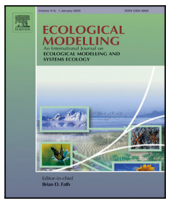
Ecological Modelling 501 (2025) 110956

Contents lists available at ScienceDirect

Ecological Modelling

journal homepage: www.elsevier.com/locate/ecolmodel



Machine learning emulators of dynamical systems for understanding ecosystem behaviour

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ARTICLE INFO

Dataset link: https://github.com/oriol-pomarol/hillslope_project

Keywords:
Artificial neural networks
Eco-geomorphology
Complex system dynamics
Minimal modelling
Emulators

ABSTRACT

Minimal models (MM) aim to capture the simplified behaviour of complex systems to facilitate system-level analyses that would be unfeasible with more sophisticated numerical models. However, the choices involved in minimal model development heavily rely on expert knowledge, a source of bias that can interfere with good modelling practices. In this paper, a new method is proposed in which a machine learning (ML) model is trained with transient data generated by a detailed physically-based numerical model, predicting the rate of change of the target state variables given their current value and additional drivers. The trained model is then used to mimic the analysis made with traditional minimal models. This approach (ML-MM) is deployed in a semiarid hillslope ecosystem characterising its soil and vegetation components. The ML-MM outputs share most of the general features with previous expert-based results but show a better ability of the hillslope to (1) recover its vegetation, (2) resist total disappearance of the soil and (3) reach substantially higher soil depths in steady state. Furthermore, a new intermediate stable equilibrium is found between the already known healthy and degraded ones, revealing a more complex pattern of ecosystem collapse that avoids a critical shift, as supported by numerical model simulations. The transient behaviour is also investigated, from which we conclude that the system can exhibit strong reactivity, that is, an initial deviation away from equilibrium after a perturbation. In conclusion, the present study demonstrates the potential of ML-MM to obtain new scientific insights on complex systems that might be missed by expert-based alternatives. Hence, minimal models may benefit greatly from incorporating detailed numerical models and data-driven simplification in their development process. Ultimately, this methodology could be applicable to many fields of study and even be expanded to observational data, enhancing our understanding of real-world complex system dynamics.

1. Introduction

Mathematical theoretical models are commonly used in ecology to explain the behaviour of natural phenomena. Following the definition by Onstad (1988), such models explicitly express the assumptions in a theory or set of hypotheses to mathematically describe a natural system, in a way that is applicable to a large number of cases. In particular, numerical or simulation models make use of complex differential equation models that are computationally solved for predicting the evolution of natural systems from its most fundamental components. Onstad (1988) claimed that, even at his time, the increase in computational power had facilitated the development of increasingly complex models, limited in their system descriptions only by knowledge availability. Given their use of the best information available, Logan (1994) defended the use of "big ugly" models for improving scientific understanding. However, such models have been criticised for being "hard to develop, hard to communicate and hard to understand" (Nes and Scheffer, 2005), as supported by other authors (Grimm, 1994; Scheffer and Beets, 1994). Grimm (1999) even identified in his review of individual-based modelling in ecology that the use of bottom-up approaches does not suffice to answer relevant questions at a system level.

Conversely, a top-down approach can be followed where the main processes are parsimoniously described at a macroscopic level (Batterman and Rice, 2014). This type of models, which we refer to as minimal models, are typically used to characterise specific aspects of complex systems by using a small set of ordinary differential equations and parameters that explain their general behaviour. They can operate under multiple names such as simple models (Bader et al., 2008; Doherty and

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https://doi.org/10.1016/j.ecolmodel.2024.110956
Received 24 September 2024; Received in revised form 1 November 2024; Accepted 19 November 2024
Available online 3 December 2024

Christensen, 2011), conceptual models (Grimm, 1994), demonstration models (Evans et al., 2013), or reduced models (Jiang et al., 2018). There are many examples of minimal models in a broad range of both social and natural scientific domains. For instance, in economics Grüne-Yanoff (2009) supported the use of minimal models as a way to judge one's confidence in given hypotheses. In environmental sciences, Quinn et al. (2017) used them as a tool to inform policy making. In ecology, the use of minimal models has been particularly popular, a classic example being the Lotka–Volterra predator–prey models (Volterra, 1926), which are still used as a starting point for studying population dynamics, such as in Naik et al. (2023). Minimal models have an ongoing relevance within the broader ecology field, with many examples of recent publications (Marsland et al., 2020; Tyutyunov and Titova, 2021; Díaz-Sierra et al., 2024). Because of the simplicity of minimal models, they require significantly lower computational costs than their numerical counterparts, enabling powerful mathematical analysis. For example, bifurcation analyses (Kooi, 2003; Troost et al., 2007; Mohd, 2019; Naik et al., 2023) study the asymptotic behaviour of the system when one or more parameters are varied, which can help in discovering tipping points (Jiang et al., 2018; Quinn et al., 2017; Scheffer et al., 2009). Minimal models can also assist in characterising the often more important transient behaviour (Hastings, 2004). For instance, these models can help to find and characterise a system's reactive behaviour (Mari et al., 2017; Yang et al., 2023), an initial change away from the final equilibrium of one or more state variables after a perturbation. These analyses provide a more complete picture of the dynamics of complex systems that enhances our fundamental understanding of them.

Despite their usefulness, minimal models have also been questioned, as they can easily become disconnected from reality. Hall (1988) found a poor fit between several such models and observational data, recommending against their use. One of the reasons is the arbitrariness of the choices made by modellers when deciding which aspects of the system dynamics should be ignored or greatly simplified (Evans et al., 2013), which are often driven by habits rather than empirical evidence (Babel et al., 2019). Among others, this may cause the model to disproportionately concentrate on one of multiple factors that can potentially explain a phenomenon (Nes and Scheffer, 2005; Scheffer and Beets, 1994). These limitations indicate that minimal models often suffer from insufficient consideration of assumptions, which is one of the main deficits in good modelling practice highlighted by Jakeman et al. (2024). Thus, an approach that combines the detailed system representation of large numerical models with the explanatory power and computational speed of minimal models, overcoming the selection bias introduced by expert-based simplification, would be highly desirable. There have been some attempts to reconcile both minimal and numerical models by using them in concert, starting from a complex model and deriving simplified versions of it (Nes and Scheffer, 2005; Doherty and Christensen, 2011). Nevertheless, in Nes and Scheffer (2005) the simplification process is still mostly reliant on expert knowledge, and in Doherty and Christensen (2011) it consists only in a coarsening of the spatial grid and re-calibration, the latter being computationally expensive. Recently, machine learning (ML) has emerged as an attractive tool for obtaining emulator models, also referred to as surrogate models, that can reduce the computational complexity of expensive numerical models in scientific and engineering domains (Alizadeh et al., 2020). For example, ML is being used to accelerate the evaluation of large environmental models (Lu and Ricciuto, 2019) or replace time-consuming parameterisations (Krasnopolsky and Fox-Rabinovitz, 2006). Emulators can also be used to model system dynamics; for instance, Deshmukh and Allison (2017) proposed the use of surrogate models to predict the state derivatives of dynamical systems for mechanical design optimisation, similar to the dynamical emulation modelling concept introduced by Castelletti et al. (2012). ML has even been used for performing bifurcation analysis of dynamic systems (Beregi et al., 2023; Galaris et al., 2022; Hassona et al., 2021). In ecology in particular, there have been attempts to use ML to predict the existence of tipping points, providing an early warning signal for their occurrence (Bury et al., 2023; Deb et al., 2022). However, no studies were found that use ML emulators with the purpose of performing a full scientific analysis of complex ecological system dynamics with the aim of obtaining new scientific insights, as currently done with minimal models.

In this paper, a novel approach is presented where ML is used to derive an emulator of a complex numerical model, taking the role of a minimal model. Because the model simplification process is automated by the learning capacity of an ML algorithm, the computational efficiency in relation to the fit to the original model's outcome (given the available inputs) can be optimised. We hypothesise that such model could therefore portray more complex and realistic system-level behaviour compared to expert-based alternatives, while enabling complex analysis of its dynamics that is unavailable with numerical models. Our research aims are defined by the following questions: (1) can we generate a ML emulator from a detailed numerical model of a geo-ecological system that is able to reproduce its dynamics, and (2) can such model provide novel scientific knowledge about the system, not captured by an equivalent expert-based minimal model.

