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Analyzing regime shifts in agent-based models with equation-free analysis

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Abstract: Conventional tools to analyze regime shifts in ecosystems, e.g. stable state and bifurcation analyses, are increasingly adapted to investigate social-ecological systems. The challenge lies in combining the analysis of system dynamics with the analysis of transient dynamics emerging from adaptive and heterogeneous agents. A typical question is, to which extent do micro level interactions contribute to a macro level outcome? We demonstrate the application of a new tool, equation-free analysis, for evaluating the state space from an agent-based model (ABM) on lake restoration. By sidestepping the requirement of an equation describing a systems macroscopic behavior, equation free analysis enables system level tasks (such as bifurcation analysis) to be performed on micro level models. This is particularly beneficial for agent-based models that aim to explain macro level patterns and include more parameters than one can feasibly analyze by simulation experiments alone. In our example on lake restoration, the macro scale pattern is the ecological regime shift between the clear and turbid water state. This regime shift can be influenced by micro level decisions from lake users affecting the main driver through alternative strategies. To find out which strategies are more effective to restore the lake into the desired clear state, we linked the resulting bifurcation diagram from the equation-free analysis to simulation experiments along the alternative trajectories. Concluding, we describe suitable steps for integrating the equation-free analysis with more traditional agent-based model analyses and discuss the difficulties and advantages therefrom.

***Keywords**:* social-ecological interaction; equation-free; steady state analysis; regime shifts; shallow lake restoration;

1 UNDERSTANDING REGIME SHIFTS

Non-linear transitions in ecosystems were often described as regime shifts by identifying dominant reinforcing feedbacks for alternative stable states (Scheffer 2009). A regime shift is a macroscopic pattern where the system's state variable undergoes a non-linear, persistent change while the driver changes relatively little. One example for this phenomenon is the ecological regime shift in shallow lakes where a slight increase in nutrient concentration can cause a drastic shift from clear to turbid water which affects the whole lake ecology in terms of plankton and fish assemblages (Scheffer 1989). The behavior of regime shifts is conventionally modelled by differential equations. While ecological shifts have been investigated a lot through modelling but also empirical methods (Biggs et al. 2012), the dynamic interaction of humans with ongoing regime shifts has received little attention in models so far (Lade et al. 2013). One potential reason for this unbalanced representation of human-environmental interaction is the difficulty to represent human decision-making which is partly addressed by agent-based models. But until today, this approach had the drawback that it was impossible to analyze macroscopic patterns, such as stable states, without running large sets of simulations covering all suitable parameter variations and combinations. To overcome this barrier, we present a new tool here, the equation-free analysis.

Treating the model as a black-box, the equation-free analysis is capable to derive system scale patterns that are represented e.g. in bifurcation diagrams. We introduce in the following section how it works and then exemplify its applicability by the analysis of a coupled agent-based, system dynamics model. In this case study, we look at shallow lake restoration and how individual agent traits may influence the state of the lake. Finally, we discuss the difficulties and advantages for analyzing ABM's with the equation-free analysis.

