Quantifying the Safe Operating Space for Land-System SDG Achievement via Machine Learning Meta-Modelling and Scenario Discovery

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Key Points:

- We trained five machine learning meta-models to mimic the performance of the Land-Use Trade-Offs (LUTO) model of Australia's land system sustainability
- The XG-Boost algorithm was able to reproduce LUTO outputs with 96% accuracy.
- We performed 480,000 meta-model simulations and found 5.82% new pathways meeting five SDG targets for 2050.
- Scenario discovery revealed the precise policy settings to achieve five SDG targets for 2050.

Abstract

We developed a machine learning based meta-model to identify sustainability pathways through rapid scenario generation and defined the safe operating space for achieving them via scenario discovery. We trained a meta-model to replicate the Land-Use Trade-Offs integrated model of the Australian land system. Latin hypercube sampling was used to create many scenarios exploring the impact of uncertainties in key drivers including future socio-economic development, climate change mitigation, and agricultural productivity at a granular level. Economic and environmental impacts were evaluated against nationally downscaled SDG targets. Scenario discovery revealed new pathways to achieving five SDG targets for 2050 which required crop yield increases above 1.78 times, a carbon price above 100 AU\$ tCO_2^{-1}, a > 9% biodiversity levy on carbon plantings, and carefully regulated land-use policy. Machine learning based meta-modelling teamed with scenario discovery revealed the policy and scenario settings required for a sustainable future for the Australian land sector.

1 Introduction

A sustainable land sector is key to achieving several of the 17 Sustainable Development Goals (SDGs) and 169 targets (UN, 2015) representing the shared environmental, social, and economic aspirations of all UN member nations (Herrero et al., 2021). However, the feasibility of achieving multiple SDG targets in the land sector has been questioned due to the inherent trade-offs involved and calls have been made to redouble efforts in the search for sustainable future pathways (Gao and Bryan, 2017). Multiple land-use models have been developed both as stand-alone models and as a part of multi-sectoral integrated assessment models to understand the complex relationships and dynamics underpinning land-system sustainability (Hurtt et al., 2011, Schaldach et al., 2011, Souty et al., 2012, Van Asselen and Verburg, 2013, Meiyappan et al., 2014, Wise et al., 2014, Bryan et al., 2016b, Zilli et al., 2020, Liu et al., 2021). However, land-use futures are characterised by substantial complexity and uncertainty driven by the large potential range in input data, model parameter specifications, and the scenario assumptions involved in land-use modelling, and the sporadic and incomplete consideration of these interacting uncertainties (Moallemi et al., 2020a). There is now an urgent need for the comprehensive exploration of this uncertainty space to better account for the diversity of plausible land-use futures and identify pathways to achieving the SDGs.

A common way of coping with such uncertainties has been to characterize scenarios that provide a structured account of plausible futures (Moallemi et al., 2020a) derived from a predefined set of scenario configurations, harmonized under a set of policy and developmental assumptions (Moss et al., 2010, Van Vuuren et al., 2011, O'Neill et al., 2017). However, the number of scenarios considered for the analysis of land-use futures is typically limited due to the complexity and data (including spatial data) requirements of the models, and hence, the time taken to run each simulation. For example, Sands et al. (2013) modelled 12 scenarios of future agricultural resources and land-use using the FARM model, Soergel et al. (2021) modelled four scenarios from the Shared Socio-economic Pathways (SSPs) for understanding development pathways for climate action using the MAgPIE model, Wang et al. (2022) modelled three scenario combinations of SSPs and Representative Concentration Pathways (RCPs) using the PLUS model to assess land-sector carbon storage under climate change. Recently, international collaborative modelling studies have extended the number of scenarios analysed to hundreds or even thousands (McPhail et al., 2020). For example, the ScenarioMIP (O'Neill et al., 2016) approach considered combinations of SSPs and RCPs as alternative future pathways, each modelled using a number of integrated assessment models, generating a scenario database of 1184 distinct views of the future (IPCC, 2014). Bryan et al. (2016a), modelled 648 scenarios of future land-use change in Australia using the Land-Use Trade-Offs (LUTO) model but still only managed to sample the six input parameter uncertainty dimensions at between two and four levels (e.g., low, medium, high estimates). Hence, modelling even a thousand or so scenarios still involves only a coarse sampling of the variance in forcing data and model parameters, effecting only a partial, intermittent coverage of the uncertainty space (Morris et al., 2022). A much more granular exploration of the uncertainty space is required, assessing many scenarios to help find nuanced pathways to achieving the SDGs in land systems (Gao and Bryan, 2017).

