes of interest, while also being capable of performing specific tasks and gaining insights into the real-world process or system [33]. With the increasing availability of data, simulation models can now be developed

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with greater sophistication, allowing for a deeper understanding of the behavior of the system and improved decision-making in real-world scenarios [18, 23, 29].

When constructing simulation models, one of the initial techniques employed to enhance validity is performing a face validity assessment [20]. Face validity is a subjective measure that evaluates the degree to which a simulation model and its outcomes appear plausible to an expert, based on the realism of the simulator [10, 27]. This involves having individuals, often experts, assess the realism of the model and/or its behavior [28]. Face validity can help identify potential issues or limitations in the simulation model, and can be determined through a combination of expert judgment, comparison with empirical evidence, and critical evaluation of the model's design and assumptions. Despite its potential utility during the early stages of simulation model development, face validity has been subject to criticism from the scientific community [25]. For example, a review of face validity assessment [15] identified concerns regarding inconsistency and inadequate guidance during the expert evaluation phase.

Process mining has emerged as a promising tool for conducting data-driven validation checks of simulation models. This technique involves analyzing event logs to discover, monitor, and improve processes within a system [1]. By applying process mining techniques to simulation output and using appropriate data processing and visualization methods, practitioners can identify patterns and anomalies in a model's behavior. This allows for a comparison with the real system underlying the model, and for the identification of discrepancies or errors in assumptions or parameters [3]. For instance, streaming process mining can be employed for real-time analysis of event data [8], providing continuous feedback on simulation processes. As a result, the correctness of the model implementation can be verified and the simulation model's capability to perform its intended tasks can be ensured through validation, increasing its utility for decision-making in various fields. Despite its potential, research on evaluating the effectiveness of process mining techniques in conducting face validity assessments is limited.

In this article, we explore the application of process mining techniques to assess the face validity of agent-based simulation models. Process mining has demonstrated its utility in the domain of agent-based simulation modeling, including model verification and performance analysis [5, 9, 35]. These techniques can also be used to analyze various properties, including agent behavior [14, 37]. However, available studies do not cover agent-based simulations that are characterized by for example numerous interactions, heterogeneous populations, and complex topologies. Additionally, the evolving nature of agent behavior and their available knowledge are often overlooked [4, 6], raising concerns about model validity. Leveraging process mining techniques to support face validity assessments can enhance the validity of agent-based simulation models.

This paper aims to demonstrate and evaluate the application of process mining techniques for assessing face validity of agent-based simulation models. We apply process mining techniques to extract insights from the event logs generated by the simulation model. Subsequently, we perform a face validity assessment using the insights obtained from process mining. To illustrate our approach, we

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employ a well-researched agent-based simulation model, namely the Schelling model of segregation, and demonstrate how a face validity assessment can be conducted using process mining techniques. Through this assessment, we aim to determine if insights obtained through process mining tools can be used to assess whether an agent-based model appears reasonable in the context of face validity.

The remainder of the paper is structured as follows. Section 2 provides a literature review of existing methods that use process mining to analyze or evaluate agent-based simulation models. Section 3 outlines the research design used for the study. The experimental results are discussed in Section 4. Finally, Section 5 provides conclusions and recommendations for future research.

2 Literature review

Several studies have explored the use of process mining to extract knowledge from agent-based simulation models. In [9], the authors integrate process mining and multi-agent models using Petri-net semantics to monitor and debug multi-agent systems during the development phase. They analyze agent interactions within simulated organizations and present a plug-in for recording interaction logs. The article uses agent interaction protocol diagrams as a descriptive form that combines organizational and control-flow information, which can be mapped to executable Petri nets. This enables mining results to be used for validating and verifying actual behavior during the design phase [9]. In [12], the authors develop a hierarchical Markov model to capture high and low-level behavior in business processes using an event log and process description. They aim to understand agent behavior from both control-flow and organizational perspectives and compare the results with those from existing process mining techniques using an agent-based simulation platform. In [19], the authors enhance MAREA, a multi-agent simulator, to enable process mining analysis. They formalize its architecture and show how a multi-agent system can record event logs for later process mining analysis. The authors extract event logs from simulations, implement a model of a trading company, and perform process structure verification and social network analysis with process mining [19]. The work discussed in [4] proposes an agent-based simulation framework that can discover and analyze emergent behavior arising in cyber-physical systems. They show a form of agents' self-learning capabilities by incorporating knowledge obtained from process models into the agent decisions. In [6], the authors propose an approach to extract agents' underlying models from log data generated from their behaviors, utilizing process mining. The authors demonstrate this approach using the Schelling model of segregation, showing how agent models can be extracted utilizing process mining techniques. In the present paper, we adopt their approach in our research design (see Section 3). The work of [36] introduces an agent-based simulation environment for process discovery and conformance checking and describe how to handle the XES format to import data into the NetLogo platform.