2 A NEW WAY TO ANALYSE ABM'S MACROSCOPIC BEHAVIOR

2.1 Path following

Path following and bifurcation analysis are well established mathematical tools for analyzing non-linear system dynamics (Seydel and Hlavacek 1987, Doedel et al. 1991). From a known steady state in a system, i.e. a stationary or periodic solution, these techniques analyze how these states respond with changes to a driver parameter in the system. As the parameter is varied the previous solutions are 'followed', providing a much more efficient method for analysis than repeatedly computing the steady state from arbitrary initial conditions as the driver parameters is varied. The basis of path following techniques is a two-step process, prediction and correction. Firstly, from a known steady state, which can be obtained from an initial simulation, a prediction is made for the steady state under some small variation to the driver parameter. Secondly, this prediction is improved upon using standard corrector or root-finding algorithms such as Newton-Rhapson (Ryaben'kii and Tsynkov 2006). This framework provides a simple and efficient way of analyzing non-linear systems and is illustrated in Figure 1. The steady state of a model described by $F(x,\theta)$ for variable(s) x and parameter(s) θ, is computed by obtaining the x_1 that, for θ_1, satisfies $F(x_1,\theta_1)=0$. This solution can be 'followed' as θ changes by predicting x_2 based on the value x_1 (white circle in Figure. 1). The prediction yields $F(x_2,\theta_2)\approx 0$ which is then corrected using the root-finder algorithm until $F(x_2,\theta_2)=0$. Repeating this process enables the following of unknown steady states (blue line in Figure. 1).Typically a secant or gradient-based method is used to extrapolate a prediction based on two previous steady states x_i and x_{i-1} using a small step in the parameter δs,

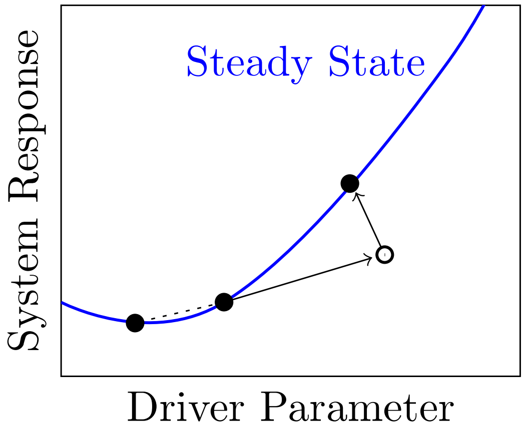

Figure 1 Path Following Framework. Using previously obtained steady states (black) a prediction can be made for the steady state at a new parameter value (white). Coupling this with a standard root-finding algorithm enables this prediction to be iteratively improved upon until it converges to the unknown steady state path (blue). This method can be used to efficiently 'follow' the steady state of a system under the variation of a driver parameter.

Equation 1

$$x_{i+1} = x_i + \frac{x_i - x_{i-1}}{\sqrt{{x_i}^2 - {x_{i-1}}^2}}\delta s.$$

Here $\sqrt{{x_i}^2 - {x_{i-1}}^2}$ is the Euclidean distance between x_i and x_{i-1}. The initial two points can be obtained from simulation then all successive points can be obtained from correcting steady state predictions. For a small step parameter δs, predictions are sufficiently close to converge within a few iterations of the root-finding algorithm and is thus much more efficient than computing the steady state for x_{i+1} directly. Furthermore, this method can follow both stable and unstable paths, which may not be possible with simulation of the micro level model. The presence of any unstable states is essential in understanding transient dynamics and any regime shifts that occur in the system. This framework can be coupled with other standard algorithms for detecting bifurcations, such as tipping points or the emergence or disappearance of steady states. Understanding how a system responds to changes in a driver parameter can improve our knowledge of its behavior and can aid decision-making.

2.2 Equation-free analysis

Section 2.1 outlines the benefits and methodology for the use of path following and bifurcation analysis for non-linear systems. Although well established in their use, their application is limited to deterministic systems where the macro level equations are known. The development of equation-free (EF) analysis Theodoropoulos et al. (2000) has side stepped these limitations. By replacing the macro level equation, $F(x,\theta)$, with an ensemble of appropriately initialized micro level models, the requirement of an explicit equation has been avoided, hence the name equation-free.

On the macro level, a separation of time scales between variables causes a bottleneck where the fast, high order, variables are bound by the slow, low order, ones. This allows the macro behavior to be characterized by a few low order variables (Kevrekidis and Samaey 2009). Often this is much less than the number of dimensions in the micro level model and reduces the system to its core dependencies. Typically EF methods involved three steps, *Lifting*, *Evolving*, and *Restricting* illustrated in Figure 2.