Models are increasingly used to support robust decision making through exploratory modelling and scenario discovery in order to deal with uncertainty (Kwakkel, 2019, Moallemi et al., 2020b). Scenario discovery works with a dataset consisting of the outputs of many scenario runs spanning the full range of uncertainty in model input parameters to identify regions in the uncertainty space that are of interest and can answer questions about requisite input parameter settings (Halim et al., 2016, Kwakkel and Jaxa-Rozen, 2016). For example, Bryant and Lempert (2010) used scenario discovery to investigate the policy settings necessary to ensure greenhouse gas emissions and economic targets were met for the United States to reach a goal of 25% of its electricity generation from renewable sources by 2025. Lamontagne et al. (2018) used scenario discovery to estimate the climate change mitigation costs based on the range of climate change scenario assumptions, while Eker et al. (2019) used it to identify the range of behavioural factors required to navigate towards a more sustainable diet. Effective scenario discovery capable of supporting granular and specific policy recommendations requires a dense sampling of model runs across the uncertainty space, but land-use models generally take too much compute time to create a dense enough sampling. For example, the 648 future Australian land-use scenarios modelled by Bryan et al. (2016a) took around one week to process despite employing an advanced column generation algorithm (Nazari et al., 2015) and parallel computing on a high-performance computer cluster (Bryan, 2013, Gao and Bryan, 2016). Hence, meta-models (i.e., parsimonious, fast, statistical or machine learning models which closely mimic the behaviour of the original, complex, process-based simulation model) are required to produce many simulation runs which densely span the input parameter uncertainty space and facilitate scenario discovery of sustainable futures (Angione et al., 2022).

In recent years, machine learning has been used to mimic complex systems models and the resulting meta-models have been used for uncertainty assessment across diverse socio-economic and environmental processes such as groundwater (Miro et al., 2021), traffic (Edali and Yücel, 2019), soil carbon (Luo et al., 2013), asset price (Lamperti et al., 2018), and social care provision (Angione et al., 2022). However, very few studies have developed surrogate meta-models of land-use change. Harrison-Atlas et al. (2021), used a Gaussian process-based surrogate modelling approach employing convolutional neural networks to understand wind power modelling impacts on land-use. Van Strien et al. (2019), fitted a support vector machine to identify stable and unstable equilibria in an agent-based model of land-use change in a Swiss mountain region. These results demonstrate the potential for machine learning as a suitable approach to surrogate meta-model development for mimicking the behaviour of complex land-use models as a basis for scenario discovery.

In this study, we created a machine learning based meta-model to capture the behaviour of a complex land systems model—the LUTO model of Australian continental land-use futures and used it to generate many scenarios which comprehensively span the input uncertainty space for multiple factors influencing future land-use in Australia. We then used the meta-model in an exploratory analysis, performing scenario discovery to assess land-use change implications for the SDGs based on the highly granular set of scenario runs. We assessed and compared the ability of different machine learning methods to mimic the LUTO model in terms of accuracy and resource requirements and assessed the sensitivity of the meta-model outputs to variation in key model parameters and scenario assumptions. Via scenario discovery, we then used the machine learning based meta-model outputs to identify critical scenario parameter and policy settings which define the safe operating space required to set Australia's land system on more robust future pathways to achieving multiple SDG targets.

2 Methods

2.1 Land-use model

LUTO is a complex, integrated, non-linear land system model incorporating multiple interacting components including land-use, food demand, agricultural productivity, climate change, water resources, bioenergy, and biodiversity at a 1.1 km ×1.1 km pixel resolution which projects land-use change based on different social, ecological, climatic, economic, and policy scenarios (Bryan et al., 2016b). Scenario configuration settings were specified for a number of uncertainty dimensions resulting in 648 scenarios of land-use futures, with each generated from a combination of parameter settings designed to cover a range of sustainability outcomes under plausible global, national, socio-economic, and environmental futures (Bryan et al., 2015a, Bryan et al., 2015c, Connor et al., 2015, Gao and Bryan, 2017) (Table 1). Uncertainty dimensions included four modelled global socio-economic and climate outlooks (L1, M2, M3 and H3), domestic land-use policies, productivity growth rates, land-use change adoption hurdle rates (i.e., the profitability multiplier required to motivate land-use change), and land-use change capacity constraints. Each global outlook is comprised of global emissions abatement efforts and the resulting RCP and climatic warming, in addition to population growth and GDP scenario settings. Each of these dimensions affects land-use change responses in LUTO via their effect on the relative profitability of land-uses including agricultural production versus a raft of new land-uses (i.e., Carbon Plantings, Environmental Plantings, Biofuels, Wheat Food/Biofuels, Wheat Food/Bioenergy, and Woody Perennials Bioenergy). Each scenario consists of annual time series from 2013 to 2050 (38 years) resulting in an overall data set containing 24,624 (648 scenarios × 38 years) individual land-use projections.

Table 1: Downscaled scenario settings and configuration used for LUTO (Gao and Bryan, 2017) to generate the 648-scenario output.