To illustrate the usefulness of this approach, we investigate the soil and vegetation response in a semi-arid hillslope ecosystem as a case study. A ML minimal model (ML-MM) based on the numerical model described in Karssenberg et al. (2017) is deployed and used to examine the ecosystem dynamics, characterising its multiple equilibrium states and understanding its transients. The results are compared to the expert-based minimal model defined in that paper, showing that we can learn new scientific knowledge that was previously obscured. In particular, the ML-MM displays a more complex transition from healthy into a collapsed system state that can avoid previously assumed tipping points via a multistability of coexisting states (Rietkerk et al., 2021). The presented approach can have wide applicability in other fields where multiple equilibrium states exist in complex systems, or to study their transient behaviour, and could potentially be deployed on observational data.

2. Methods

Our approach for the deployment and use of ML minimal models consists of four steps (Fig. 1). First, a numerical model is needed that describes the system of interest with the highest level of detail available. Such models capture the system behaviour through a time-transfer function, which describes the change in the state variables as a function of their current status, external drivers and additional parameters. Second, the numerical model is used to generate transient simulations, from which a subset of state variables and parameters of interest is stored. These simulations should cover the feature space of the variables of interest as thoroughly as possible. If the model is spatially explicit, the outputs should be spatially aggregated across the entire grid to ensure that the relationship between the variables can be studied at system level. Furthermore, if the interest lies in longer timescale processes, the data may be temporally averaged into longer time steps to reduce computational costs. Third, an ML model is trained on the processed data, taking the subset of state variables and drivers as input features and the simulated rate of change of the state variables as response variables. In this way, the ML model learns the equivalent of the time-transfer function for a particular variable subset at system level. Finally, the response of the ML model is analysed across the input feature domain to study its dynamical properties. More advanced techniques such as bifurcation analysis can also be performed to better understand the behaviour of the system.

In this paper, the previously described methodology is employed to study a semi-arid hillslope ecosystem, specifically its soil and vegetation interactions, as a proof of concept. The interest of this type of ecosystem lies in the critical shift that can occur when it is forced from a healthy into a degraded state by an external variable, such as

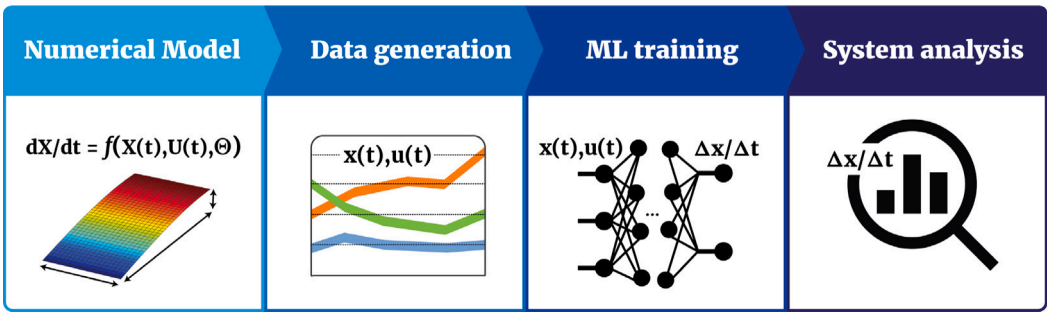

Fig. 1. Schematic showing the steps involved in ML minimal model implementation. $X(t)$, $U(t)$ and Θ represent the state variables described by the numerical model, its drivers and parameters respectively, while $x(t)$ and $u(t)$ are the corresponding spatially aggregated subset.

grazing pressure, after exceeding a tipping point (Rietkerk and van de Koppel, 1997). To assist in the correct management of such ecosystems, it is crucial to correctly model their dynamical properties. For that purpose, Karssenberg et al. (2017) introduced an expert-based minimal model, validated by comparing its predicted behaviour with that of a more complex, spatially explicit numerical model. This minimal model displayed a healthy state at low grazing pressure, for which there is sufficient rainfall to sustain the vegetation cover and sufficient soil. At high grazing pressures, the system collapses towards a degraded state with null soil depth and vegetation after undergoing a critical shift. However, it is not clear that the numerical model supports that claim, so in this study we take a step further and propose an ML minimal model (ML-MM) directly trained on the numerical model data. In the following subsections, the specific application of the four steps mentioned above is described for this case study.

As a prior step to the full implementation, the expert-based minimal model (Appendix A) was used as a data generating source to guide the design of the presented methodology. This allowed to speed up the tuning process significantly and enable a system-level comparison for the ML outcomes. The strategy that resulted in the best ML performance was chosen and assumed to be valid for the data generated with the numerical model as well, given the similarity of the task.

2.1. Numerical model

The spatially explicit numerical model thoroughly describes the hydrological, vegetation and geomorphological processes on a semi-arid hillslope. The model is not driven for a specific location, but rather generally describes this type of ecosystem, for which plant growth is considered to be constrained only by water availability, assuming sufficient nutrients are present in the soil. The hillslope is modelled using a 2-m spaced grid measuring 80 × 40 m, with the field equations being solved at each grid point. The model takes extensive formulations and parameters from previous literature, so here we only provide a high-level description of the modelled processes; for detailed specifications refer to Appendix A in Karssenberg et al. (2017).

The hydrology in this model is driven by stochastic rainstorm events that are introduced following a gamma distribution. Precipitation can be intercepted by the canopy or reach the soil, where it can either infiltrate or produce surface runoff. A simple soil water storage is considered that is updated by the infiltration and evapotranspiration processes. The vegetation subsystem is modelled by its biomass, which can expand through spatial diffusion that is mainly limited by water availability. On the other hand, surface runoff and grazing reduce the amount of biomass. The soil subsystem is characterised by soil depth, which increases by bedrock weathering. The soil material is redistributed by soil creep and overland flow erosion, transfer and deposition. In the model, vegetation growth together with rainfall associated processes (e.g., runoff and erosion) are simulated weekly. Soil formation and soil creep are much slower processes and are therefore updated annually to speed up computation.

Table 1
Range of values for each of the input variables to which they can be shifted.

Variable	Range
Biomass (B)	$[0, 3]$ kg/m^2
Soil depth (D)	$[0, 0.6]$ m
Grazing pressure (g)	$[0, 3]$ kg/m^2/yr

In particular, we are interested in the vegetation and soil evolution and how they are affected by the grazing pressure, replicating the analysis by Karssenberg et al. (2017) as a starting point. Hence, only biomass and soil depth state variables are stored to disk, and the grazing pressure is and fed to the system as an external driver. The remaining model parameters were left at their default values.

2.2. Data generation

The training and validation data were generated with the spatially explicit numerical model and consisted of two hundred 10 000-yr transient simulations runs. The grazing pressure was set to a constant value across all grid points, and was given an empirically-found probability of 0.002 every half year to switch to a random value drawn from a uniform distribution within the range described in Table 1. The resulting data was aggregated to a half yearly time step by computing the median to speed up ML training and simulation times while ensuring sufficient detail in the outputs. Finally, the time series of the spatially averaged biomass, soil depth and grazing pressure were stored to be used as training data for the ML-MM.

Because simply changing the grazing pressure would not be sufficient for the transient simulations to explore all the regions in the biomass and soil depth space, a probability for the spatial average of these variables to suddenly shift to another value every half year was introduced as well. Table 1 contains the ranges to which the state variables values could jump to. The spatial pattern was preserved during those shifts, adding or subtracting the corresponding difference to each pixel and capping negative values at zero. In this occasion the chance was empirically set to 2%, which results in simulations that can explore multiple starting system states for each value of the grazing pressure (Fig. 2). For lower probabilities, the simulations could not explore all of the input space, biasing the response in those regions. However, it was to remain as small as possible in order to produce longer transients that result in realistic spatial patterns and allow to sample closer to the area around the system equilibria, crucial for characterising system dynamics.