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The efficacy of using process mining techniques to assess the outcomes of agent-based simulation models remains under-studied, resulting in limited research in this domain. Although there is existing literature on the use of process mining for performance analysis of agent behavior in agent-based simulation systems (e.g., waiting times, anomalies, etc.), the applicability of process mining techniques for conducting face validation for agent-based simulation models is a topic that has received limited attention in the research community. A knowledge gap in the process mining discipline is the lack of guidelines for balancing quality dimensions, such as fitness and precision, when assessing the face validity of agent-based simulation models. Nevertheless, there have been initial attempts to compare different agent-process mining configurations, including multiple process mining discovery algorithms [5], agent rule settings [4, 5], and variation in the number of events [2]. However, these investigations are still preliminary and have explored only a limited set of variations. Furthermore, they are not specifically focused on face validation. In [3], the authors present an approach for assessing the face validity of agent-based simulation models through process mining. However, their focus is on outlier behaviors, and their six-step approach is not described in detail, but rather outlines what should be done. Although their approach is illustrated through its application to the Schelling model of segregation, it lacks detailed descriptions of how each step can be implemented. To address this gap in the literature, we aim to demonstrate and evaluate the applicability of readily available process mining techniques for determining the face validity of a well-established agent-based simulation model.

Overall, the combination of process mining and agent-based simulation has promising potential for gaining insights into complex systems, enhancing simulation model verification and validation, and improving agent decision-making. Our proposed analysis framework is novel in that it employs a data-driven approach to extract performance metrics, taking into account both the features of an agent-based simulation model and the outcomes of process mining techniques. Ultimately, this approach can aid in developing better simulation models, achieve a deeper understanding of the underlying mechanisms of agent-based simulations, and making more informed decisions through the application of process mining techniques.

3 Research design

Figure 1 outlines the research design, which consists of several phases. This illustration is adapted from the approach proposed by [6]. In the following part, we provide a detailed account of the execution of each phase.

3.1 Problem context

For our study, we have selected the Schelling model of segregation as our case study and use it as an illustrative example throughout our explanation of the research design used for conducting a face validation assessment.

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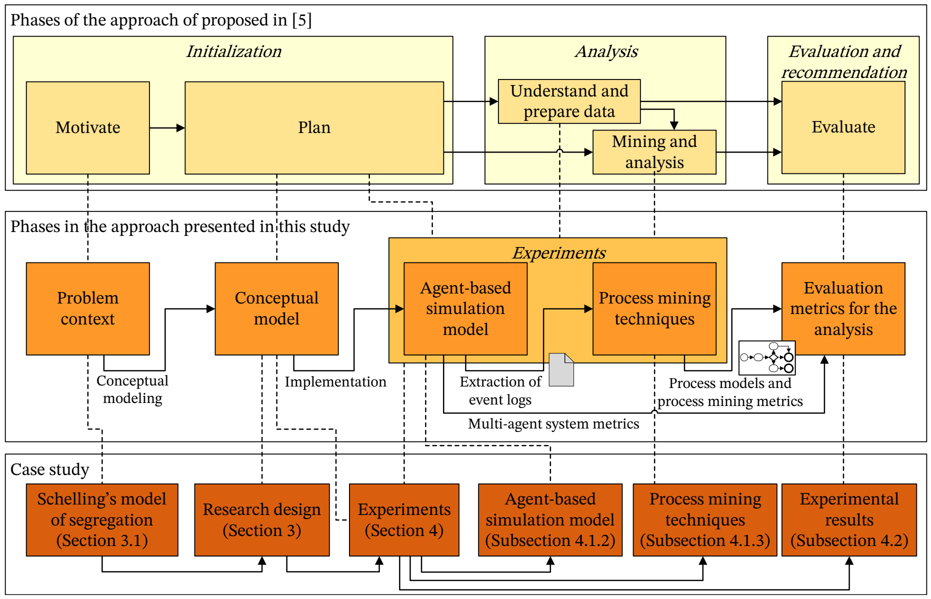

Fig. 1: Research design.