Name	Global Outlooks			
	L1	**M3**	**M2**	**H3**
Temperature Increase in 2100 (°C)	1.3-1.9	2.0-3.0	2.0-3.0	4.0-6.1
Representative Concentration Pathway (RCPs)	2.6	4.5	4.5	8.5
Population Outlook	1	3	2	3
Global Population in 2050 (billion people)	8.1	10.6	9.3	10.6
World GDP per capita in 2050 (US$2010 thousand)	20.0	18.6	19.3	18.6
World GDP in 2050 (US$ trillion)	161.6	197.0	179.1	197.8
Global abatement effort	Very strong	Strong	Modest	None
Emissions per capita in 2050 (tCO2yr-1)	2.3	4.7	5.4	8.7
Cumulative emissions (GtCO2e)	1437.0	2091	2091	2823
Coverage abatement policy	All sources	All sources except livestock		No sources
Carbon price(AU$ tCO2-1)	200	119	59	0
Grain price (% increase from 2010 to 2050)	75	118	11	61
Livestock price (% increase from 2010 to 2050)	147	112	22	61
Oil price (% increase from 2010 to 2050)	42	44	45	43
Biodiversity Fund				
Carbon	AU$125 million p.a. baseline budget for biodiversity payments, 0% levy on carbon plantings			
Balanced	AU$125 million p.a. baseline budget for biodiversity payments, 15% levy on carbon plantings			
Biodiversity	AU$125 million p.a. baseline budget for biodiversity payments, 30% levy on carbon plantings			
Production growth rate				
Low	0% p.a. increase in total factor productivity of agriculture, 0% p.a. increase in carbon plantation productivity			
Medium	1.5% p.a. increase in total factor productivity of agriculture, 0.75% p.a. increase in carbon plantation productivity			
High	3% p.a. increase in total factor productivity of agriculture, 1.5% p.a. increase in carbon plantation productivity			
Land-use change adoption hurdle rate				
1x	Land-use changes when a new land-use becomes more profitable than agriculture			
2x	Land-use changes when a new land-use becomes more than twice as profitable as agriculture			
5x	Land-use changes when a new land-use becomes more than five times as profitable as agriculture			
Land-use change capacity constraints				
Unconstrained	No limit to the rate of land-use change. Assumes that all labour, capacity, material, technological requirements for land-use change are met.			
Constrained	Rates of land-use change were constrained to that observed previously or reasonably expected. Reforestation limited to 100,00 ha yr-1, increasing by 7% p.a. for the 10 years after the first year it occurred, then by 10% p.a. thereafter. Biofuels feedstock demand was limited by the rate at which processing capacity could be developed which started at 400 ML p.a. in 2013 and increased by 50 ML p.a. to 2015 then by 100 ML p.a. to 2020 and by 400 ML p.a. thereafter. Bioenergy feedstock demand was similarly limited to 0.2 PJ p.a. in 2013 increasing by 2.5 PJ p.a. after 2015.			
Global Climate Model (GCM)				
CanESM	Significant warming, wetter in north and south, drier in central arid areas			
MPI-ESM-LR	Significant warming, wetter in north, drier in south and central arid areas			
MIROC5	Mild warming, wetter throughout			

2.2 Machine learning meta-modelling of scenario projections

2.2.1 Data preparation

We prepared the data in tabular format with all inputs and outputs for each scenario/year in the same row. We transformed the categorical variables to numerical dummy variables representing the presence or absence of each category as 1 or 0 (i.e., Constraint Settings: Unconstrained = 0, Constrained =1; each of three GCMs: present =1, absent =0; and each of four Global Outlooks: present =1, absent =0). All 17 input and output variables were linearly transformed to a fixed range of [0, 1] by subtracting the minimum value of the feature and then dividing by the range. We also transformed and cleaned the data to remove redundant and unimportant information for the model (known as *feature selection* in machine learning) (Supplementary Tables S1 and S2).

2.2.2 Meta-model preparation

The primary advantage of using a meta-modelling approach is to reduce the time required to run each simulation and rapidly generate many predictions using the trained model. As speed and accuracy are important but likely vary between machine learning methods (Angione et al., 2022), we trained five different types of machine learning algorithms and tested their ability to accurately reproduce LUTO model outputs based on different scenario and model input parameter settings. We focussed on decision-tree type models selected due to their short training times, low hyper-parameter tuning requirements, and demonstrated performance with structured/tabular data prediction problems (whereas neural networks tend to perform better with unstructured data such as images and text) (Rudin et al., 2022).

Linear Regression (LR) was selected as a basic linear method for prediction and forecasting (Kashinath et al., 2021). Gradient Boosted Regression Trees (GBRT) was selected as an ensemble learning method that constructs a strong learning model by sequentially aggregating a set of weak classification and regression tree sub-models (Friedman, 2001, Friedman, 2002). Random Forest (RF) was selected as a technique for classification and regression (Ho, 1995) that combines several base models to produce one optimal predictive model. Multivariate Adaptive Regression Splines (MARS) was selected as an extension of linear regression that can capture non-linearities and interactions between variables (Friedman, 1991). Finally, Extreme Gradient Boosting (XGBoost) was selected as a tree-based algorithm optimized via parallel processing, tree pruning, efficient missing value handling, and regularisation to avoid overfitting or bias (Ma et al., 2020, Janizadeh et al., 2021).