2.3. ML training

The processed simulations were fed to the ML model, each time being treated as a separate data point. The biomass, soil depth and grazing pressure for a specific time step were given as inputs, and the rates of change of the biomass and soil depth between that time step

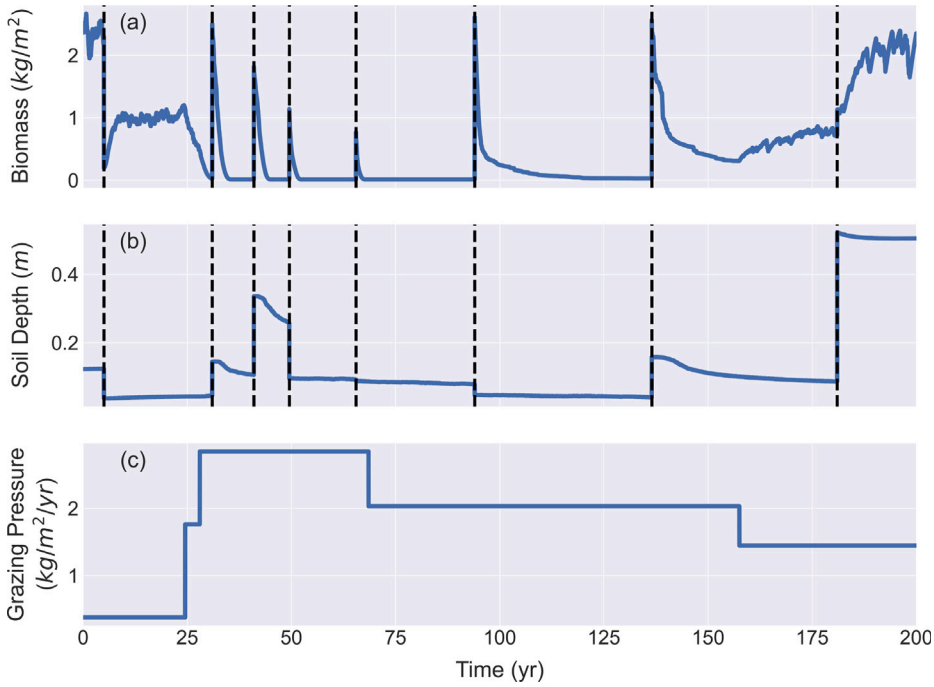

Fig. 2. First 200 yr of a numerical model simulation from the training data, showing the spatial average of the (a) biomass, (b) soil depth and (c) grazing pressure. The stochastic shifts in the state variables are represented by a vertical dashed line.

and the next as outputs. By doing this, the ML model aims to capture the equivalent of the time transfer function in numerical modelling, which explains the change in the system given its previous state and additional drivers or forcing parameters. This function is defined in Eq. (1) for the ML-MM,

$$\left(\frac{B(t+1)-B(t)}{\Delta t}, \frac{D(t+1)-D(t)}{\Delta t}\right) = \mathbf{ML}\left(B(t), D(t), g(t)\right) + \mathbf{e} \quad (1)$$

where B and D and g represent the biomass, soil depth, and grazing pressure respectively, t a specific simulation time step, **ML** the two-output machine learning model and **e** the prediction error that it tries to minimise.

Two of the most popular machine learning algorithms (Pichler and Hartig, 2023) were tested, random forest (Breiman, 2001) and fully-connected artificial neural network (Rumelhart et al., 1986). Although the former achieved satisfactory results, especially at emulating forward simulation, it produced rough or noisy response surfaces that are arguably less realistic. This perceived noise further affects the calculation of the predicted output's derivatives, necessary for some analyses. For these reasons, the neural network architecture was ultimately chosen, implemented in Python using version 2.4 of the Keras library (Chollet et al., 2015). Several network hyperparameters were tuned, namely the number of layers and units, activation functions, number of epochs and learning rates. Furthermore, L1 regularisation was introduced to the weights to reduce the effect of spurious correlations. The final values for these hyperparameter are presented in the Results section; the remaining ones were left at their default values.

Of all the generated simulations, 70% were selected at random and assigned for training, resulting in a total of 27 436 806 training points after removing the state variable shifts. 10% of the simulations were used for hyperparameter tuning and the remaining 20% as a test set for independent validation, corresponding to 3 919 932 and 7 839 210 data points respectively. Because an exhaustive search of ML model structure and hyperparameters was computationally unfeasible, they were iteratively adjusted based on empirical results. The model was qualitatively evaluated by visual inspection of the outputs at a key grazing pressure values (as in Fig. 4) and by comparing the ML predictions to the numerical data in the test set, both visually (see Fig. 3) and by computing the R^2 value between the two using version 1.2.0 of the scikit-learn library (Pedregosa et al., 2011).

2.4. System analysis

Once the ML-MM has been trained, one can study its response to get a better idea of the system dynamics. Similar to the numerical model, there is the option to run it forward in time by iteratively calling the ML model. However, because the number of state variables considered by the ML model is reduced to only two, a similar approach to Karssenberg et al. (2017) can be followed where the rates of change of the biomass and soil depth are represented as surfaces in the state (or feature) space at a fixed grazing pressure, enabling a quick overview of each variable's dynamics. More interestingly, one can find the nullclines, system states for which the rate of change is zero that represent the asymptotic state of the represented variable if the other one was kept constant. These nullclines are often found analytically (Rietkerk and van de Koppel, 1997; Karssenberg et al., 2017, e.g.,), but can also be found with numerical methods by finding regions in which the rate of change is zero with arbitrary precision. For this study, a fine square grid of 4800 × 4800 was defined in the feature space, limited by the values given in Table 1 except for an increased soil depth maximum of 0.8 m. The nullcline condition was obtained by comparing the absolute value of the rate of change with an empirically-determined threshold, 10^{-3} kg/m^2/yr and 10^{-6}/yr m for the biomass and soil depth respectively. This same procedure can be repeated with the expert-based minimal model enabling a direct comparison.

To study the behaviour of the system as a whole, the two variable's rates of change must be combined. In particular, for obtaining the asymptotic states of the system, the overlap of the nullclines for both a biomass and soil depth nullcline must be retrieved. Such points can correspond to stable or unstable equilibria, which was determined by the sign of the gradient for each of the variables' rate of change with respect to that same variable. A bifurcation analysis was then performed, by which the equilibrium points of the system were obtained for the full range of grazing pressure values in Table 1. Furthermore, to study the transient behaviour, both rates of change were simultaneously used to visualise the direction of the system in the feature space using

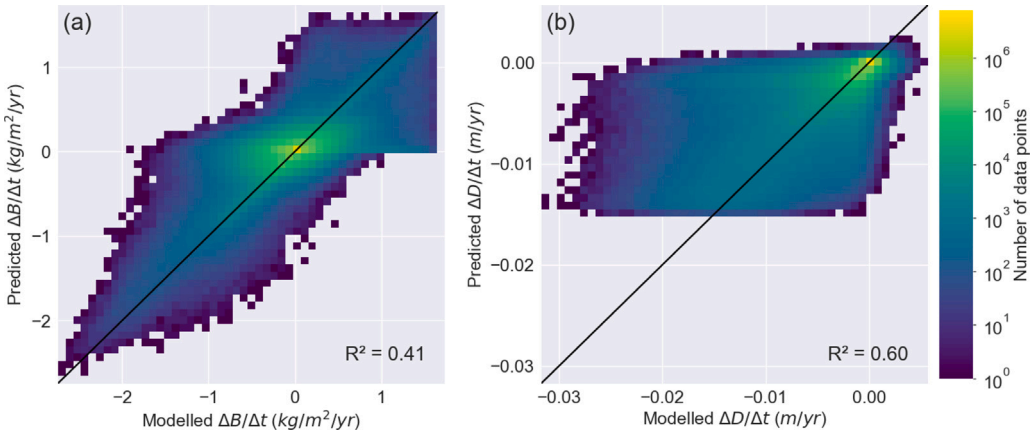

Fig. 3. Predicted compared to modelled rates of change for the testing data of (a) biomass and (b) soil depth. The colour scale represents the number of data points in logarithmic scale, binned into a 50 × 50 grid. The 1:1 line (in black) implies a perfect model fit.