Introduction to the case study. The Schelling model of segregation is a widely recognized and influential social simulation model [34] that has been applied in various fields of research, including sociology [11]. This model illustrates how individual preferences can result in large-scale social patterns, even without explicit discrimination or prejudice [30]. The Schelling model of segregation was developed by economist Thomas Schelling to explain how segregation can occur even when individuals do not have a strong preference for living among people of their own race or ethnicity [31]. The Schelling model has served as a basis for developing other simulation models that explore social phenomena, such as the spread of infectious diseases [17] and the formation of social networks [16].

In this model, a grid representing a housing market is randomly populated with individuals who are characterized by a "tolerance threshold". This threshold represents the proportion of neighbors of the same race or ethnicity required for an individual to feel satisfied with their living situation. As the simulation progresses, dissatisfied individuals move to new locations on the grid in search of neighborhoods that meet their tolerance thresholds. This process can result in highly segregated neighborhoods as individuals with similar characteristics cluster together, attracting more individuals with those same characteristics. Clustering can occur when individual preferences are moderate rather than extreme.

Performance analysis in terms of extracting agent rules and patterns, and evaluating task or function performance (e.g., time, costs, quality, etc.) from the Schelling model of segregation through process mining can be valuable, as it can provide insights into underlying mechanisms and identify previously unknown patterns or relationships, improving our understanding of complex systems, and avoiding biases or assumptions inherent in pre-specified rules. This can lead to a more objective and accurate understanding of the system's behavior, facilitating its future development. Furthermore, the Schelling model of segregation is illustrative for understanding how individual preferences can shape large-scale patterns. Its versatility and simplicity make it a suitable starting point for exploring various agent phenomena (e.g., social cohesion and equality) and their resulting process models. The literature also reports examples of model extensions (see e.g., [22, 32, 34]). Additionally, this study aims to build upon the research conducted by [6] by using their case study as a foundation for further investigation.

Motivation for performance analysis in the context of face validity. While process mining techniques have shown promise in extracting knowledge from agent-based simulation systems, an analysis can provide a better understanding of their benefits and limitations, particularly with regard to face validity. It is important to address questions such as: What is the optimal number of event logs required for effective knowledge extraction?, Which process discovery algorithm is most suitable for a given scenario?, What biases are associated with these algorithms?, and How can they be mitigated? Additionally, investigating the scalability of process discovery mining algorithms for event logs generated by agent-based simulation models and quantifying the computational time required for knowledge extraction using these techniques is relevant. Answering these questions can provide context, such as scalability, timeliness, and quality of results, for determining the face validity of agent-based simulation models through process mining techniques.

Addressing the questions raised in this paper can help develop a deeper understanding of process mining's potential as a tool for face validity, and inform the design of innovative algorithmic process mining solutions specifically tailored for agent-based modeling and simulation. In [37], the authors called for efforts to design process mining techniques specifically for agent-based simulation systems. A systematic analysis can be a step towards achieving this goal.

To assess face validity, we incorporate features such as heterogeneous agents, network typologies, and agent rule behavior into Schelling's model by varying the parameters of the underlying agent model. These features help to make the model more realistic and representative of real-life settings. This approach can enhance our understanding of emergent phenomena in agent-based modeling and simulation. Heterogeneous agents represent a more realistic view of the world, where individuals have different characteristics, capabilities, and behaviors. Network typologies are important because agents often interact within a larger environment or network, and the structure of the network can have a significant impact on the behavior of the system. Finally, considering agent behavior is key because it allows us to model the decision-making logic of individual agents.