Each of these methods incorporate hyper-parameters which need to be tuned based on the data type, expected result, and runtime requirements. For our study, the hyper-parameters of these machine learning approaches were optimized using the random search method and the grid search method as these methods have been demonstrated to efficiently improve performance (Zhang et al., 2021). Finally, a single set of optimal hyper-parameters were selected for each model by comparing the performance indicators and results over the iterations.

2.2.3 Training and testing

In this study, we randomly split the LUTO model output dataset (Bryan et al., 2015b) of 24,624 rows (648 scenarios by 38 years) into training and test datasets at a ratio of 4:1. The five machine learning methods were trained using a training dataset (19,700 rows) and their projection accuracy was evaluated and compared using a test dataset (4,924 rows). To reduce any potential bias produced by train-test data splitting, all five machine learning methods were trained and evaluated using five-fold cross-validation which randomly divides the dataset into five training datasets and five test datasets. All results presented in this paper were averaged over the five-fold cross-validation outputs. The five machine learning methods were implemented using the Regressor modules of the Python 3.7 scikit-learn library on a standard laptop computer with an Intel(R) Core(TM) i7-4710MQ CPU@2.50 GHz, 8.00 GB RAM, and Windows 10 Professional (64-bit).

We selected the root mean square error (RMSE) and the coefficient of determination (R^2) to evaluate meta-model performance, measuring the deviation between the observed (i.e., LUTO projections) and predicted (i.e., meta-model outputs) values (Eq. 1) and degree of fit of the meta-model (Eq. 2), respectively.

$$RMSE = \sqrt{\sum_1^n \frac{(y_i - \hat{y}_i)^2}{n}}, \text{ ………………………… (Eq. 1)}$$

$$R^2 = 1 - \frac{\sum_1^n (y_i - \hat{y}_i)^2}{\sum_1^n (y_i - \bar{y})^2}, \text{ ……………………………... (Eq. 2)}$$

Where y_i represents the actual values, $\hat{y}_i$ is the predicted value, and *n* is the number of observed values in the test dataset samples and $\bar{y}$ is the mean of the *y* values.

2.2.4 Influential features

The best performing machine learning meta-model (i.e., XGBoost) was selected and analysed to verify the underlying relationships between model inputs and outputs and to quantify the influential predictor variables. To quantify the influence of explanatory variables we excluded each explanatory variable from the whole dataset then applied five-fold cross-validation where for each fold a new model was trained and the number of times features appeared in the tree-based model was counted to help split into the leaf nodes. Following this, we assessed the importance of the features using the Python scikit-learn inspection module (Pedregosa et al., 2011). Based on this influence value we ranked all the input features (1 to 17, with 1 being the most influential and 17 the least) for each output variable. We then identified the most influential features in the overall model for use in scenario discovery by averaging these influence rankings across all output variables.

2.2.5 Model implementation and scenario discovery

The best performing meta-model was then used to run many simulations (termed pathways) of Australian land-use futures. Based on the minimum and maximum values of the LUTO model parameter and scenario settings (Table 1) we produced a dense, high-resolution Latin hypercube sampling (Abyani and Bahaari, 2020, Morris et al., 2022) of the model input parameter and scenario uncertainty space. Plausible input parameter ranges were specified separately for the years 2030 and 2050 and those value ranges were used to define the uncertainty bounds for those years. We then took a Latin hypercube sample of 10,000 samples across each of the 24 possible combinations for each of three GCMs, four global outlooks, and two constraint settings which gave us a total of 240,000 unique scenarios for the year 2030 and 240,000 unique scenarios for 2050.

We then used exploratory modelling and scenario discovery to search for future pathways to sustainability for Australia’s land sector in the output dataset based on specified targets. We identified land-sector relevant Sustainable Development Goals (i.e., 2, 6, 7, 13, and 15), relevant indicators, and targets downscaled for Australia for 2030 and 2050 at three levels of ambition (Low, Moderate, and High) from Gao and Bryan (2017). Sustainability targets were specified for a series of six indicators (note that SDG 2 has two indicators/targets) which align with key meta-model output variables (Table 2) and we quantified the number of scenarios achieving these land-sector SDG targets.

Table 2: Description of land-sector relevant SDGs, indicators, and nationally downscaled targets for 2030 and 2050 and three levels of ambition for Australia's land sector (Gao and Bryan, 2017).

