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FEATURE IMPORTANCE FOR UNCERTAINTY QUANTIFICATION IN AGENT-BASED MODELING

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ABSTRACT

Simulation models are subject to uncertainty and sensitivity, meaning that even small variations of input can cause considerable fluctuations in the output results. Consequently, this can amplify the uncertainty associated with the simulation, thereby limiting the confidence one can have in its outcomes. To mitigate these effects, this paper suggests using a cooperative game theory-based feature importance method, which can identify uncertainty in a dataset, and provide additional insights that could be used in the development or analysis of a simulation model. A predator-prey scenario was considered, demonstrating its usefulness in identifying important parameters or features. By identifying the most influential parameters or features, this approach can help improve the accuracy, explainability, and reliability of simulation models as well as other models with highly variable input parameters.

1 INTRODUCTION

A single simulation run can provide valuable insights but cannot account for all the sources of uncertainty and variability in the modeled system (Ritter, Schoelles, Quigley, and Klein 2011). Therefore, multiple simulation runs with varying input parameters, initial conditions, or model assumptions are necessary to explore a wide range of possible outcomes, especially for agent-based models that simulate individual agent behavior and interactions within a larger system. However, multiple simulation runs can also introduce uncertainty when different results are observed, making it difficult to discern the significance of each input variable in the agent-based model. Given that agent-based models are inherently stochastic and sensitive to small changes, multiple simulation runs are crucial to fully explore the range of possible outcomes and evaluate the uncertainty associated with the model results (Windrum, Fagiolo, and Moneta 2007; Collins, Jayanetti, Grigoryan, and Chatfield 2023). Although running multiple simulations can help identify aggregate patterns and emergent behaviors not apparent in single simulations, it can be computationally expensive and time-consuming. The sheer volume of data generated from multiple simulation runs can also make it challenging to identify and interpret the most significant results.

Running multiple simulations or experiments with varying conditions or parameters can produce different results, making it challenging to determine the most accurate result (Sargent 2004). Uncertainty quantification (UQ) plays a significant role in addressing this challenge by identifying, quantifying, and reducing uncertainties associated with models, algorithms, and predicted quantities of interest (Ghanem et al. 2017). UQ is particularly important when accurate predictions or decisions are required, but underlying models or data are incomplete, imperfect, or subject to variability. As Begoli et al. (Begoli, Bhattacharya, and Kusnezov 2019) note, predictions without UQ are neither predictions nor actionable.

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Addressing uncertainty in agent-based models (ABMs) poses several challenges. One of the main obstacles is the complexity of these models, which often have high-dimensional feature spaces with numerous parameters, initial conditions, and rules governing agent behavior. This complexity makes it challenging to identify the sources of uncertainty and the impact of each parameter on the model output. Furthermore, the stochastic nature of ABMs can pose another challenge by leading to high variability in the model output. Running multiple simulations considering different conditions can help capture the collective trends and novel phenomena that arise from agent interactions and are not observable in single simulations (Ali, Shafiee, and Berglund 2017). ABMs often rely on incomplete or imperfect empirical data, leading to additional uncertainty (Bruch and Atwell 2015). The model's assumptions about the behavior and interactions of agents may also not accurately reflect the real-world system being modeled, adding to the uncertainty.

Sensitivity analysis has been widely used to address the challenges associated with uncertainty in ABMs (Marino et al. 2008). However, the objective of sensitivity analysis is to improve the robustness of a model by examining how changes in the inputs of a model affect its outputs (Ten Broeke, Van Voorn, and Ligtenberg 2016). While sensitivity analysis can identify the most influential parameters and assumptions, it may not provide additional insights into the underlying mechanisms driving the model output (Thiele, Kurth, and Grimm 2014).

Feature importance techniques from explainable artificial intelligence (XAI), on the other hand, could be useful in addressing these limitations. By providing additional insights into the relative importance of model features, XAI methods can enhance the initial information and help clarify and better explain the model (Grigoryan 2022). This can lead to a more comprehensive understanding of the model's behavior and improve the accuracy and reliability of its predictions.