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3.2 Conceptual model

Figure 2 presents an overview of the conceptual model that underlies our simulation. The model consists of three main components: input parameters (Step 1 in the figure), model implementation (Steps 2.a, 2.b, and 2.c), and output evaluation metrics (Steps 3.a and 3.b). Below, we provide a brief description of these components. A more detailed account can be found in the experiment section (Section 4).

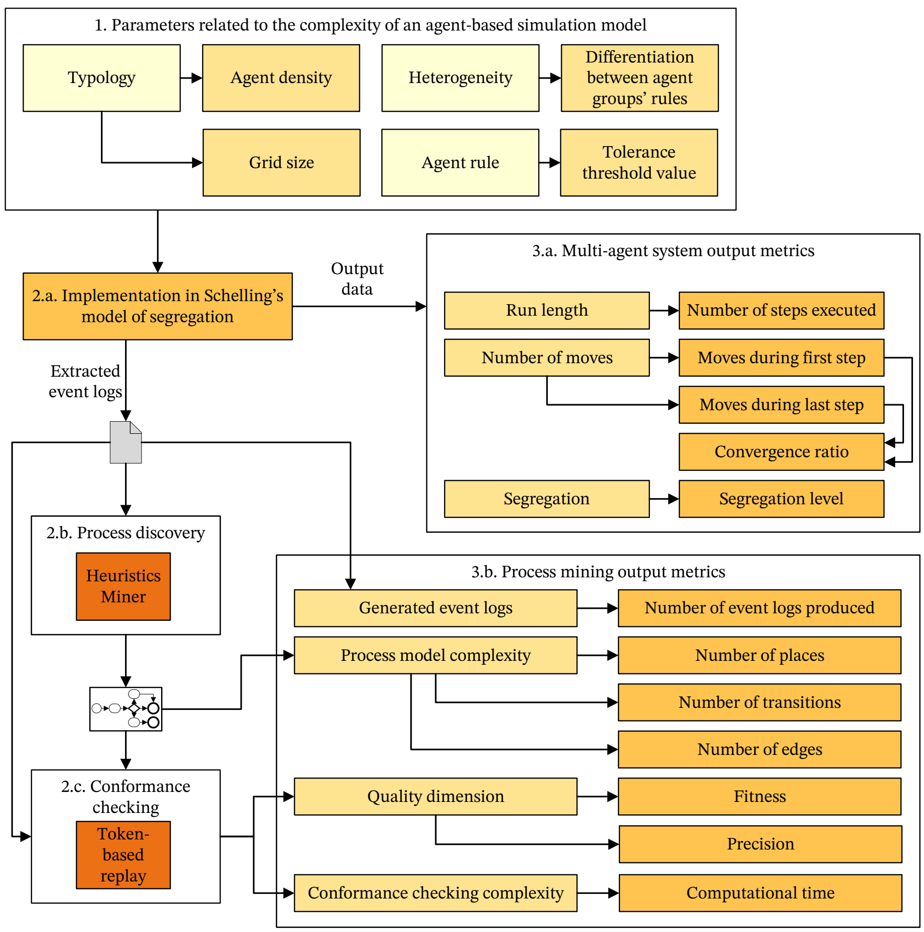

Fig. 2: Conceptual model of the simulation study.

Input parameters. To evaluate the face validity of the model, we systematically vary its input parameters, assuming that these variations will affect the

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emergent behaviors that result from agent interactions. To produce a range of results, we select three types of parameters: typology, heterogeneity, and agent behavior rules. By varying these parameters, we anticipate observing changes in the frequency and nature of interactions between agents and their environment, which can help to determine the model's face validity.

Model implementation. For the implementation of our simulation model, we based our design on the approach proposed by [6]. Additionally, we have used an existing simulation implementation developed by [13] for verification purposes. However, we have made modifications to suit our specific research needs. Figure 3 shows a flowchart that represents the logic of our simulation model.