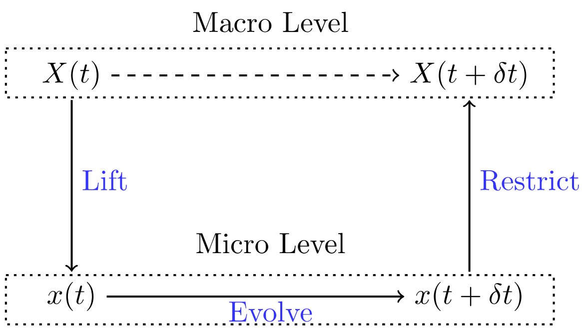

Figure 2 The Equation-free framework. The macro state $X(t)$ is Lifted to the micro level $x(t)$ which is simulated forward in time for some small time window δt (Evolve). Typically an ensemble of independent micro models is used and the macro state at $X(t+\delta t)$ is then estimated from the distribution of microstates at $x(t+\delta t)$ (Restrict). This framework bypasses the need for equations to govern how the system varies from$X(t)$ to $X(t+\delta t)$ explicitly.

The Lifting step is where the state of the macro system is *Lifted* to the micro level models. Lifting requires that all parameters, variables, and any dependencies between them are initialized in accordance with the macro state as in Figure 2. The Lift step is problem dependent as it requires the model to be initialized to a specific state equivalent to $F(x,\theta)$ in Section 2.1. The Evolve step is simply running the micro level simulations forward in time for some small time window. In general this time window is significantly shorter than running the simulation from an arbitrary initialization, in (Thomas et al. 2016) authors required less than 1% of the simulation time for in the Evolve step compared to direct simulation in some cases. This highlights the computational efficiency of this method, in addition to the analytical benefits that are not possible with direct simulation. Generally, an ensemble of independent micro models is used to account for variability in the outcomes through stochasticity in the system or varying initial conditions. The Restrict step estimates the macro state from the distribution of the ensemble of micro models, i.e. the state of the ensemble of micro states is restricted to the core dependencies on the macro level. The separation of time scales (fast high orders and slow low orders) means that the macro state can be characterized by a slow manifold of the low orders and the high orders can be ignored. Therefore the micro state (also with high and low order variables) can be 'Restricted' to only the low orders to described the macro state - i.e. we can use the low order to make an approximation of the state and ignore the high order terms. Likewise we can 'Lift' the fewer orders (only low) of the macro state to the micro state. It is possible that some systems may have the same number of orders in both the micro and macro levels (i.e. all low orders characterizing the slow manifold), but there will never be more on the macro level than the micro level. The choice of macro variable(s) is problem specific, however the mean of the ensemble results can be used in some cases (Thomas et al. 2016). The Lift, Evolve and Restrict operators replace $F(x,\theta)$ in Section 2.1 and enable path following by varying x until we have $F(x,\theta,t=t+dt)-F(x,\theta,t=t\,)\leq \epsilon$, where ϵ is some small level of tolerance due to the stochasticity in the system.

EF analysis has provided significant insight into the macro level behavior of systems where only a micro level simulation, such as agents, rules or a probabilistic model, exists. Analysis with EF methods has been applied to problems in a diverse areas including; stochastic systems (Barkely et al. 2006); bio-chemical and engineering systems (Kevrekidis and Samaey 2009); civil violence (Zou et al. 2012); model validation (Tsoumanis et al. 2012); biological system (Erban et al. 2006); traffic flows (Marschler et al. 2014); infections and disease (Gross and Kevrekidis 2008); social networks

(Tsoumanis et al. 2010) and consumer lock-in (Avitabile et al. 2014). This type of analysis is completely generic and has even been applied to physical experiments where input parameters are much more constrained than in computational studies (Sieber 2008).