This paper aims to demonstrate the use of feature importance measures from explainable AI as a means for uncertainty quantification. To achieve this, we revisit a classical predator-prey model involving two interacting species: a predator (rotifer) and a prey (unicellular algae). The following section provides a background on agent-based models and cooperative game theory. Section three discusses the feature importance method. Subsequently, we present the results of our analysis in Section Four, followed by concluding remarks in the final section.

2 BACKGROUND

This section presents an overview of the concepts of agent-based models, feature importance, and cooperative game theory.

2.1 Agent-Based Models

An agent-based model (ABM) is a type of computational model that simulates the behavior of individual agents and their interactions with each other and their environment (Macal and North 2009). Each agent in an ABM is programmed with a set of rules and behaviors that govern their actions, and the model is designed to track the interactions between agents over time. ABMs are used in a variety of fields, including economics, ecology, sociology, and epidemiology, to study complex systems and understand the emergent behaviors that arise from interactions between individual components.

A classical example of an ABM is the predator-prey model, which simulates the interactions between populations of predators and prey in an ecosystem. In this model, agents are divided into two categories: predators and prey (Grimm and Railsback 2005). Each predator agent is programmed to seek out and consume prey agents, while each prey agent is programmed to avoid predators and reproduce. The Lotka-Volterra equations also referred to as the predator-prey equations, are a pair of differential equations that capture the dynamics of interacting populations (Brauer, Castillo-Chavez, and Castillo-Chavez 2012). These equations enable the model to track the populations of predators and prey over time, unveiling emergent behaviors such as population cycles and extinction events as a result of the interactions between agents. Specifically, the equations are given by:

The Lotka-Volterra equations, also known as the predator-prey equations, can be represented as a single equation:

$$\begin{aligned} \frac{dx}{dt} &= \alpha x - \beta xy, \\ \frac{dy}{dt} &= \delta xy - \gamma y. \end{aligned} \tag{1}$$

In Equation 1 x represents the population of the prey species, y represents the population of the predator species, and α, β, γ, and δ are positive constants representing the growth rates and interaction strengths between the populations. A predator-prey model is a useful model for studying the dynamics of ecosystems and understanding the impacts of environmental factors on populations of animals.

One example of a predator-prey model from agent-based modeling is the "wolf-sheep predation model," which simulates the interactions between wolves and sheep in a given ecosystem (Wilensky and Rand 2015). In this model, agents representing wolves and sheep move around the environment and interact based on specific rules, such as the wolves hunting the sheep and the sheep trying to avoid them. Another example, which we have considered in this paper is the rotifer-algae predator-prey model (Blasius, Rudolf, Weithoff, Gaedke, and Fussmann 2020). Rotifers and algae are common microorganisms found in aquatic environments. Rotifers typically have a transparent, elongated body with a distinctive head crowned by cilia. In Figure 1, the rotifer is described with yellowish/orange pigment. The cilia create a rotating motion, resembling a spinning wheel, as they move through water. Algae, on the other hand, encompass a diverse group of photosynthetic organisms ranging from microscopic single-celled forms to large, multicellular seaweeds. Algae can exhibit a wide array of colors, including green, red, and brown. They play a critical role as primary producers, converting sunlight, water, and carbon dioxide into organic compounds through photosynthesis. Furthermore, algae serve as a fundamental food source for numerous aquatic organisms. In Figure 1, the depicted algae are prominently green in color.

The interaction between these two species is of ecological importance, as it affects the balance of the ecosystem. In the rotifer-algae model the agents are assumed to interact with each other based on simple conditions such as feeding and reproducing, and their individual behaviors can lead to the emergence of complex patterns at the system level. In the rotifer-algae model, each rotifer and algae agent has its own set of attributes and behaviors, such as movement, feeding, and reproduction. Rotifer-algae system incorporates various environmental factors such as light, temperature, and nutrient availability. By simulating the behavior of individual agents, the model can predict the emergent effects of adaptive behavior and the impact of different conditions on the system as a whole.