Target ambition	**2030**	**2050**
SDG 2 Economic returns (total net economic returns to all land-uses [2010 AU$ billion yr^{-1}])		
Weak	≥32.96	≥40.80
Moderate	≥37.77	≥54.39
Ambitious	≥41.98	≥67.99
SDG 2 Food/fibre production (total value of agricultural production [2010 AU$ billion yr^{-1}])		
Weak	≥53.0	≥66.1
Moderate	≥55.3	≥77.7
Ambitious	≥64.6	≥111.4
SDG 6 Water resource use (agricultural irrigation and water intercepted [gigaliters yr^{-1}])		
Weak	≤10676.7	≤10676.7
Moderate	≤9697	≤9697
Ambitious	≤8737.3	≤8737.3
SDG 7 Renewable energy (Biofuels (mobile transport fuel) production [petajoules yr^{-1}])		
Weak	≥40.6	≥85.8
Moderate	≥145.0	≥286.9
Ambitious	≥313.3	≥590.3
SDG 13 Emissions abatement (megatons of CO2 yr^{-1})		
Weak	≥55.5	≥160.9
Moderate	≥108.4	≥274.8
Ambitious	≥178.0	≥411.1
SDG 15 Biodiversity and land degradation (biodiversity services [% of maximum])		
Weak	≥10	≥10
Moderate	≥15	≥15
Ambitious	≥20	≥20

Scenario discovery (Lempert et al., 2008) was then used to identify the regions of the model input space containing a high proportion of future pathways which achieve multiple sustainability targets. This safe operating space defined by influential input variable ranges were identified where multiple targets can be achieved. Mapping the number of scenarios in relation to the top four most influential input variables (found through influential feature ranking), we visualised the density of the scenarios clustered in two-dimensional space (divided into bins). Via this process we identified critical levels of influential input variables likely to lead to desirable outcomes (i.e., meeting targets) versus undesirable outcomes (i.e., failing to meet targets). To quantify this likelihood, we assessed the purity of regions of interest in the input data space by quantifying the probability of scenarios meeting targets for meta-model outputs (Serra and Tagliaferri, 2019).

$$Purity\ (\%) = \frac{D}{N} \times 100, \ldots\ldots\ldots\ldots \text{(Eq. 3)}$$

Where *D* is number of scenarios meeting the desired target in an input data region and *N* is the total number of scenarios in the region. The safe operating space was defined by combinations of influential input variable ranges necessary to achieve multiple SDG targets with >80% purity.

3 Results

3.1 Meta-model selection

Overall, the classification and regression tree based algorithms performed well on these datasets given the non-linearity in the data. XGBoost outperformed the other models in terms of R^2 (0.9694) and had the second highest RMSE (0.00379) (Table 3), hence it was selected for further analysis and scenario discovery (Table 2).

Table 3: Average and standard deviation (in brackets) of test dataset accuracy metrics from each machine learning method under five-fold cross-validation averaged across all outputs.

Metrics	**Machine learning method**				
	LR	GBRT	RF	XGBoost	MARS
R^2	0.55924 (0.29)	0.66259 (0.11)	0.8355 (0.05)	**0.9694 (0.046)**	0.5438 (0.091)
RMSE	0.05679 (0.023)	0.0157 (0.006)	0.00571 (0.002)	0.00379 (0.0021)	0.00343 (0.0024)
Training Time (Minutes)	0.01723	14.4555	4.94144	5.48626	6.497
No. of Hyper-parameters	0	5	2	6	9

3.2 Parameter influence

Out of the 17 input features, the five most influential features were Yield Increase (Crops), Constraint Settings, Carbon Price, Hurdle Rate, and Biodiversity Fund. Conversely, the least influential features overall were Global Outlook, Yield Increase (Trees), and GCM (Figure 1), although these features were influential for some individual outputs. Figure 1 shows the most influential features by output type, for example the four most influential features for Economic Returns related outputs were Yield Increase (Crops), Carbon Price, Constraint Settings, and Hurdle Rate (Figure 1).

Input /Output

Influence Ranking (1 being high and 17 being low)