With EF analysis it is now possible to perform system level tasks where the macro behavior is unavailable explicitly (Kevrekidis et al. 2003). As such we can now perform statistical, equilibrium, tipping point, regime shift and dynamical analysis directly to microscopic models to extract insight into the macro dynamics. One significant barrier for this type of analysis is the lack of a general tool for application to problems. To date applications are implemented specifically for the problems under investigation. Recently, an open-source algorithm has been developed that can apply EF analysis to any external simulator (Thomas et al. 2016). In their paper, the authors apply their EF tool to a number of agent-based models to demonstrate its ability to extract insight from models without knowledge of the underlying dynamics or internal workings.

3 CASE STUDY: SHALLOW LAKE RESTORATION

Alternative stable states in a shallow lake are characterized by either clear or turbid water driven by the concentration of nutrients in the lake. The main anthropogenic drivers are nutrient flows from overabundant fertilizers in agriculture, insufficient, municipal sewage treatment, but also insufficient private sewage treatment. Shallow lakes can be restored towards a clear state by effectively reducing the inflow of nutrients (Jeppesen et al. 2005), however, in many cases the nutrient reduction is insufficient (Søndergaard et al. 2007). While there is plenty of ecological and technical knowledge available, we address the gap of integrating human-lake interactions that may slow down or reinforce restoration processes.

3.1 Model description

We use a coupled social-ecological simulation model that links the system dynamics in a lake to the social system consisting of a regulating municipality and individual house owners (Figure 3, Martin & Schlüter 2015). The lake system is a reimplementation of a minimal model of differential equations by Scheffer (1989) that allow regime shifts between the clear and turbid state driven by the nutrient concentration. The clear state is characterized by a low nutrient level with few planctivorous fish (bream) and abundant piscivorous fish (pike). This relation switches to the opposite in the turbid state.

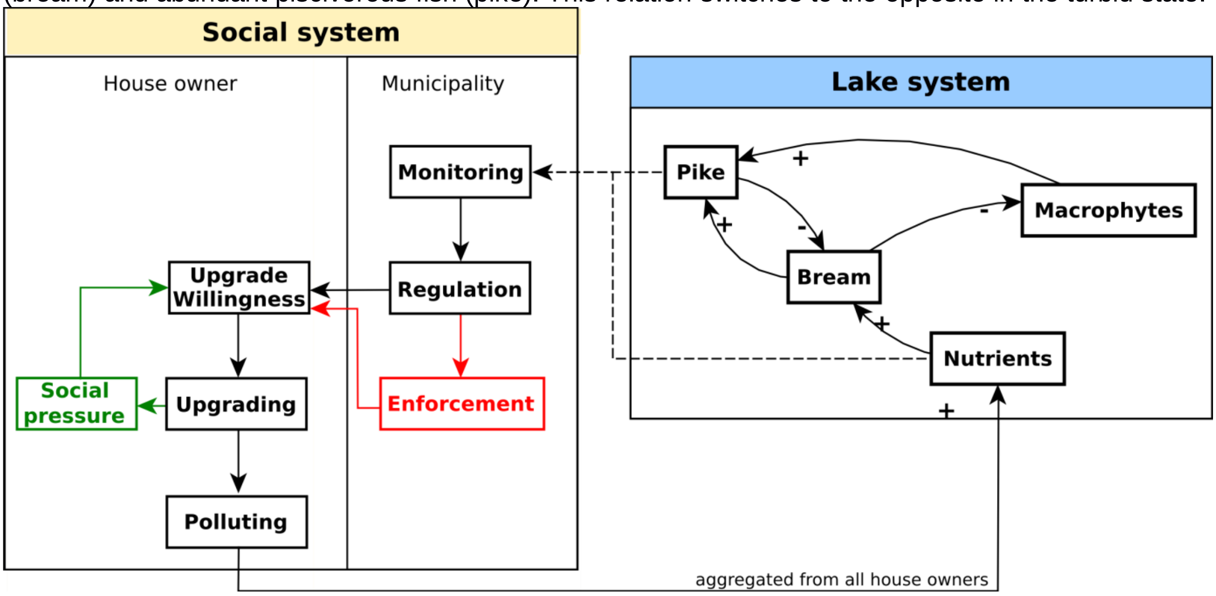

Figure 3 Coupled social-ecological model with three alternative social mechanisms to reduce nutrient outflow from private sewage: social pressure or central enforcement. Boxes in the lake system denote stocks (Scheffer 1989) and boxes in the social system describe processes carried out by the 'house owner' agents or the 'municipality' respectively.