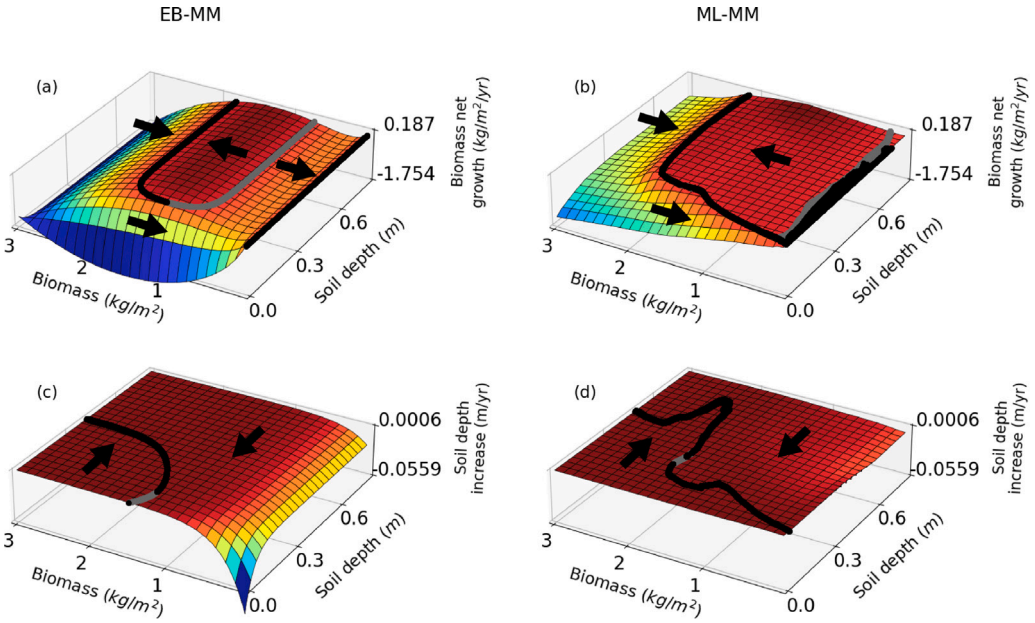

Fig. 4. Predicted rate of change values of the expert-based minimal model for (a) biomass and (c) soil depth, and of the ML minimal model for the same variables, (b) and (d) respectively. The stable nullclines are represented by black dots and the unstable ones by grey ones. The arrows indicate the direction of change in the system if keeping the complementary variable constant. The responses have been plotted for a grazing pressure value of 1.76 kg/m^2/yr.

the streamplot function in Matplotlib (Hunter, 2007). Finally, specific forward simulation runs were performed with the numerical model to explore if some of the system characteristics found using the ML minimal model could be traced back to its parent model.

3. Results

3.1. Model-generated data

For the training data, the grazing pressure followed a uniform distribution within the range described in Table 1, as expected from the generation process. Because the soil depth and biomass are updated by the model every time step, it resulted in more complex distributions that nonetheless remained roughly bounded to the ranges from that table. For the soil depth, the lower part of its spectrum was slightly over-represented, lowering the median to 0.26 m. The biomass showed an even more complex behaviour; a large portion of its values concentrated close to zero, and the rest followed a bimodal distribution with peaks at roughly 1.25 and 2.4 kg/m^2. The rates of change of both variables had a large number of values near zero that rapidly decreased with the variables absolute value. For the soil depth, the rates of change were considerably small and negatively skewed, bound between $-1.74 \cdot 10^{-2}$ and $3.35 \cdot 10^{-3}$ m/yr, and for the biomass they were higher and less skewed, reaching a similar order of magnitude to that of the variable's range, from -1.46 to 0.83 kg/m^2/yr. Full summary statistics for the generated data as well as their correlation matrix are provided in Appendix B.

3.2. Model tuning and evaluation

The hyperparameter tuning preformed with the expert-based minimal model generated data resulted in a deep artificial neural network with seven hidden fully-connected layers that features an increasing number of units (9, 27, 81, 162, 324, 648 and 1296) between the input and output layers of sizes 3 and 2 respectively. The ReLU activation function was ultimately chosen, and the learning rate was set to 10^{-5} as it produced a smoother training. The training was stopped at 200 epochs, after which the model did not improve significantly. Finally, the regularisation strength was set to 10^{-5}. The training time for the ML model was 20.97 h on a cluster computer using one CPU core from an

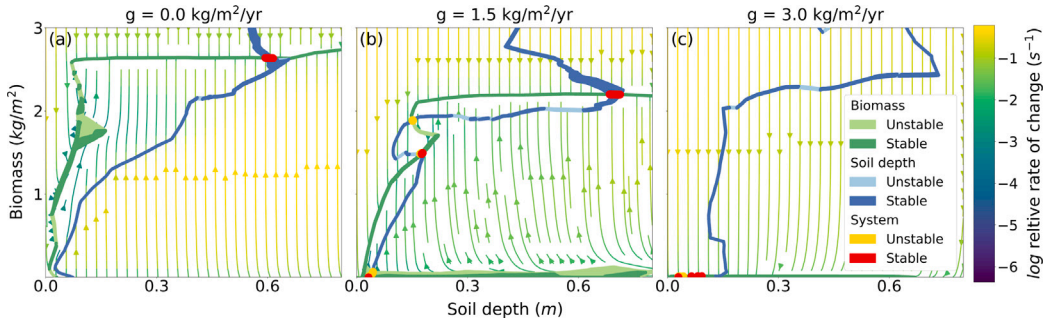

Fig. 5. Streamplot of the system response for three different values of grazing pressure. The arrows point at the direction of the system's change in the biomass and soil depth space, and the colour represents the base-10 logarithm of the change's magnitude. The points at which the rate of change for the biomass and soil depth are zero are represented in green and blue respectively, using the corresponding light version for unstable states. The points at which both coincide are represented in red if both are stable, indicating a full system equilibrium, and in yellow otherwise.

AMD EPYC 7451 24-Core Processor and a GTX 1080 Ti graphics card. With the optimised hyperparameters, the ML model achieved extremely high accuracy and precision for the full range of simulated values in the expert-based data, as evidenced by its coefficients of determination (R^2) of 0.99996 and 0.999996 for the biomass and soil depth rates of change respectively.

Ultimately, the credence in the ML-based surrogates is heavily constrained by how well they can reproduce the behaviour of the original model, in our case the numerical model. To evaluate the model's predictive performance, Fig. 3 plots the predictions of the ML minimal model (ML-MM) against the numerical simulated values used as ground truth for the independent validation data. There is a clear correlation between the outputs of both models, as demonstrated by R^2 values of 0.41 and 0.60 for the biomass and soil depth rates of change respectively. This indicates the suitability of ML-MM for representing the numerical model, despite some limitations. In particular, the spread of measurements around the diagonal is rather wide, indicating a lack of precision that could be attributed to the stochastic nature of the numerical model. On top of that, there is bias for some predicted variable values, as ML tends to smooth out the output distribution, predicting more values closer to zero. This may also cause an underestimation of high rate of change values for both biomass and soil depth. Lastly, ML-MM fails to predict any large negative rates of change for the soil depth, as they are caused by stochastic storm events in the numerical model.

3.3. Comparison of system dynamics

To compare the dynamics of the expert-based and ML-based minimal models, Fig. 4 shows the rates of change in the biomass and soil depth space for a fixed grazing pressure of 1.76 kg/m^2/yr. The result is a 3D surface representing each of the outputs, in which the nullclines (i.e., regions in which the rate of change is zero) have been highlighted in black if stable and grey if unstable. This helps to visualise the system dynamics as described by both models. In general terms, similar features can be observed in both models. For instance, for high values of biomass or low values of soil depth, $\Delta B/\Delta t$ is negative in both models, meaning that the hillslope will decrease its biomass as the soil cannot sustain it. However, for medium levels of biomass and moderate to high soil depths, the models present positive $\Delta B/\Delta t$ values indicating that the vegetation will recover back to the nullcline-defined amount, where they would remain stable if the soil depth was fixed. A similar analysis can be performed on the $\Delta D/\Delta t$ plot, where the system change is on the soil depth axis instead. There, positive values are found mainly at high biomass and low soil depth, as the former mitigates soil erosion enabling it to increase, and the rest of the domain displays negative values.

Despite the similarities, three main characteristics appear in ML-MM that significantly differ from those of the expert-based minimal model. First, for low (but not zero) values of biomass, the latter predicts a collapse of the biomass as represented by negative values in $\Delta B/\Delta t$, but ML-MM predicts positive values instead, indicating a full recovery. Second, in the vicinity of the coordinate origin, $\Delta D/\Delta t$ remains positive for ML-MM but is highly negative in the expert-based model. Lastly, it is worth noting that the $\Delta D/\Delta t$ nullcline reaches much higher values of soil depth in ML-MM. While the exact positioning of such nullcline is difficult to capture in this region, as it is mostly flat, this can have important consequences in the predicted location of the full system equilibria.