1 5 9 13 17

	Input /Output	Crop Price (multiplier)	Biodiversity Fund (% levy on carbon plantings)	Carbon Price (AU$/tonne CO2)	Constraint Setting	Electricity Price (AU$/MWh)	Hurdle Rate	Livestock Price (multiplier)	Global Outlooks: L1	Global Outlooks: M2	Global Outlooks: M3	Global Outlooks: H3	GCM: CE2	GCM: MPI	GCM: MR5	Oil Price (AUC/litre)	Yield Increase Crops (multiplier)	Yield Increase Trees (multiplier)
Economic Return	Beef (AU$)	8	6	1	4	9	5	3	14	13	12	16	15	11	10	7	2	17
	Carbon plantings (AU$)	8	2	1	3	9	6	5	12	15	14	15	13	10	11	7	4	15
	Cattle total (AU$)	7	8	1	5	9	4	3	13	10	14	16	15	12	11	6	2	17
	Crops (AU$)	2	8	10	6	4	5	3	14	9	13	16	15	11	12	7	1	17
	Dairy (AU$)	9	11	1	8	6	5	3	10	4	15	16	14	12	13	7	2	17
	Environmental plantings total (AU$)	9	2	1	3	8	6	4	14	15	13	16	12	10	11	7	5	17
	Environmental plantings: biodiversity payment top-up(AU$)	9	2	1	3	8	6	4	14	15	13	16	12	10	11	7	5	17
	Environmental plantings: carbon price (AU$)	12	1	3	5	7	2	8	6	15	14	16	13	11	10	9	4	16
	Horticulture (AU$)	1	11	6	9	4	8	10	15	3	7	16	14	13	12	5	2	17
	Sheep (AU$)	7	6	1	5	10	4	3	11	14	13	16	15	9	12	8	2	16
	Wheat biofuels (AU$)	5	7	11	2	10	4	3	15	16	13	14	12	6	8	9	1	17
	Wheat food/bioenergy (AU$)	6	7	2	5	3	4	8	16	12	15	14	13	9	10	11	1	16
	Wheat food/biofuels (AU$)	3	7	9	2	8	1	4	13	16	11	15	14	10	12	6	5	17
	Woody perennials bioenergy (AU$)	6	2	5	1	7	4	8	11	12	12	12	17	16	9	10	3	12
	Woody perennials biofuels (AU$)	6	12	4	2	10	5	11	16	14	15	3	13	7	8	9	1	17
Area	Beef (ha)	8	6	2	1	7	5	3	13	15	12	16	14	11	10	9	4	16
	Carbon plantings (ha)	9	3	2	1	7	6	5	12	15	13	15	14	11	10	8	4	15
	Cattle total (ha)	8	6	2	1	7	5	3	11	15	13	16	14	12	10	9	4	16
	Crops (ha)	8	5	4	1	9	2	6	11	14	12	16	15	10	13	7	3	16
	Dairy (ha)	8	6	3	4	9	2	5	13	14	12	16	15	10	11	7	1	17
	Environmental plantings total (ha)	9	2	1	4	7	3	6	12	15	13	16	14	11	10	8	5	16
	Environmental plantings: biodiversity payment top-up (ha)	9	2	1	4	7	3	5	14	15	13	16	12	11	10	8	6	17
	Environmental plantings: carbon price (ha)	9	2	4	5	6	1	12	3	15	14	16	13	10	11	8	7	17
	Horticulture (ha)	2	8	9	4	10	3	6	11	14	7	16	15	13	12	5	1	17
	Sheep (ha)	9	5	7	2	8	3	1	14	15	12	16	13	10	11	6	4	16
	Wheat biofuels (ha)	5	6	11	2	10	4	3	16	13	14	15	12	7	9	8	1	17
	Wheat food/bioenergy (ha)	6	7	2	5	3	4	8	16	12	15	14	13	9	10	11	1	17
	Wheat food/biofuels (ha)	5	7	9	2	11	1	8	6	15	10	14	16	12	13	4	3	17
	Woody perennials bioenergy (ha)	6	2	4	1	7	5	8	9	12	12	12	17	16	10	11	3	12
	Woody perennials biofuels (ha)	8	9	3	2	11	5	12	15	14	16	4	13	7	10	6	1	17
Biodiversity	Biodiversity service (% of maximum)	9	1	2	5	7	3	4	12	14	13	15	17	11	10	8	6	16
	Payment expenditure (AU$)	9	1	2	3	7	6	5	13	15	12	15	14	11	10	8	4	15
Emissions	Bioenergy: net emissions abatement (tCO2e)	8	2	3	1	9	5	7	10	10	10	10	15	17	16	6	4	10
	Biofuels: net emissions abatement (tCO2e)	7	8	10	2	11	3	4	12	16	13	15	14	6	9	5	1	17
	Carbon sequestration carbon plantings (tCO2e)	9	5	2	1	6	7	4	14	15	12	15	13	11	10	8	3	15
	Carbon sequestration environmental plantings total (tCO2e)	11	2	1	4	6	3	7	12	15	14	16	13	8	9	10	5	16
	Carbon sequestration environmental plantings: biodiversity payment top-up (tCO2e)	11	2	1	4	7	3	5	13	15	14	16	12	9	10	8	6	16
	Carbon sequestration environmental plantings: carbon price (tCO2e)	6	2	3	5	4	1	12	8	15	14	16	13	9	11	10	7	16
	Food/fibre production: avoided emissions (tCO2e)	9	7	5	1	6	2	4	12	15	13	14	16	10	11	8	3	17
	Total carbon sequestration (tCO2e)	9	7	2	1	6	5	3	13	15	12	16	14	11	10	8	4	16
	Total emissions abatement (tCO2e)	8	7	2	1	6	5	3	14	15	12	16	13	11	10	9	4	16
Energy	Energy: bioenergy from biomass (GJ)	8	3	2	1	9	5	7	10	10	10	10	17	16	15	6	4	10
	Energy: biofuels from biomass (GJ)	5	12	2	3	6	4	8	15	14	15	11	13	9	10	7	1	15
	Energy: biofuels from grain (GJ)	5	7	11	2	10	4	3	16	15	13	14	12	6	8	9	1	17
	Energy: biofuels from wheat residue (GJ)	7	9	8	2	11	3	4	12	16	13	15	14	6	10	5	1	17
	Energy: total from bioenergy (GJ)	8	3	2	1	9	5	7	10	10	10	10	17	16	15	6	4	10
	Energy: total from biofuels (GJ)	7	8	9	2	11	3	4	12	16	13	15	14	6	10	5	1	17
	Energy: total from biofuels and bioenergy (GJ)	7	8	9	2	11	3	4	12	16	13	15	14	6	10	5	1	17
	Feedstock: biomass for bioenergy (tonnes)	8	3	2	1	9	5	7	10	10	10	10	17	16	15	6	4	10
	Feedstock: biomass for biofuels (tonnes)	5	12	2	3	6	4	8	15	14	15	11	13	9	10	7	1	15
	Feedstock: grain for biofuels (tonnes)	5	7	11	2	10	4	3	16	15	13	14	12	6	8	9	1	17
	Feedstock: total biofuels (tonnes)	7	8	10	2	11	3	4	12	16	13	15	14	6	9	5	1	17
	Feedstock: wheat residue for biofuels (tonnes)	7	9	8	2	11	3	4	12	16	13	15	14	6	10	5	1	17
	Production: biofuels from biomass (ML)	5	12	2	3	6	4	8	15	14	15	11	13	9	10	7	1	15
	Production: biofuels from grain (ML)	5	7	11	2	10	4	3	16	15	13	14	12	6	8	9	1	17
	Production: biofuels from wheat residue (ML)	7	9	8	2	11	3	4	12	16	13	15	14	6	10	5	1	17
	Production: biofuels total production (ML)	7	8	9	2	11	3	4	12	16	13	15	14	6	10	5	1	17
Food/Fibre	Beef (head)	7	8	5	2	6	4	10	3	16	13	15	14	12	11	9	1	17
	Cattle total (head)	7	9	5	3	2	4	10	6	16	13	15	14	12	11	8	1	17
	Crops (tonnes)	10	5	9	3	7	4	8	2	16	13	14	15	11	12	6	1	17
	Dairy (head)	6	11	8	4	5	3	7	13	16	12	15	14	10	9	2	1	17
	Horticulture (tonnes)	2	9	10	6	11	5	4	14	16	13	12	15	8	7	3	1	17
	Sheep (head)	10	6	5	2	7	3	9	4	16	13	15	14	8	12	11	1	17
	Total food/fibre production (AU$)	10	8	9	2	5	4	6	3	16	13	14	15	11	12	7	1	17
Water	Agricultural water use (ML)	5	6	7	3	8	2	4	12	14	10	16	15	11	13	9	1	16
	Surface water resources intercepted (ML)	9	7	1	2	6	3	4	12	15	13	16	14	11	10	8	5	16
	Total change in water use (ML)	8	7	1	2	6	3	4	12	15	13	16	14	10	11	9	5	16
	Total water resources intercepted (ML)	8	7	1	2	6	3	4	12	14	13	16	15	10	11	9	5	16
	Overall Influence Rank	7	5	3	2	8	4	6	11	14	15	10	17	12	13	9	1	16