For the social system, we assume that nutrient levels increase through insufficient private sewage systems. This may cause harmful algae blooms and pike levels drop while bream become abundant. So together, the nutrient and the pike level serve as suitable indicators for the municipality to decide on thresholds that, in case they are crossed, require a response. Beyond monitoring, the municipality is responsible for legislation and informing private house owners on requirements for upgrading their on-site sewage systems. House owners are then in a high-cost and low-benefit situation (Wallin et al. 2013), so their general willingness to upgrade (wtu) is assumed to be low. We implemented two scenarios to improve their willingness to upgrade the sewage system, namely through 'social pressure' and 'central enforcement', to eventually reduce the nutrient flow into the lake. Simulations run with annual time steps for the social system and daily steps for the ecological system in NetLogo.

3.2 Simulation experiments

First, we start with no social-ecological feedback and use the equation-free analysis to extract the macro level dynamics of the isolated lake system. This not only provides verification of the model implementation, but also provides a based line from which we can assess the impact of house owners and scenarios. Without any social influences (nutrients = constant) the equation-free method determines, and follows, the steady states in the levels of bream, pike and vegetation as the level of the initial nutrient concentration is varied. The so-called *lifting operator* here is simply defined as initializing the level of each of the populations as there are no other variables in the isolated lake system. The work-flow for the equation-free analysis of the lake model is as follows: for a given level of initial nutrients, perform the *lift operation* to initialize the population levels for *N* independent microscopic models (the ABM) at time $t = t_0$, perform the *evolve operation* and run each simulation for some small time window $t = t_w$, estimate the macro state at time $t = t_w$by performing the *restrict step*. In this specific case, it is sufficient to take the mean of the *N* independent ABM simulations at $t = t_w$. Note, this mean is calculated using the bootstrap method (Efron and Tibshirani 1993) so it does not require any assumptions of normality across the *N* simulation outcomes.

For the second experiment, we look at the coupled social-ecological system and address the question which of the two social scenarios is more effective in restoring the lake to the clear state. Now the initial nutrient concentration is at the level of a turbid lake and it is reduced to an intermediated level depending on how fast house owners respond. The two scenarios are evaluated at three different values of the willingness-to-upgrade with the equation-free analysis to determine whether the social responses are sufficient to reach the clear state.

4 RESULTS

4.1 Bifurcation analysis from ABM simulations

Combining the in section 3.2 described process with a root finding algorithm enables the computation of steady states in the system. That is, we evaluate if the macro state at $t = t_0$ is (approximately – due to noise) the same as the macro state at $t = t_w$. Once a steady state has been obtained, for a small perturbation to the driver parameter, here initial nutrient level, we use the predictor discussed in section 2.2 to efficiently 'follow' how the steady state changes with this driver. This enables efficient computation of the steady states and additionally enables the analysis of unstable states. Obtaining the steady states using equation-free analysis required a simulation time (t_w) of a few 10's of ticks due to the predictor-corrector procedures. In contrast, running a single ABM simulation directly requires a few 1000's ticks to converge to a steady state. Clearly if one is running a large number of independent simulations to alleviative noise, or analyzing a large parameter range, equation-free analysis will be significantly faster than performing batch simulations.