The agents interact with each other based on their proximity and the conditions governing their behavior (Figure 1). For example, a rotifer may move towards an algae if it is hungry and within a certain distance, and then feed on the algae if it is close enough. Similarly, algae may reproduce when it has enough nutrients and space.

2.2 Feature Importance

Uncertainty quantification encompasses a wide range of methods and tools used to critically evaluate simulation models. This includes processes such as verification and validation (V&V) (Lynch, Gore, Collins, Cotter, Grigoryan, and Leathrum 2021), sensitivity analysis, and uncertainty propagation (Ten Broeke, Van Voorn, and Ligtenberg 2016). In this paper, we suggest considering the feature importance measures to address the uncertainty quantification by identifying the most important features that contribute to the model outcome. Feature importance is a technique used in explainable artificial intelligence to evaluate and explain the importance of different features (variables) in a model's prediction (Adadi and Berrada 2018). Explainable Artificial Intelligence (XAI) focuses on solving "black-box" related uncertainties

Figure 1: Rotifer-algae predator-prey system. Image used with permission from SciencePhoto - Image ID C025/3764, Request ID 904451.

when explanations are crucial. Explainable AI program launched in 2017 (Adadi and Berrada 2018), emphasized the need to create models that are both highly accurate and easily understandable by humans, thereby allowing them to effectively utilize and manage the new insights of intelligent systems. The main objective of XAI techniques is to improve the explainability of the model's decision-making logic and the reasoning behind model recommendations and suggestions. Gregor and Benbasat (1999) describe explainability as a "declaration of the meaning of words spoken, actions, motives, etc., with a view to adjusting a misunderstanding or reconciling differences". Explainability also helps to understand the system's malfunctions or anomalies.

When features are uncertain or poorly characterized, the output of the model may also be uncertain or unreliable. By quantifying the impact of these important features on the output, we can better understand the sources of uncertainty and develop strategies to reduce it. Therefore, feature importance analysis could be an essential tool in the UQ process, allowing for a more comprehensive assessment of the reliability, accuracy, and explainability of agent-based models. Measuring the importance of features in a model can be accomplished using various approaches, including permutation feature importance (Altmann, Toloşi, Sander, and Lengauer 2010), and cooperative game theory-based solutions (Štrumbelj and Kononenko 2014). Cooperative game theory-based approaches are known for their ability to yield fair assessments of feature importance values (Lundberg and Lee 2017). By ranking the features by importance, we can focus on the most important features when making decisions about how to reduce uncertainty and improve the model's reliability and accuracy.

2.3 Cooperative Game Theory

Cooperative game theory is a branch of game theory that focuses on the analysis of cooperative, or coalition, games (Fudenberg and Tirole 1991). In cooperative games, players form coalitions and work together to achieve a common goal or outcome. The goal of cooperative game theory is to understand the ways in which players can form coalitions and allocate resources in order to achieve the most favorable outcome for all parties involved (Fudenberg and Tirole 1991; Collins, Thomas, and Grigoryan 2019). A cooperative game in characteristic function form is defined as a 2$-$tuple $\Gamma = (N, v), N$ being the set of players $N = \{1, 2, 3, ..., n\}$ and v being the value function. The players form coalitions, which refer to the formation of sub-sets of players. For a set $A; C_A$ denotes the subsets of A, i.e., $C \subseteq A$, and P_A denotes the partitions of A. For a set of players N, a coalition is any subset of N, and N is the grand coalition. A partition of N is the splitting of all the players into disjoint coalitions. The value v of a coalition is non-negative and it is the characteristic function and satisfies the $v(\emptyset) = 0$.

An outcome of a game Γ is a pair (P,x), where: $P = (C_1, C_2, ..., C_k) \in P_N$ is a coalition structure (CS), and $x = (x_1, ..., x_n)$ is a payoff vector, which distributes the value of each coalition in P. Cooperative game theory is used in a variety of fields, including economics, political science, and computer science, to study problems such as resource allocation, bargaining, and voting systems. By analyzing the ways in which players can cooperate and form coalitions, researchers can gain insights into the dynamics of complex social and economic systems.