3.4. Stability analysis of ML-MM

In the previous sub-section, the system dynamics have been studied only at a single grazing pressure value and considering the two system components separately for comparison purposes. To provide a full stability analysis of the ML-MM model, the 2D system dynamics are illustrated in Fig. 5 with the help of streamplots, which show the direction and magnitude of change of the system in the biomass and soil depth space. Three grazing pressures are shown that are representative for the three different phases observed in Fig. 6, which presents the values of the biomass and soil depth at the equilibrium points for the whole range of trained grazing pressures.

For low values of grazing pressure, exemplified in Fig. 5 with a value of $g = 0$ kg/m^2/yr, the system tends to a healthy equilibrium at roughly $B = 2.5$ kg/m^2 and $D = 0.6$ m for any initial state. This phase is characterised by a fast recovery of its biomass, then the soil slowly adjusts until equilibrium is reached. When the system starts at low soil depths, a collapse of the biomass may occur at first, followed by a slow recovery along the biomass nullcline. This type of reactive behaviour can also be found in the expert-based minimal model but with a smaller magnitude and only for a more limited range of soil depths. Even in the event that soil depth and biomass are initially zero, the soil can increase through bedrock weathering, enabling biomass to also grow in it, slowly heading to full recovery.

For intermediate values of grazing pressure, represented by $g = 1.5$ kg/m^2/yr, the healthy equilibrium occurs at a gradually lower biomass values as the grazing pressure increases (Fig. 6), until a tipping point at $g = 2$ kg/m^2/yr is reached causing this equilibrium to disappear. For starting soil depths larger than approximately $D = 0.2$ m, the system is able to return to the healthy equilibrium. However, for low values of biomass we see that the soil depth can also display reactive behaviour, as it is initially reduced away from equilibrium but recovers after the biomass has been restored. Another visible equilibrium point is the collapsed or degraded state, at null biomass and residual soil depths. Only extremely low values of soil depth lead to this state during this phase. In the close vicinity of such equilibrium, there is an unstable equilibrium are. Surprisingly, another separate stable equilibrium appears at $B = 1.5$ kg/m^2 and $D = 0.2$ m, its biomass value decreasing with the grazing pressure. This new equilibrium acts as a

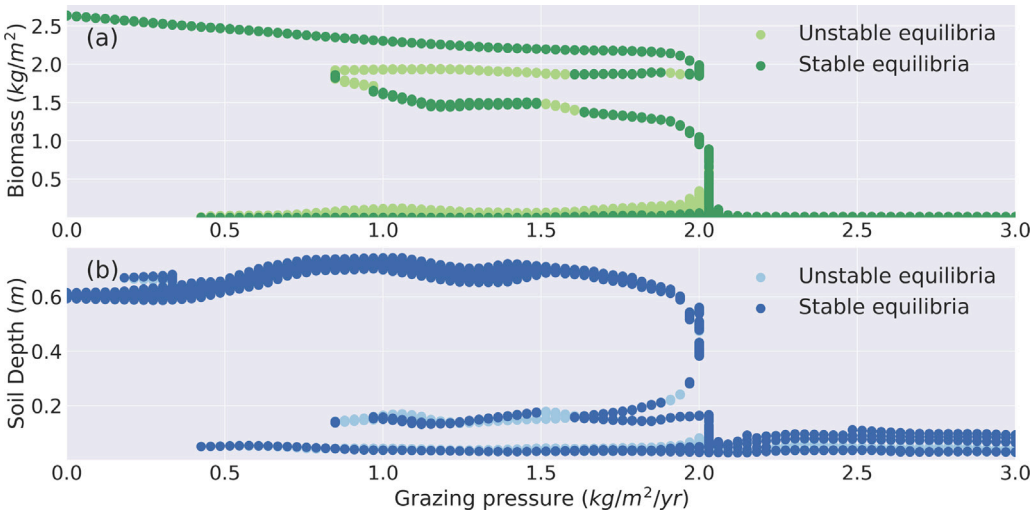

Fig. 6. Representation of (a) biomass and (b) soil depth system equilibrium values as a function of the grazing pressure.

buffer between the healthy and degraded ones, which attracts systems at lower soil depth and biomass. An unstable equilibrium is located between this and the healthy equilibrium. It should be mentioned that the stability of these new equilibria is sometimes changing, which indicates some instability in the ML predictions.

Finally, the third phase for higher grazing pressures features again a single stable point, the degraded state, due to the collapse of the biomass nullcline that is now only a line at null value. All starting points end up in this degraded state after a fast collapse of the biomass, followed by a slower soil depth stabilisation. Surprisingly, the equilibrium soil depths can reach slightly higher values compared to the same state in the previous phase, possibly as a result of systems starting at higher soil depths not being fully depleted when collapsing, in contrast with collapsed states that remain stable at smaller soil depths for lower grazing pressures.

From Fig. 6 it becomes apparent that system follows a hysteresis cycle, as the healthy and degraded states can coexist for some grazing pressure values. This implies that the system takes different paths when moving from low to high grazing pressures compared to the opposite; in the first case the collapse occurs at about $g = 2.0$ kg/m^2, but in the second case a full recovery does not take place until $g = 0.5$ kg/m^2. In terms of duration, the hillslope collapse unfolds much faster than its recovery, since soil restoration is a much slower process than its depletion. This behaviour can become even more complex if stochasticity is introduced. In that case, the system might make an early transition, which would temporarily lead to an intermediate state before making the full shift.

The appearance of intermediate equilibrium points between healthy and degraded equilibria can also be observed in numerical model simulations, as illustrated in Fig. 7. This is one of the realisations of the simulation that was carried out for the purpose of finding evidence of such intermediate equilibria in the numerical model, which were generated with a linear increase of grazing pressure until the expected tipping point is reached, then kept constant for the remaining time steps. The example realisation shows an initial healthy state (HS), before the grazing pressure tipping point is reached, showing high values of biomass and soil depth. Next, a pseudo-stable state (PS) occurs to which the system transitions after having reached the tipping point, for which both variables take intermediate values. This stage can consist of multiple shifts with varied intensity, and its duration cannot be exactly defined. Finally, the system reaches a stable equilibrium in the transitioned state (TS), for which the state variables reach even lower values for the rest of the simulation.

In Fig. 8 the spatial pattern of biomass and soil depth for the numerical model are presented for three representative points of the three phases described in the previous step. For the first point (HS), representing the healthy state, the spatial pattern is relatively homogeneous with high values of biomass and soil depth at all points of the spatial grid. In the second (PS), it can be observed that the top part of the hillslope has collapsed through the creation of rills in the soil depth that cannot sustain the biomass in that area. Finally, for the third point (TS), the biomass can only exist in the lower half of the hillslope, and the soil depth has also mostly collapsed in a similar way, although a stable layer of soil depth appears at the top of the hillslope due to the creep process that tends to produce a concave shape in the hillslope.

For other realisations of this simulation for the same grazing pressure pattern, a similar behaviour was observed; the system remained in one or more pseudo-stable states after partial collapses of the biomass and soil depth which often also featured slow biomass degradation, eventually reaching a similar final state similar to the transitioned state in Fig. 7. These sharp transitions between stable or pseudo-stable states were found to occur after a heavy rainfall event, which produces significant overland flow that causes an abrupt depletion of a large portion of the biomass. This effect is especially strong in the top part of the hillslope. In the next time step, the vegetation can only recover in the less-damaged bottom part, which causes the soil depth to collapse shortly after for the areas where the vegetation has perished. Ultimately, a stable degraded state with null biomass is reached in the top part of the hillslope, but a healthy equilibrium is still maintained in its lower part, reaching an overall intermediate state. The values of biomass and soil depth in the transitioned state coincide reasonably well with the intermediate equilibrium predicted with our stability analysis for a grazing pressure of $g \approx 1.9$ kg/m^2/yr (Fig. 6).