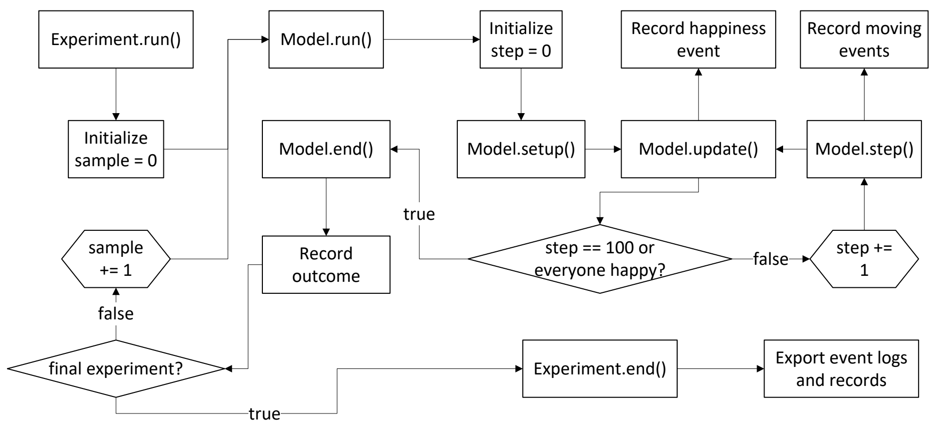

Fig. 3: Flowchart of the simulation model setup.

The simulation model tracks several updates discretely, including (1) when an agent's happiness changes, (2) when an agent moves from one location to another, and (3) when the simulation reaches its final state, either because all agents are satisfied or because it has reached a predetermined number of steps. The data from the simulations can provide valuable insights into the model's validity. Through analysis of these recorded events, simulation modelers can determine if the model behaves as expected and accurately represents the real-world system being studied. The model records events in chronological order to support process mining algorithms. This approach is appropriate since agent-based simulation can be regarded as a type of discrete-event simulation [21].

The segregation level in this model is calculated only after the model has stopped running. Specifically, this calculation happens after the last `Model.update()` call, which follows the last `Model.Step()` call. If the model runs for fewer than 100 steps, it means all agents are happy and the model has reached maximal segregation.

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Evaluation metrics. We use evaluation metrics related to the multi-agent system and process mining techniques to assess our system's validity. These metrics are depicted in Figure 2. The process mining metrics include measurements based on both process discovery and conformance checking. We chose these metrics for their simplicity, allowing for a rapid assessment of the model's plausibility. We chose a straightforward approach instead of using more complex analytical metrics. As our research is an initial step in this field, this ensures that our findings are easily accessible and understandable.

4 Experiments

We conducted a series of experiments by adjusting the selected parameters to different levels. In the following part, we provide details about the experimental setup and present the experimental results.

4.1 Experimental setup

Here, we outline the setup for our agent-based simulation model and the process mining techniques, followed by a brief description of their implementation.

Agent-based simulation model. For the analysis, we varied one parameter at a time while keeping all others constant. This allows us to isolate the effect of a parameter on the system's behavior and identify its level of influence. The following parameters were set to fixed values: density = 0.70, grid size = 20, ruleset type (homogeneous/heterogeneous) = homogeneous, tolerance threshold = 0.55, maximum number of steps = 100, and number of agent groups = 4. "Ruleset type" means either all agent groups have the same tolerance threshold (homogeneous population) or all but one group have the same threshold (heterogeneous population). Each parameter setting was executed once, and all runs employed the same random seed values. Single-run assessments can provide valuable insights and guide early model development, as is common for face validity assessments. However, it is important to acknowledge the inherent variability in stochastic simulations when interpreting the results.

Process mining techniques. As a process mining discovery algorithm, we used the Heuristics Miner. This algorithm uses the Directly-Follows Graph to handle noise and identify common constructs (e.g., dependencies between two activities) [38]. Its output is a Heuristics Net, which includes the activities and their relationships, and can be converted to a Petri net. The resulting model has three elements: places (states or conditions for a trace, shown as circles), transitions (actions that move the trace between states, shown as rectangles), and edges (flow of work between places and transitions, shown as arrows).

Event logs are stored in the XES format, using the `agentID` as the case identifier. Activity names include `move_location`, `change_happy_X_Y`, and `change_`

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unhappy_X_Y, where X represents the total number of direct neighbors and Y represents the number of direct neighbors from the same group as the case agent. Upon application of a process discovery algorithm, activity names can be transformed into transitions. For the timestamp, we used a similar approach as described by [6]. We assigned a sequential counter to each step in the model's execution, based on the chronological order of its occurrence.