Figure 1: Influence of 17 input parameters on the 68 outputs. Colours in the grid cells represent the total ranking position, and numbers in the grid cells represent the influence rankings.

3.3 SDG target achievement

SDG target achievement varied substantially between future pathways for both 2030 and 2050. By design, weak targets were more achievable than moderate and ambitious ones. Moderate and ambitious targets tended to be achieved by more pathways for 2050 targets than for 2030. For example, Biodiversity services targets for 2050 were achievable under 53.56%, 41.31%, and 32.75% of future pathways across the weak, moderate, and ambitious levels (Table 4), whereas for 2030 the target was achieved at only 1.796%, 0.294% and 0.047% of future pathways. Some targets (e.g., ambitious targets for Water Resource Use and Food Production targets for 2030 and 2050) were not achievable under any pathways (Table 4).

Table 4: The proportion (%) of pathways where each target is achieved for the year 2030 and 2050.

	Year 2030			Year 2050		
	Weak	Moderate	Ambitious	Weak	Moderate	Ambitious
Economic Returns	12.432	1.494	0.116	48.717	17.512	2.196
Food Production	21.904	12.040	0.000	25.220	0.898	0.000
Water Resource Use	66.239	0.506	0.000	11.761	0.588	0.000
Biofuels Production	70.187	19.458	6.685	71.685	22.495	11.155
Emissions Abatement	13.429	6.550	2.673	46.083	26.976	13.635
Biodiversity Services	1.796	0.294	0.047	53.558	41.307	32.755

Many scenario runs also revealed the trade-offs and joint achievement of multiple sustainability targets. For example, two, three, four, and five moderate 2030 targets were achieved under 7.1%, 1.19%, 0.06%, and 0% of future pathways, while for 2050 moderate target achievement was considerably higher at 14.98%, 12.38%, 3.90%, and 0% of future pathways, respectively (Table 5, Figure 2). No pathways achieved all six targets simultaneously at any level of ambition.

Table 5 – Level of SDG target achievement under future pathways.