Cooperative game theory has been applied in XAI to allocate feature importance values in a fair manner considering their marginal contributions to the model performance (Lundberg and Lee 2017). The next section presents the feature importance method.

3 METHODS

The approach presented in this paper utilizes the Shapely value cooperative game theory solution concept (Eq. 2) (Grigoryan and Collins 2021). This approach is model-agnostic, making it applicable to post-hoc data analysis regardless of the specific modeling technique employed.

$$\phi_i(v) = \sum_{s \subseteq N \setminus \{i\}} \frac{|S|!(|N| - |S| - 1)!)}{|N|!}(v(S \cup \{i\}) - v(s)) \tag{2}$$

Our approach determines the important features by analyzing empirical data collected about the simuland (system under study). A simulation designer could use this knowledge in the development of the simulation model, i.e., which features they should focus their attention on during the simulation design. The important features could also help inform which features to focus on during the sensitivity analysis stage of a simulation project. This is important because developing targeted sensitivity analysis methods has been identified as a key challenge for agent-based modeling (Ten Broeke, Van Voorn, and Ligtenberg 2016). Moreover, our approach can also assist in identifying and eliminating irrelevant features, which could lead to model complexity and reduced simulation performance. The feature importance method employs a feature importance evaluation algorithm to calculate the importance values of features from the behavioral space, resulting in a list of the most significant features that impact the system behavior. By focusing on important features, simulation designers can create more efficient models and avoid wasting resources on simulating irrelevant features, which could result in longer simulation run times and higher computational costs. Additionally, the knowledge gained from identifying important features can also facilitate the parameterization of the simulation model, which is crucial for model calibration and validation. With this information, simulation designers can more accurately set and test the parameters of the model, leading to improved confidence in the model's results and predictions. Overall, our approach can help streamline the simulation design process and lead to more explainable and accurate simulation models.

To determine the importance of a feature, the model's performance is evaluated by comparing the model performance value with and without that feature using the Shapley value (Eq. 3). This approach shares similarities with feature ablation techniques as it involves systematically assessing the impact of removing a feature on the model's overall performance **??**. Various performance indicators such as multiple determination R^2 or AIC values can be employed for the evaluation of feature importance. For instance, in the context of regression models, one approach to estimate feature importance is by analyzing the changes in R^2 values that occur when a specific feature is included or removed from the model (Eq. 3).

$$U_i = R^2 - R^2_{-i} \tag{3}$$

Algorithm 1 presents a concise summary of the sequential steps required to calculate the feature importance value. The algorithm extracts simulation model output and identifies various feature combinations, then conducts regression models for each combination. The resulting R^2 values are used as fresh data to define the game in characteristic form for n features in lexicographic order. The algorithm assesses all permutations and generates feature importance values that represent

Algorithm 1: Shapley value feature importance explanaitons

Collect data about the simuland;
Identify all possible feature combinations for each feature $x_1, x_2, \ldots, x_3$;
Estimate regression models and extract R^2 values for each feature combination ;
Define the game (N, v) in characteristic form and compute Shapley regression values;
Return the computed feature importance values

the incremental contributions of each feature. The data and the R code can be accessed online from https://github.com/grigoryangayane/Predator-prey-model-feature-importance.