To perform conformance checking, we utilized the token-based replay method. This approach is widely employed to verify whether a trace conforms to a given (process) model, indicating that transitions can be executed without any tokens missing during the process. Token-based replay involves comparing a trace and a Petri net model from the initial position to detect the executed transitions and any tokens that may have been added or removed during the process instance [26]. In case the final marking is mandatory, a fitting trace should reach the final marking without any tokens missing or remaining.

Implementation. We implemented the experiments using Python 3.6.9 and utilized the AgentPy 0.1.5 [13] and PM4PY 2.7.2 [7] libraries. The computational resources used in our experiments consisted of a 6-core Intel(R) Core(TM) i7-8750H CPU, which runs at a maximum of 3.29GHz, and 16GB of RAM. No multi-threading was used.

4.2 Experimental results

There are various techniques for conducting face validity assessments for agent-based simulation models [20]. Due to space constraints and to avoid overwhelming the reader with excessive data (e.g., particularly for process models that typically contain numerous nodes and edges), we selectively report key results. Our intention is not to conduct a thorough statistical analysis of the outcome, but rather to present intuitive methods for supporting face validity assessment through the use of process mining techniques. Below, we present a graphical representation, immersive assessment, and sensitivity analysis technique.

Graphical representations. Figure 4 shows a generated process model that can be used to evaluate the overall system flow, including general flows that match real ones. For example, we observe that many traces of agents who became happy (green box in Figure 4) go to the end node (see the blue arrow) and do not move anymore, while many unhappy agents (red box) generally move to a different location. Based on this simple observation, the model's face validity can be deemed plausible.

Immersive assessment. A human expert can view the simulation model's execution through the eyes of the agent and evaluate its actions. For instance, one of the traces, partially depicted in Figure 5, of an agent includes: unhappy_2_1, move_location, happy_1_1, unhappy_4_1, and move_location. This suggests

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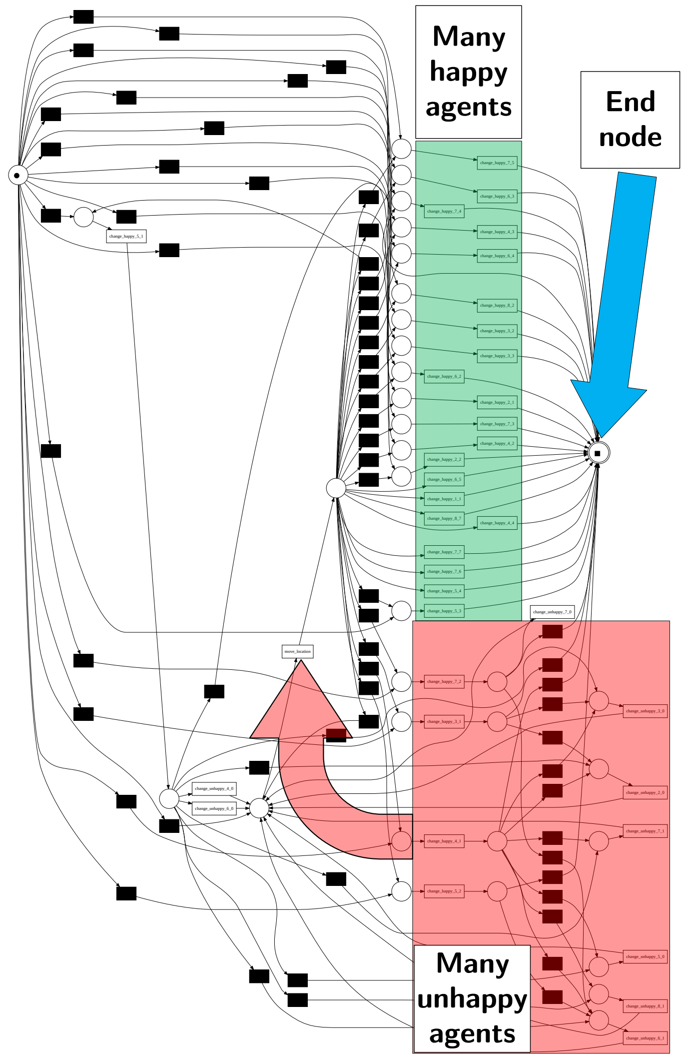

Fig. 4: High-level view of a process model from an experiment with a consistent tolerance threshold of 0.10 applied to all agents. (Note: This illustration is intended for general understanding and not for detailed examination.)

that an agent moves when it is unhappy, but can also become unhappy again when new neighbors arrive who cause the agent to move once more. This is consistent with Schelling's model and supports the face validity assessment.