The location and response of an unstable state to a driver parameter is vitally important to understand the dynamics of the system. Unstable states indicate a separation between the basins of attraction of the stable states and can provide insight into how likely a transition is to occur in a particular regime. In Figure 4 the unstable state in the pike population (center) shows the turbid state (lower red line) has a much larger proportion of the parameter space compared to the clear state (upper red line). This indicates that the clear state is much more sensitive to changes from noise or external influence, than the turbid state.

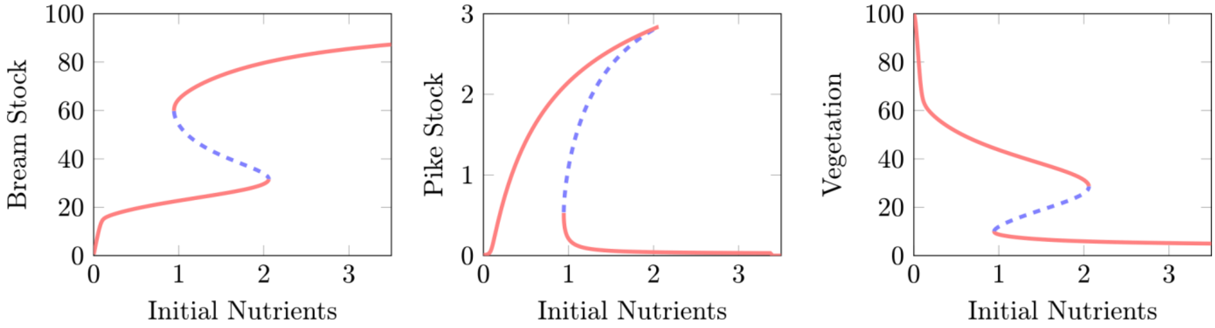

Figure 4 Bifurcation diagrams for three lake state variables. Here stable states are given as solid red lines and unstable states are dashed blue lines.

By looking at the distance between the stable and unstable states, in both the clear and turbid regimes, it is possible to assess the resilience of a state towards a transition to the other state through a 'shock' rather than via crossing the tipping point. We normalize these distances to the maximum population level over the nutrient ranges in Figure 4 and show how the separation between the stable and unstable state varies for each regime in the bi-stable region (where two stable states can occur at the same nutrient value).

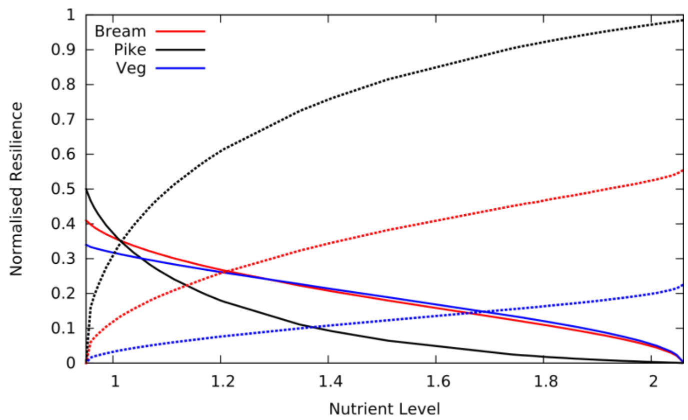

Figure 5 Resilience, here in terms of a normalized distance to the alternative state, for each population from Figure 4. The clear state's resilience is given by solid lines and the turbid state's resilience is given by dashed lines.

In Figure 5, we observe that the pike population is the least resilient in the clear state, i.e. the pike population is much more sensitive to change in the clear state than the other populations. Moreover, this sensitivity (lack of resilience) increases as it approaches the tipping point. The bream and vegetation stocks have approximately the same sensitivity in the clear state, and although pike is initially more resilient, it quickly decays to a low level of resilience. What is also striking is the extremely high resilience of the pike population in the turbid state. This indicates that in a clear state the population of pike is very sensitive to changes through external influence and is easily pushed to the turbid state without going over the tipping point. Furthermore, once in the turbid state, the population of pike becomes extremely resilient to changes. This means it will require an enormous influence to move the system back to the clear state, i.e. restoration. It is worth highlighting that as the system of bream, pike and vegetation is coupled, if one population transitions to another state (i.e. crosses the blue line in Figure 4), then it causes the other two populations – and therefore the whole system – to transition into the other state.