Simulation models and various applications, such as cybersecurity (Vernon-Bido et al. 2018), healthcare (Ghavidel, Ghousi, and Atashi 2022) and coalition formation (Grigoryan, Etemadidavan, and Collins 2022) that can generate a feature space are suitable for analysis. In this paper, we utilize a predator-prey dataset collected Blasius, Rudolf, Weithoff, Gaedke, and Fussmann (2020). The features can encompass continuous values, temporal data, or text-based information depending on the specific context and application. The dataset we considered comprises time series data from ten physical experiments involving a planktonic predator-prey system, with measured population densities of the prey (unicellular algae), predator (rotifer), and predator life stage characteristics recorded over approximately 2,000 measurement days. The dataset demonstrates predator-prey cycles of unparalleled length, making it a valuable resource for investigating the dynamics of predator-prey systems. The purpose of this study is not to explore the design or evaluation of simulation models but rather to leverage this existing dataset to examine uncertainty quantification in predator-prey models. Table 1) displayed below presents single-sample observations captured from distinct experiments (Table 1):

Table 1: Single observation instances extracted from datasets

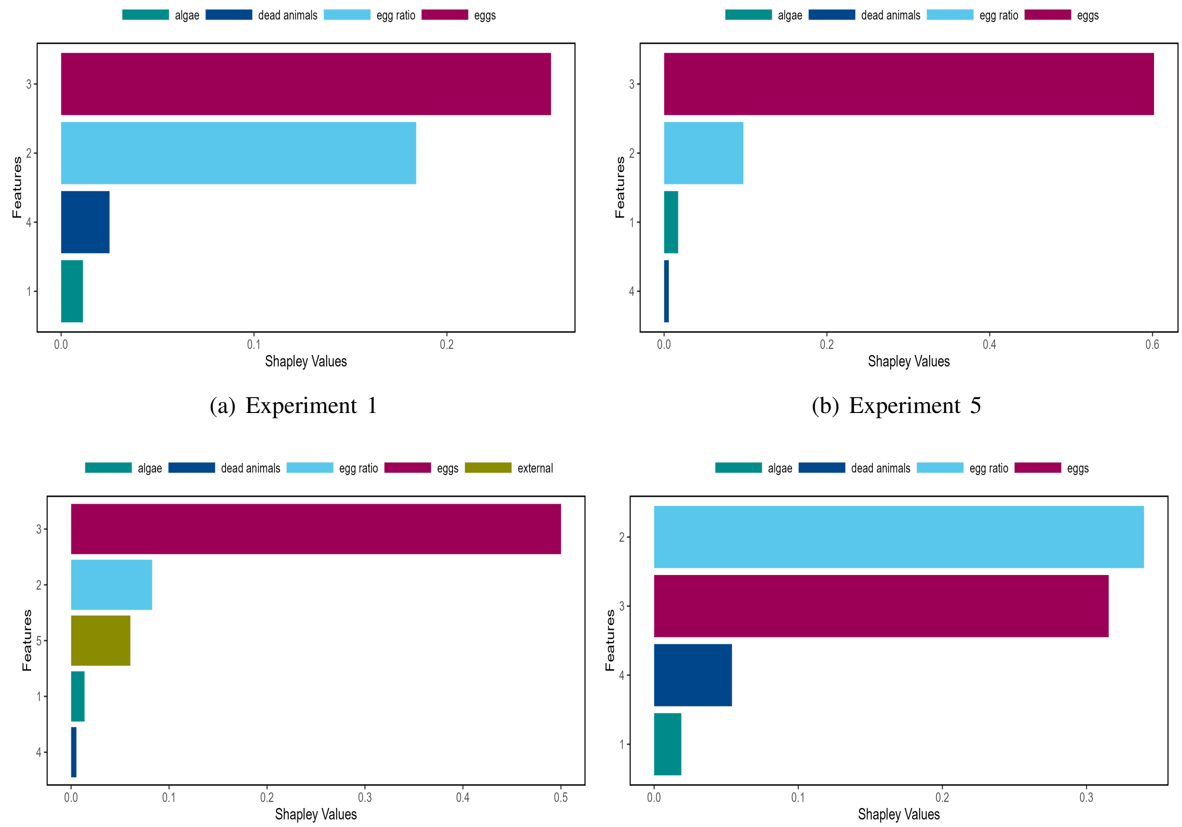
Exp/features	rotifers	algae	egg-ratio	eggs	dead animals	external
Exp1	5.42	0.83	0	0	0.4	NA
Exp5	9.83	0.73	0.27	2.61	0.4	NA
Exp8	11.04	2.83	0.67	7.42	0.4	160
Exp10	6.82	2.03	0.06	0.4	0.2	NA