Sensitivity analysis. As shown in Figure 2, we used various parameters related to the complexity of our agent-based simulation model. In this paper, we

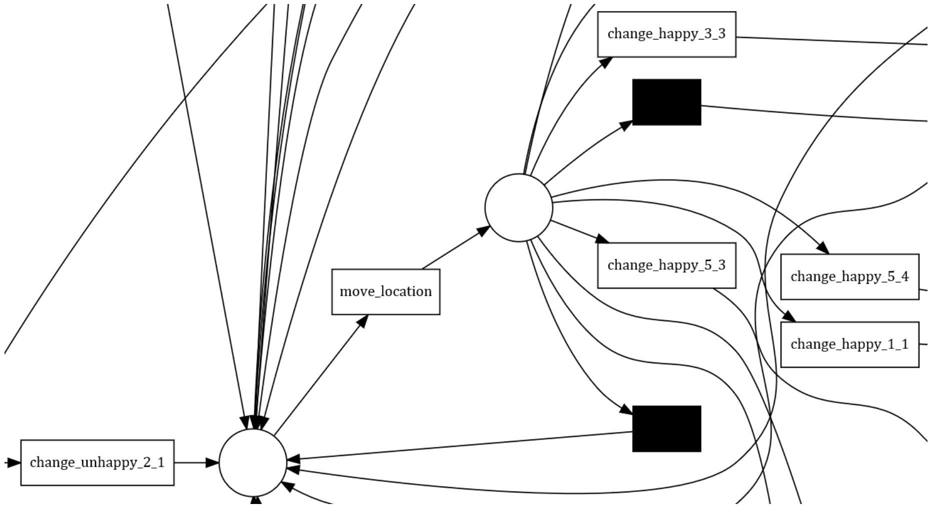

Fig. 5: A snippet of a process model near the move_location activity (experiment T13).

only vary the agent density, which represents the percentage of grids occupied by agents, due to space restrictions. Table 1 shows the resulting output metrics. To assess face validity, we consulted an expert in the field for a preliminary evaluation of general trends and extreme values in the process mining-related output metrics (highlighted in bold), allowing us to determine whether the results were reasonable upon initial examination.

The data indicates a positive correlation between agent density and the number of event logs, except for experiment T6. Experiments T10-T12 had the highest agent densities and similar number of event logs, suggesting consistent agent moves. However, the ratio of moves varied, indicating fluctuations during each run. Despite this, end segregation levels were identical, possibly due to reaching an equilibrium or cyclic state (e.g., an agent can repeatedly transition between unhappy and happy).

Agent density affects the complexity of the process model. At low densities, the model is less complex, while at high densities, it increases slightly. The greatest number of behaviors is captured at 60-80% density, despite the fact that the number of event logs is not as high as in, e.g., experiments T9-T12.

Fitness and agent density have a non-linear relationship. Fitness decreases as density increases from 0.10 to 0.70 but then increases again from 0.70 to 0.99. This could be due to the system's complexity, making it difficult for the process mining algorithm to accurately reproduce behavior, resulting in decreased fitness. Further increases in density may result in more predictable behavior, increasing fitness. Further analysis is needed to determine the exact cause.

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Table 1: Varying network typology, expressed in agent density.