4. Discussion

In this paper, a novel approach is presented for analysing the behaviour of complex systems. The method consists in training a machine learning emulator on transient simulations generated by a complex numerical model. This emulator acts as a minimal model, from which system dynamics can be studied. This technique is applied to explore a semiarid hillslope soil-vegetation system, comparing the resulting ML minimal model (ML-MM) with an equivalent expert-based minimal model. To enable an analysis of the system's behaviour, the rates of change must be determined for any given combination of system state variable values. Machine learning is able to sufficiently reproduce this relationship for the hillslope ecosystem, as demonstrated by the high accuracy of the ML-MM on the spatially and temporally averaged transient simulation data generated with a complex numerical model. An artificial neural network was considered more suitable than a random

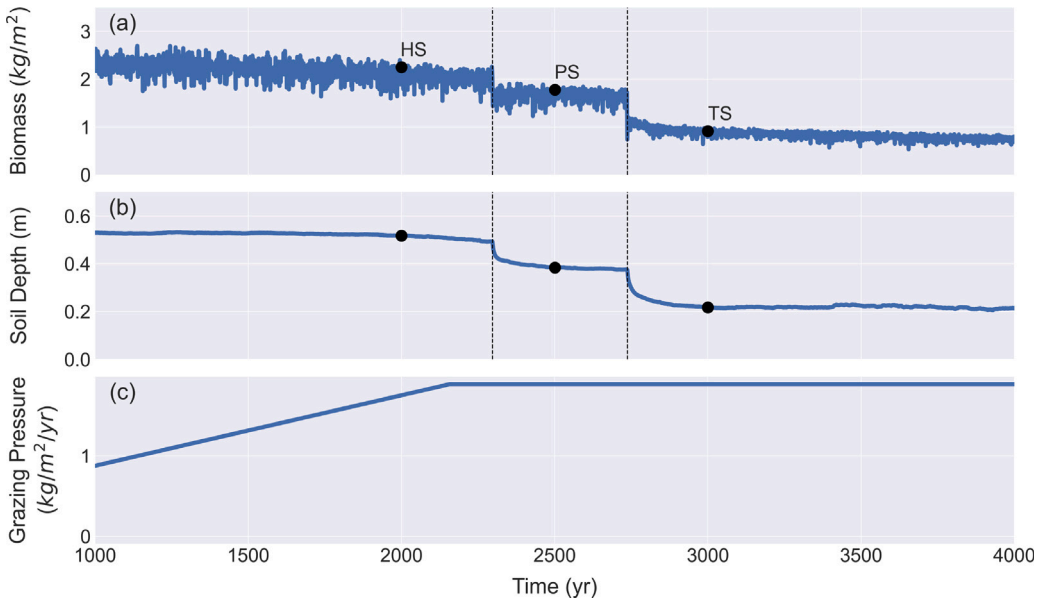

Fig. 7. Results of the simulation that aimed at finding intermediate equilibrium states, showing the spatial average of (a) biomass, (b) soil depth and (c) grazing pressure. Three representative points of the healthy state (HS), pseudo-stable state (PS) and transitioned state (TS) are highlighted, the black vertical lines indicating the boundaries for these regions.

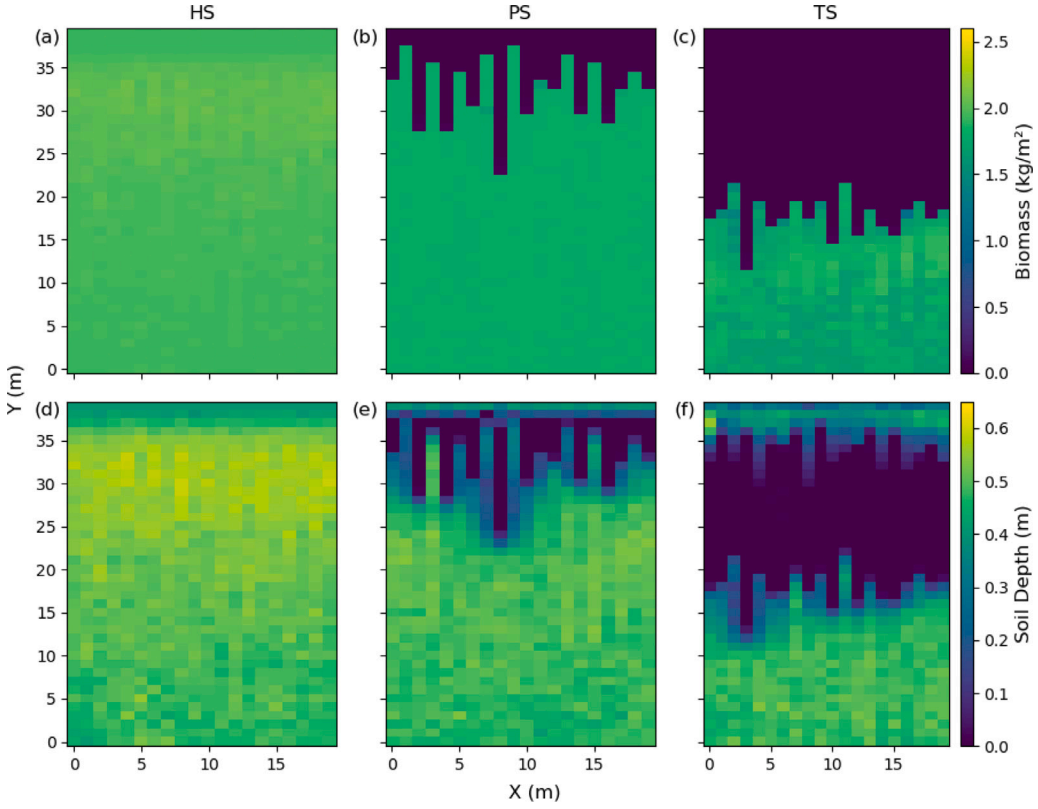

Fig. 8. Spatial pattern of the biomass simulated with the numerical model for (a) healthy state, (b) pseudo-stable state and (c) transitioned state, and same for the soil depth in (d), (e) and (f) respectively. X and Y refer to the spatial coordinates of the hillslope other than its height.

forest alternative for this task due to the continuity in its output and improved performance, the latter corroborated by many examples in similar fields (e.g., Angione et al., 2022).

The response of the ML-MM shares most of the general features with the expert-based one but differs in some key aspects. For instance, it shows a tendency of the hillslope to recover its vegetation in low biomass but high soil conditions, in contrast to the collapse predicted by the expert-based minimal model. It also displays a positive (but low) soil depth equilibrium at low biomass, preventing the system from total collapse, which can recover back to a healthy equilibrium as opposed to the expert-based degraded state which remains stable at null soil depth and biomass even in the absence of grazing pressure. Finally, the ML-MM predicts significantly higher asymptotic soil depths for the healthy state. These examples provide valuable insights at certain

characteristics of the hillslope ecosystem that the expert-based minimal model is clearly misrepresenting.

Further analysis of the dynamical properties of the ML-MM unveils additional patterns, highlighting the efficacy of this type of model in facilitating a better understanding of complex systems. An analysis of asymptotic behaviour was performed for a range of grazing pressure values, concluding that the system follows a hysteresis cycle between a healthy and a degraded state. This implies that the system follows a different path during its recovery compared to its collapse, the former taking place in much longer periods of time due to the slower nature of soil formation. Burg et al. (2015) already demonstrated the appearance of hysteresis even for a minimal soil-vegetation model, and Karssenberg et al. (2017) showed it for the numerical model used in our study, giving more confidence in the ML-MM output. Interestingly, a new intermediate equilibrium between the healthy and degraded ones is found for moderate values of grazing pressure that was not characterised by the expert-based minimal model. Similar behaviour can be observed in the numerical model simulations, demonstrating that the hillslope ecosystem can follow different routes, staying in transitional states for large periods of time before decaying from healthy to degraded equilibrium. A closer look at the spatial pattern shows that in this staged collapse certain regions are already in a degraded state while others remain healthy, coinciding well with the multistability of coexistence states described in Rietkerk et al. (2002), by which complex systems can avoid tipping points.

To study the transient behaviour of the ML-MM, the response of the ML-MM is examined at specific grazing pressures, which enables a study of the full evolution of the system for any given initial state. An interesting aspect of transient characterisation is the reactivity of the system, an initial change away from its final equilibrium when a perturbation is introduced. This behaviour is strongly manifested in the ML-MM for low initial values of soil depth and grazing pressure but high biomass. In that scenario, there is an initial collapse of the biomass that eventually recovers to a healthy state after a lengthy process constrained by soil formation. Although the expert-based minimal model predicts some reactivity, the magnitude and spectrum of initial conditions it covers are much larger in the ML model. Moreover, the soil depth is also found to show reactive behaviour, which was overlooked by the expert-based model.