The model uses several features to investigate the dynamics of planktonic freshwater organisms and rotifers. These features include the total number of rotifers, unicellular green algae, produced eggs, and dead animals. Additionally, the egg ratio, which measures the reproductive status of the population by dividing the total number of eggs by the total number of animals, is considered as another potential predictor of rotifer numbers. The study also examines the influence of external factors, such as spatial structure, immigration, or environmental perturbations, to investigate the potential for persistent cycles.

While there are multiple features linked to the number of rotifers, identifying which of these features plays the most significant role in predicting rotifer numbers remains an essential question. Understanding the relative importance of each feature can provide valuable insights into the underlying mechanisms driving the dynamics of the rotifer population and inform the development of more accurate and effective predator-prey models.

4 RESULTS

The aim of this study was to examine the importance of various features in predicting rotifer numbers. The results of the analysis are presented in Figure 2 and 3. In Experiment 1, the number of eggs was found to be the most crucial feature for predicting rotifer numbers, followed by the egg ratio. Surprisingly, the number of algae and dead animals were found to play the least important roles.



(a) Experiment 1 (b) Experiment 5

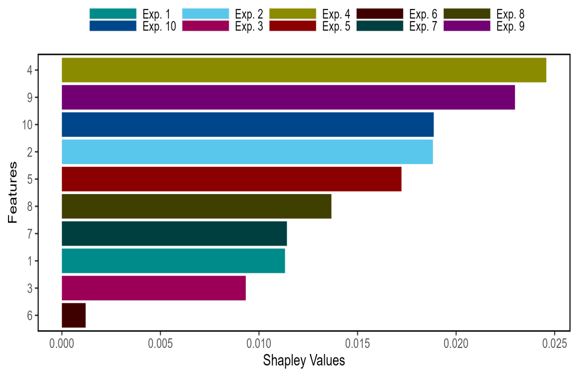
(c) Experiment 8 (d) Experiment 10

Figure 2: Shapley feature importance analysis results from different experiments.

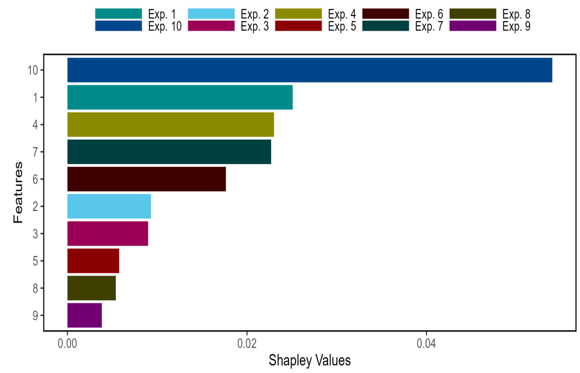
Similar results were obtained in Experiments 2, 3, 4, 6, 7, and 9, and therefore, the figures for these experiments are not included. In Experiment 5, the same feature importance pattern was observed, but the egg ratio had a slightly smaller importance value. In Experiment 8, the feature external was identified as the third most important feature, whereas in the other experiments, it had an importance value of 0. In Experiment 8, the number of eggs was the most crucial feature for predicting rotifer numbers, followed by egg ratio and external factors. The number of algae and dead animals were again found to play the least important roles. In Experiment 10, the egg ratio was found to be relatively more important than the feature eggs. This was followed by dead animals, and then the number of algae. These results suggest that the importance of different features in predicting rotifer numbers can vary across different experiments, and that it is important to carefully examine the results in the context of each specific experiment.