#	Varying parameter	Multi-agent system output metrics					Process mining output metrics						
	Agent density (%)	Number of runs until the threshold is reached	Number of moves			Segregation level	Number of event logs produced	Number of places	Number of transitions	Number of edges	Fitness (%)	Precision (%)	Computational time (MM:SS.ss)
			First run	Last run	Ratio								
T1	0.10	100*	36	10	0.28	0.77	**1966**	**14**	**38**	**76**	**100.00**	40.83	**00:09.36**
T2	0.20	100*	80	10	0.13	0.87	3837	21	67	134	97.50	**20.84**	00:16.11
T3	0.30	100*	90	1	0.01	0.99	5118	29	94	188	96.67	42.49	00:34.56
T4	0.40	100*	146	1	0.01	0.98	6301	33	121	242	96.25	39.07	00:25.87.
T5	0.50	100*	184	1	0.03	0.70	16730	44	172	344	90.50	36.22	01:29.87
T6	0.60	100*	211	2	0.01	0.93	14912	51	227	454	82.50	43.88	04:13.67
T7	0.70	100*	257	26	0.10	0.89	19208	56	245	490	**73.93**	42.67	06:10.48
T8	0.80	100*	295	93	0.32	0.41	29014	57	**256**	**512**	78.75	44.80	08:10.22
T9	0.90	100*	334	319	0.96	0.26	35663	**63**	233	466	85.83	**47.70**	**14:28.97**
T10	0.97	100*	362	257	0.71	0.28	**39724**	49	146	292	96.39	43.89	12:03.88
T11	0.98	100*	375	355	0.95	0.28	**39724**	54	147	294	98.98	38.40	12:30.71
T12	0.99	100*	384	371	0.97	0.28	**39724**	44	123	246	98.99	36.07	08:57.56

*: the maximum number of steps is reached

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4.3 Discussion

In this section, we will provide an analysis, interpretation, and discuss the implications of the experimental results. Our experiments show that changing the parameters of the agent-based simulation model leads to different emergent behaviors and outcomes, as shown by process mining techniques. This suggests the model is sensitive to changes in input parameters, which is important for face validity. However, we also observed that the results obtained from parameter combinations can result in process mining outcomes that need more examination to match with real-life scenarios.

Face validity is important in agent-based simulation [20], especially when interpreting experiment results, but caution should be exercised. In agent-based modeling, analysts usually do not limit themselves to only examining inputs, such as initial conditions and model specifications, to explain results. Nor do they consider the results to be solely the final state, without taking into account the history or paths taken to reach that state. Unless one is modeling a one-shot game or similar scenario, applying process mining in the manner presented in this study may not be sufficient. Analysts often plot results temporally and use other techniques to evaluate simulations that evolve over time. The variables examined are not limited to those that are measurable in experiments but may also include latent variables or other key model variables, whose physical significance may be unclear, in order to observe how they unfold over time and explain models and results.

While process mining allows for the identification of individual agent behavior in multi-agent systems, examining collective emergent behavior on various levels is also important. To address this, we propose future investigations into both individual and group levels, possibly using hierarchical or relationship-based methods. For example, object-centric process mining can enhance the analysis of an agent-based system by focusing on individual objects or entities. This, in turn, can help to identify emergent behaviors at the group or population level, particularly among populations with specific characteristics (e.g., outliers).

5 Conclusion

This paper presented a study on the application of process mining techniques for assessing the face validity of agent-based simulation models. We proposed an approach that leverages process mining as a tool for conducting face validity assessments and illustrated its effectiveness using the Schelling model of segregation. Our approach demonstrated the potential of process mining techniques to augment the face validity assessment process, thereby contributing to the development of valid agent-based simulation models. Through a proof-of-concept implementation, we showed how a human expert can assess a simulation model and its outcomes using process mining. This knowledge can ultimately aid in the development of valid agent-based simulations, providing accurate representations of real-life systems.

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Future research directions include exploring the applicability of process mining to other types of agent-based simulation models, and developing more automated methods for face validity assessment of agent-based simulation models through process mining. One avenue to explore is the integration of statistical methods, such as Latin hypercube sampling or orthogonal sampling, to generate a sample set of agent model parameters, and then selectively and systematically assess the resulting simulation model and its outcomes by a human expert through process mining. Another direction includes deploying mixed methods using multiple approaches to conduct validation analysis. Furthermore, while the utilization of process mining techniques represents a valuable approach in augmenting the face validity of agent-based simulation models, further elucidation regarding their differentiation from conventional approaches may be advantageous. This could include a more detailed explication of the application of process mining techniques in the evaluation of temporally evolving simulations and their distinction from alternative methodologies employed. By addressing this concern, we could offer a more comprehensive understanding of the unique contributions afforded by process mining techniques.

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