Limitations, potential uses and implications

Because the purpose of this paper is mainly to present the ML-MM approach, many aspects of its practical application in this specific case study could be improved. For example, exploring a larger number of ML architectures and hyperparameters could likely lead to a better fit between the ML and numerical model outputs. This would in turn reduce the variability in the ML-captured equilibrium lines, reducing the uncertainty of the positioning of the equilibrium points, crucial for ecosystem management. Furthermore, while the process described to generate the training data with the numerical model allows the creation of sufficiently accurate ML responses, it is by no means optimised in terms of computational efficiency. Given that the purpose of an emulator model is to speed up computation, the sampling process in the data generation phase would need to be largely optimised for practical purposes. For example, instead of generating transient simulations, the space of system states could be explored with a more efficient sampling technique, reducing both the time spent in data generation and ML model training. However, the success of the transient simulation as a training dataset suggests the potential for deriving minimal model directly from observed data, so long as it is diverse and comprehensive enough for the ML model to properly capture the behaviour of the system. Illustratively, Lapeyrolerie and Boettiger (2023) showed that ML models trained on ecological data that did not showcase a critical transition failed to predict its correct behaviour, but succeeded when it included as few as one realisation of such transition. Finally, although the use of the expert-based minimal model for accelerating our tuning process and ensure qualitative similarities between the outputs may generally not be available, similarly good results are expected if performing only a quantitative analysis on the numerical model data.

Additionally, there are some limitations inherent to the ML-MM by design. For example, this method only captures the mean behaviour of the system without considering its stochastic nature. Therefore, its predicted system evolution may deviate substantially from specific realisations of the original numerical model. Moreover, the ML-MM is purposely simplified to the minimum number of state variables and drivers that are necessary for one particular study, as to enable the analysis performed in this paper. This means, for example, that it does not explicitly take into account any climatic or weather variables for the hillslope ecosystem. Their effects, however, have an impact on the generated data and therefore in the ML-MM predictions. So, should the climate or weather patterns change, a re-training with the new data would be necessary. The same is true for all variables not considered in the model simplification process. Adding other system variables is possible, but would likely require more data generation, slowing down the model training, and would produce more convoluted output visualisations.

Nevertheless, the presented examples point to the usefulness of ML-MM to identify interesting qualitative features of ecological systems that cannot be explored with numerical models due to their computational cost and their spatial and stochastic nature. So, even if ML-MM may not capture all system features perfectly, or may even find spurious patterns from the data, it still offers promising directions for studying the original numerical model and by extension the ecological system. Furthermore, the ML-MM approach has the potential to easily adapt to any inputs and outputs, and to any spatial and temporal resolutions, making it especially useful for environmental management (Schuwirth et al., 2019). ML-based surrogates have already been proven suitable for landscape management with very positive results (Nguyen et al., 2019). Given the increasing need for studying catastrophic shifts of increasingly complex systems in ecology (Kéfi et al., 2022), the methodology presented here gives a promising approach to automatically create minimal models that incorporate detailed process knowledge, providing more confidence in their outputs. Furthermore, there are potentially many more ways in which new scientific insights could be extracted from ML models in fields such as ecology, for example as described in Yu et al. (2021).

More generally, these findings suggest that expert-based minimal model may fail to sufficiently capture the complexity of the system, questioning the usual modelling practices for this type of models. Their use is attractive as they provide analytical formulas and ease of analysis, but they may not properly capture prominent features of the system dynamics. We sustain that well designed minimal models have the potential to yield valuable information, but the objectivity in their formulation process should be enhanced. In the ML-MM, this is achieved by initially considering all system knowledge available and the simplification process being performed by a data-driven model, reducing the risk of introducing bias. In fact, ML-MM has the potential to achieve the best possible fit with the numerical modelled (or observed) data, which can also be quantified by evaluating its performance. Interpretation still needs to be done carefully and should preferably be supported by detailed numerical simulations. Even if not used in direct application, for example because there may be concerns about its lack of a causal structure, it could still be used as a tool to inform mechanistic minimal model development. This directly addresses important challenges in good modelling practice, such as points 1.5, 1.7 and 13 in Jakeman et al. (2024). Namely, it prevents the leakage of preconceived ideas about the system under study from influencing minimal model formulation, it can help guide the level of detail necessary for optimal system description, and it promotes a more objective model development cycle. Further development of ML-MM may even allow for uncertainty estimation, for example by following the approach in Lapeyrolerie and Boettiger (2023).

5. Conclusion

In this paper, we present ML-MM, a new tool for studying the behaviour of complex systems. A machine learning model is trained on spatially-aggregated data from a detailed numerical model, predicting the change in the target system variables given their current state and specified drivers. Its system-level description and computational speed enable a mathematical analysis of system dynamics that would be impossible with the numerical model, but because it is trained to reproduce the outputs of the detailed numerical model it can provide better system description than over-simplistic expert-based alternatives. The approach is applied to a semiarid hillslope ecosystem, obtaining new insights on its dynamical properties that were not captured by an alternative expert-based approach. Most notably, the reactivity of the system is much higher than previously described, and a new intermediate stable equilibrium is discovered between the known healthy and degraded one that supports the idea that this type of system can evade tipping points through certain spatial patterns. Ultimately, this type of analysis could be implemented in many systems in ecology (e.g., predator–prey systems, lakes) but also in different fields such as economics, climate science or social hydrology to improve our knowledge of complex system's behaviour. Lastly, this study emphasises that more effort should be put into making the development of minimal models more objective, to ensure all relevant system features are sufficiently captured.

CRediT authorship contribution statement

Oriol Pomarol Moya: Writing – original draft, Visualization, Validation, Software, Methodology, Formal analysis. **Siamak Mehrkanoon:** Writing – review & editing, Supervision, Methodology. **Madlene Nussbaum:** Writing – review & editing, Supervision, Methodology. **Walter W. Immerzeel:** Writing – review & editing, Supervision, Methodology. **Derek Karssenberg:** Writing – review & editing, Supervision, Methodology, Funding acquisition, Conceptualization.

Declaration of Generative AI and AI-assisted technologies in the writing process

During the preparation of this work the authors used ChatGPT in order to suggest text reformulations and enhancements, with the aim of improving the language quality. After using this tool/service, the authors reviewed and edited the content as needed and takes full responsibility for the content of the publication.

Declaration of competing interest

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

Acknowledgements

This project was funded by both the Faculty of Geosciences, Utrecht University, The Netherlands as well as the Department of Physical Geography, Utrecht University, The Netherlands. Appreciation is extended to the reviewers of this paper for their constructive feedback and helpful suggestions during the review process.

Table B.2
Summary statistics for the biomass, soil depth and grazing pressure for the test data.

	B (kg/m^2)	D (m)	g (kg/m^2/yr)
Mean	1.25	0.28	1.51
Std	0.97	0.15	0.87
Min	0.01	0.00	0.00
25%	0.02	0.15	0.76
50%	1.28	0.26	1.52
75%	2.23	0.39	2.26
Max	3.21	0.64	3.00

Appendix A. Expert-based minimal model

The expert-based minimal model developed by Karssenberg et al. (2017) consists of two coupled ordinary differential equations for the biomass and soil depth in a semi-arid hillslope (Eqs. (A.1), (A.2)), derived by expert knowledge. In general, parameters were extracted from the literature, but some were stepwise adjusted to replicate some of the numerical model's behaviour.

$$\frac{dB}{dt} = \begin{cases} [1-(1-i)e^{-D/d}]\left[rB(1-B/c)\right] - g\left(\frac{B}{s+B}\right) & \text{for } B \geq 0 \\ 0 & \text{for } B = 0 \end{cases} \quad \text{(A.1)}$$

$$\frac{dD}{dt} = \begin{cases} W_0 e^{-aD} - e^{-B/b}\left[E_t + e^{-D/k}(E_0 - E_t)\right] - C & \text{for } D \geq 0 \\ 0 & \text{for } D = 0 \end{cases} \quad \text{(A.2)}$$

The biomass (B) rate of change includes two main terms concerning vegetation growth dynamics. The first term evaluates the effects of soil depth and biomass on growth rate, featuring $r = 2.1\,\mathrm{yr}^{-1}$ for the growth rate and $c = 2.9\,\mathrm{kg\,m}^{-2}$ for the carrying capacity. The growth rate reduction at shallower soil depths is considered by the $i = 20.7$ parameter, with $d = 0.04\,\mathrm{m}$ controlling the soil depth range. The second term applies the Michaelis equation (Noy-Meir, 1975) to model the effect of grazing g, employing a parameter $s = 0.4\,\mathrm{kg\,m}^{-2}$.