Next, we looked at the feature importance values, for selected features, across different experiments to see if the same feature importance values were observed across different experiments. Notice that the features are given different feature importance values throughout different experiments. The variability in the feature importance results across different experiments suggests that the importance of different features in predicting rotifer numbers can depend on the specific conditions of each simulation. For example, factors such as the type and quantity of food provided to the rotifers, the temperature and lighting conditions, the length of the experiment, or the presence of predators, can all affect the growth and reproduction of rotifers, and consequently, the importance of different features in predicting their numbers.

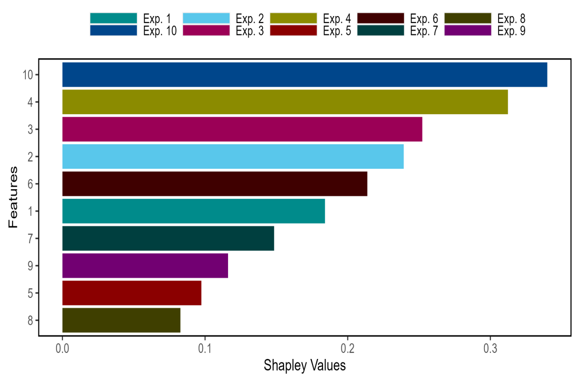
Therefore, it is important to carefully examine the results of each experiment and consider the specific conditions under which the data was generated when interpreting the feature importance results. This



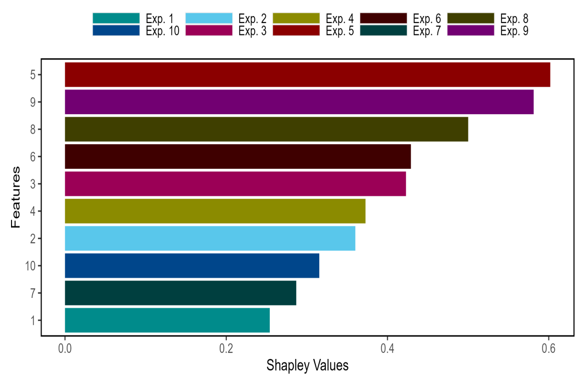
(a) Feature: algae



(b) Feature: dead animals



(c) Feature: egg ratio



(d) Feature: eggs

Figure 3: Comparing Shapley feature importance values for each feature across multiple experiments.

means that the importance of a given feature in one experiment may not necessarily be the same in another experiment with different conditions. By taking into account the specifics of each experiment, we can gain a better understanding of which features are most important for predicting rotifer numbers under different conditions, and how they may interact with other factors to influence rotifer populations.

Overall the findings of this analysis indicate that the reproductive status of the rotifer population, as measured by the number of eggs and the egg ratio, has the most significant impact on the population dynamics. Additionally, external factors such as spatial structure, immigration, or environmental perturbations can also have an impact on shaping the predator-prey cycles. Identifying these features can help in the development and validation, through sensitivity analysis, of the simulation.

Future work for this research is to repeat the feature importance approach but on the simulation output data. Comparing the rankings of the features (real-world data vs simulation data) might provide insight into the limitations of the simulation and/or add to the validation process of the simulation. Thus, feature importance might be able to aid the validation process beyond informing the features to focus on.

5 CONCLUSION

Based on the results of the feature importance analysis, we can conclude that the importance of different features in predicting rotifer numbers can depend on the specific conditions of each experiment. The variability in the feature importance results across different experiments suggests that it is important to carefully examine the results of each experiment and consider the specific conditions under which the data was generated when interpreting the feature importance results.

The findings of this analysis indicate that the reproductive status of the rotifer population, as measured by the number of eggs and the egg ratio, has the most significant impact on the population dynamics. This suggests that efforts to control or manage rotifer populations should focus on factors that affect their reproductive behavior. Additionally, external factors such as spatial structure, immigration, or environmental perturbations can also have an impact on shaping the predator-prey cycles.

Overall, the use of feature importance as an uncertainty quantification approach can aid in agent-based models by identifying the crucial factors driving system behavior, enhancing the comprehensibility of the model, and providing a more sound basis for decision-making. However, it is important to carefully consider the specific conditions of each simulation run and interpret the results in the context of those conditions.

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