4.2 Social processes and agents driving macroscopic behavior

Coupling social responses to the isolated lake dynamics opens a new perspective to analyze state transitions independent of whether they are accidentally or intendedly driven by actors. Integrating solely the house owners influence by increasing the nutrient inflow to the lake will always lead to a turbid state. But, using strategies such as central enforcement or social pressure to motivate sewage system upgrades helps to restore the lake, or prevent it from transition to the turbid state after the tipping point was crossed. Prior to any upgrades, the level of nutrients in the lake will increase and the lake will move to the turbid state – assuming it begins in a clear state. At some stage it becomes impossible to restore the lake (the point of no return) as the level of nutrients is too high and the lake momentum of transition is already too strong. Therefore as long as the house owners upgrade before this point then the lake can be restored. Due to the probabilistic nature of upgrades, the time taken to upgrade varies across simulations. Using equation-free analysis, we assess the effects of the willingness to upgrade (wtu) and the emerging ability to restore the lake to the clear state.

From Figure 6 we see that all scenarios are well described by a sigmoid function showing a reduction of the percentage of lake restorations with increasing levels of initial nutrients. The more to the right a curve lies, the higher are the tolerated nutrient levels from which a restoration back to the clear state is possible and the more time house owners have before implementing the upgrade. As the willingness to upgrade is increased, the lake can be restored from a higher initial nutrient level. This may not be surprising as higher wtu values shorten the time frame for all house owners to upgrade and enable a sufficient, accumulative nutrient reduction before the point of no return.

For a low wtu value, we see little difference between the social pressure and central enforcement scenarios with a slight advantage from the enforced scenario. However, as wtu is increased the order of the two curves switches and social pressure enables restoration at higher nutrient values. Moreover, the steepness of the central enforcement curves are approximately the same, whereas they vary in the social pressure case when comparing wtu=0.2 and wtu=0.3. This indicates a decreasing sensitivity of restoration success towards the nutrient level at higher wtu values, hence social responsiveness on the individual level can to some degree compensate for time lags in communal regulation.

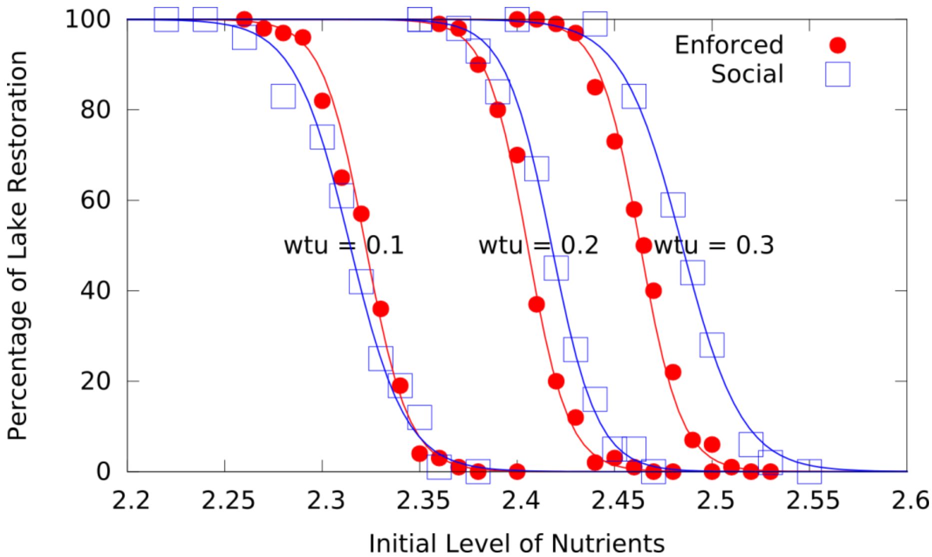

Figure 6 Restoration of the lake under different values for the willingness to upgrade (wtu) and social strategies. The y-axis shows what percentage of ABM simulations are converging to the clear state (restored) under the wtu and nutrient level for the social or enforced scenarios. Note 0 indicates a turbid end state in all simulations.