For the soil depth (D), three main terms are outlined. The first relates to soil formation due to bedrock weathering, modelled exponentially with coefficient $W_0 = 5 \cdot 10^{-4}\,\mathrm{m\,yr}^{-1}$ and decay rate $a = 4.0\,\mathrm{m}^{-1}$. The second considers water erosion, described by $E_t = 0.021\,\mathrm{m\,yr}^{-1}$ and $E_0 = 0.084\,\mathrm{m\,yr}^{-1}$, the erosion rates at null biomass and soil depth respectively. The parameters $k = 0.05\,\mathrm{m}^{-1}$ and $b = 0.28\,\mathrm{m}^2\,\mathrm{kg}^{-1}$ adjust the erosion rate according to soil depth and biomass respectively, to account for rainfall interception and runoff reduction due to increased infiltration. Lastly, soil loss due to creep is kept constant $C = 1 \cdot 10^{-4}\,\mathrm{m\,yr}^{-1}$.

Despite a valid justification of its formulation, the simplification process of this minimal model might not be sufficient to explain the complex dynamics of the semi-arid grazing system. For instance, when using it for generating transient simulations, once the system has fully collapsed it can never recover, even at zero grazing pressure, which is not the case for the numerical model. Furthermore, the evasion of the tipping points described in Rietkerk et al. (2021) is completely missed. Therefore, a ML minimal model approach might be more suitable.

Appendix B. Statistical summary of the data

This appendix contains the statistical summary of the data generated with the numerical model and aggregated spatially and temporally for the ML-MM training, as well as its outputs. For simplicity, only the results for the test data are provided, as they are nearly identical to the training data. In Tables B.2 and B.3, the data is described giving most common statistical metrics for the input and output variables of the ML-MM respectively. The predictions made by the ML-MM model are also included in Table B.3 for comparison. The number of samples in the test data is 7 839 210.

In Fig. B.9, the correlation matrix of the test data for all the input and output variables generated with the numerical model used for the

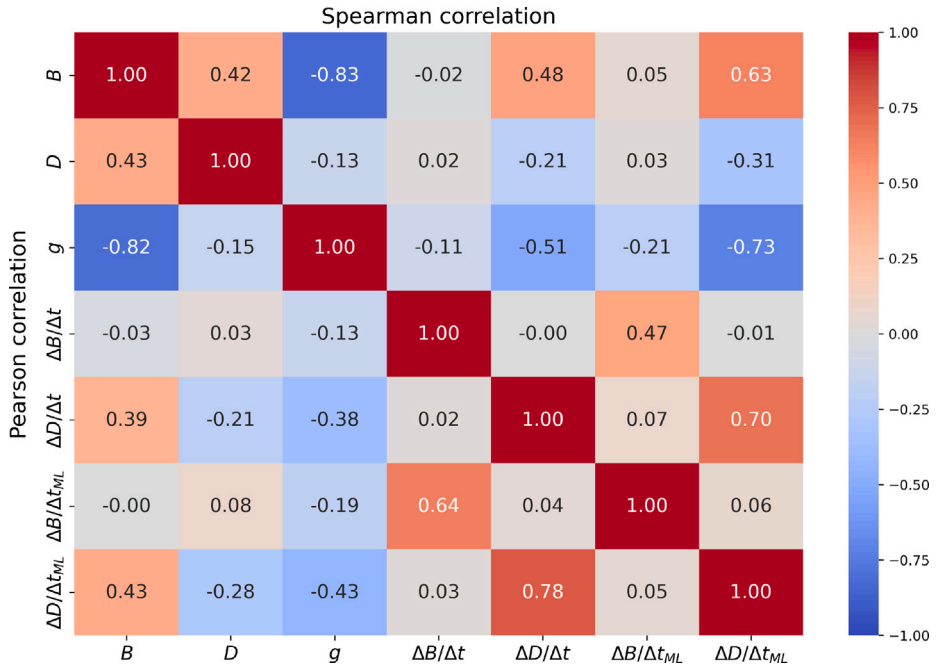

Fig. B.9. Correlation matrix of the test data for the pre-processed biomass (B), soil depth (D), grazing pressure (g) and the rates of change for the first two as predicted by the numerical model, as well as the ones predicted by the ML model. Below the diagonal, the Pearson correlation is given; above it, the Spearman correlation. The cells are coloured according to the correlation values to highlight their differences.

Table B.3
Summary statistics for the rates of change for the biomass and soil depth as generated with the numerical model (ground truth) or as predicted by the ML model for the test data.

	$\Delta B/\Delta t$ (kg/m^2/yr)	$\Delta D/\Delta t$ (m/yr)	$\Delta B/\Delta t_{ML}$ (kg/m^2/yr)	$\Delta D/\Delta t_{ML}$ (m/yr)
Mean	$-3.47\cdot10^{-3}$	$-4.54\cdot10^{-4}$	$2.53\cdot10^{-3}$	$-3.66\cdot10^{-4}$
Std	$1.12\cdot10^{-1}$	$1.25\cdot10^{-3}$	$7.35\cdot10^{-2}$	$9.22\cdot10^{-4}$
Min	$-1.37\cdot10^{0}$	$-1.59\cdot10^{-2}$	$-1.32\cdot10^{0}$	$-7.38\cdot10^{-3}$
25%	$-3.54\cdot10^{-2}$	$-4.53\cdot10^{-4}$	$-3.91\cdot10^{-3}$	$-4.14\cdot10^{-4}$
50%	$0.00\cdot10^{0}$	$-2.40\cdot10^{-5}$	$-2.95\cdot10^{-6}$	$1.97\cdot10^{-6}$
75%	$3.08\cdot10^{-2}$	$7.55\cdot10^{-5}$	$2.11\cdot10^{-2}$	$4.52\cdot10^{-5}$
Max	$8.24\cdot10^{-1}$	$2.85\cdot10^{-3}$	$8.20\cdot10^{-1}$	$1.05\cdot10^{-3}$

ML-MM training and the predicted outputs of the former is provided, using both Pearson (below the diagonal) and Spearman (above the diagonal) methods. The results show a positive correlation between biomass and soil depth, as the system equilibria usually happen at either low or high values for both biomass and soil depth. The grazing pressure shows a strong negative correlation with biomass, as should be expected from the equations, but also a weaker one with the soil depth. The latter is most probably understood from the fact that when biomass collapses, soil depth usually follows. Moving to the ground truth for the outputs, the biomass rate of change shows little correlation with any variable except the grazing pressure, for which it is moderately negative, as explained from the equations. More interestingly, the soil depth rate of change correlates moderately with the biomass and is negatively correlated with the soil depth and grazing pressure. The first two can also be derived from the equations, as the vegetations offers shelter for the soil promoting its growth, while having more soil depth diminishes bedrock weathering that reduces soil formation. The correlation with the grazing pressure is surprisingly the largest, and the disagreement between the Pearson and Spearmen correlation about its strength suggests non-linearity. This effect is most probably linked to the lowered biomass affecting also the soil behaviour, but possibly the difference in collapse speed for both variables explains this non-linearity. This may also explain why there is only little correlation between biomass and soil depth rates of change. Lastly, the outputs of the neural network model show a similar behaviour with the ground truth and high correlation with them, as one would hope to see from an emulator model. The larger differences are in the Spearman correlations of the soil depth rate of change, which are larger for the input variables, suggesting that the ML model predicts a slightly less linear behaviour between them.

Data availability

The software used in this paper can be found in the following GitHub repository: https://github.com/oriol-pomarol/hillslope_project. The data generated with the numerical modelling, which is required to run the code, has also been published (Pomarol Moya, 2024).

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