5 DISCUSSION

5.1 Lessons learned

In this paper, we have demonstrated how equation-free analysis can be used to provide insight into the behavior of complex ABMs. We show how this technique can extract bifurcation curves from ABMs without requiring an equation to describe them. Beyond insight, this can also be used for model validation and implementation verification by comparison to observations in the real-world or previous studies. We stress that the results of equation-free analysis are based on the model they are applied to – if there is a problem in the results it indicates that there is a problem in the model or its implementation. We therefore suggest this method as a means of analysis alongside the model development to ensure that it is behaving as one expects or observes in the real world. We also analyze the bifurcation diagram of the isolated lake system as a means to determine the resilience of the clear and turbid states to external influences or system 'shock'. These results clearly show that in our example case of shallow lakes, the predatory fish population is the least resilient in the clear state but also the most resilient in the turbid state. This implies that lake degradation, from clear to turbid, is achieved through small external influences far from the tipping point, whereas lake restoration, from turbid to clear, requires larger efforts even near the lipping point.

Adding a social interaction, we examine the dependence of lake restoration on the willingness to upgrade (wtu) and two reinforcement scenarios in the model. These results illustrate that with high wtu values, social pressure to upgrade is more effective than central enforcement by the municipality. Our results also indicate that social pressure is increasingly more effective in enforcing upgrades as wtu increases, though more experimentation is required to verify this. The percentage of restored lakes as a function of initial nutrient level is well described by a sigmoid curve in all cases. In this model, as with many ABMs, equation-free analysis provides access to tools such as bifurcation analysis that can provide insight in to the behavior of a model. Moreover, as we have seen in this work, probabilistic rule based models can have a response or dependence that can be captured mathematically.

5.2 Ways forward to analyze complex ABM's

As we mentioned in section 5.1, we suggest that equation-free analysis can be used in parallel to model development as a means of verification and validation. This has the potential to save the ABM programmer a lot of time by spotting errors early in the code development. Moreover, equation-free analysis can be used in a number of ABMs to understand the behavior, identify drivers, provide baseline comparisons for different scenarios, or provide insight in some other way. The algorithm used in this work can be applied to generic ABM as was developed by Thomas et al. (2016) and details of its open-source release are given in their paper. Currently a user interface for the equation-free program is under development to make it easy to use by non-experts. Although applicable to any ABM is possible in principle, in practice there are some limitations. Firstly some kind of steady state behavior needs to be observable in some dimension, such as a stable state or oscillation. Models with qualitative outcomes are not suitable for this analysis in general, though specific cases may be feasible. Second, the definition of the lifting operator is non-trivial and may be difficult to obtain for complex model. Many efforts in the equation free community are attempting to develop an automated method for determining this operation. The use of equation-free methods to analyze ABMs is in its infancy and requires much more investigation. By demonstrating its use, alongside Thomas et al. (2016) open-source program with model repository, we hope to incorporate this technique as a standard ABM analysis tool.

5.3 Conclusion

Slow processes such as human-driven eutrophication in shallow lakes, if remain unmanaged, have the unintended consequence of a regime shift that makes it difficult or even impossible to turn the ecosystem to its original favorable state (Biggs et al. 2009). Here, we presented for the first time, how human responses to regime shifts can be modeled explicitly in an agent-based model and analyzed the macroscopic behavior therefrom using the equation-free analysis. It proved to be useful for systems with clearly defined response variables exhibiting stable states and enables to link micro level processes and agent traits to macro level outcomes.

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