Year	Ambition	Target achievement (% of future pathways)				
		2 Targets	3 Targets	4 Targets	5 Targets	6 Targets
2030	Weak	42.77	10.78	1.53	0.25	0.00
	Moderate	7.10	1.19	0.06	0.00	0.00
	Ambitious	1.20	0.05	0.00	0.00	0.00
2050	Weak	24.36	26.00	21.23	5.85	0.00
	Moderate	14.98	12.38	3.90	0.00	0.00
	Ambitious	11.65	2.53	0.24	0.00	0.00

The most prospective pathways for multi-target SDG achievement was the achievement of weak targets for Economic Returns, Food Production, Biofuel Production, Emissions Abatement, and Biodiversity Services under 0.2% and 5.8% of scenarios for the year 2030 and 2050, respectively (Figure 2). Water Resource Use and Biofuels Production targets for 2030 and 2050 under weak target ambitions were more achievable (26.94% and 4.71%) than any other target pairs, whereas the Economic Returns and Food Production target pair was the least achievable (0.001% and 0.038%) for both 2030 and 2050 (Figure 2).

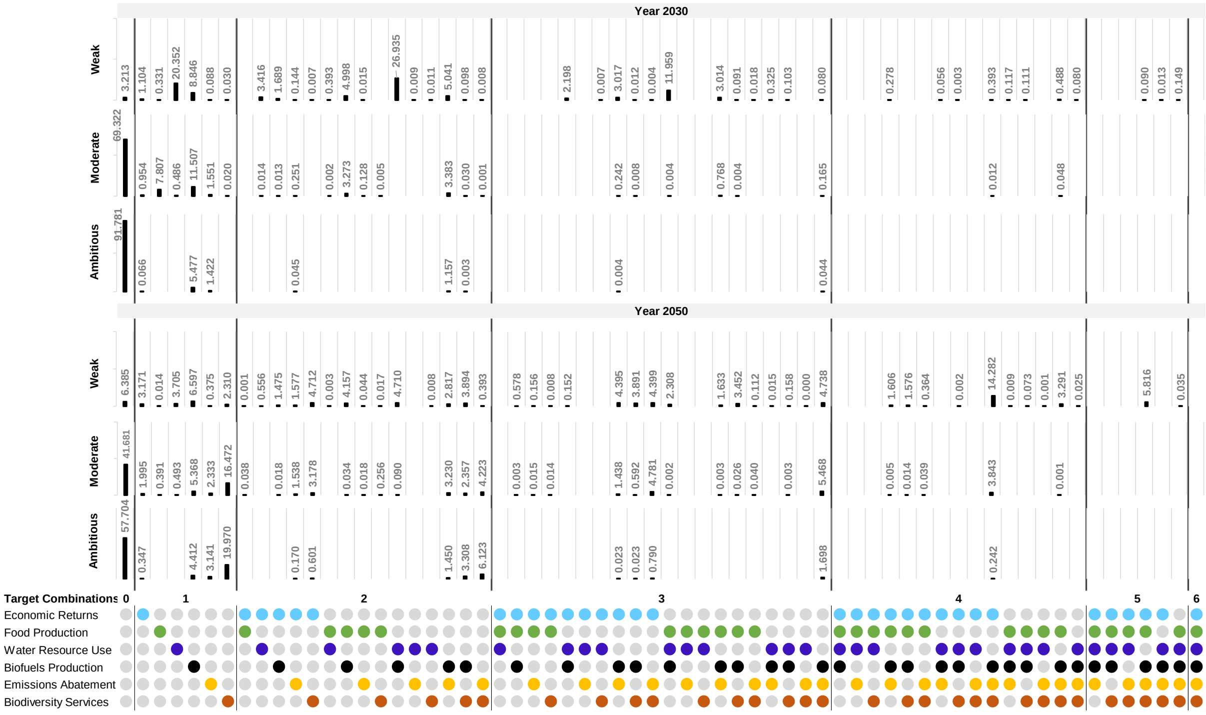

Figure 2: Future land sector SDG target achievement for Australia. a.) The bars represent the proportion (%) of scenarios meeting the weak, moderate, and ambitious targets by the year 2030 and 2050.

3.4 Identifying the safe operating space using scenario discovery

Focussing on the 5.82% of pathways meeting the weak target achievement levels for 2050 (i.e., Economic Returns, Food Production, Biofuels Production, Emissions Abatement, and Biodiversity Services targets), we picked the top four most influential parameters based on overall influence ranking and demonstrated in two-dimensional space (Figure 1). Other input parameters also influence target achievement (Figure 1) and the full list of influential parameters is provided in Table 6.

The statistical distribution of input parameter settings required to meet five SDG targets is presented in Table 6. To achieve the five SDG targets with more than 80% purity, specific scenario, policy, parameter settings were required which defined the safe operating space (Table 6 and Figure 3). Specifically, these targets were most likely to be achieved when Yield

Increase (Crops) exceeded 1.78 (multiplier), Carbon Price was above 100 AU\$ tCO_2^{-1}, the Biodiversity Fund levy on carbon plantings was above 9%, under a constrained and regulated land-use system (Table 6 and Figure 4).

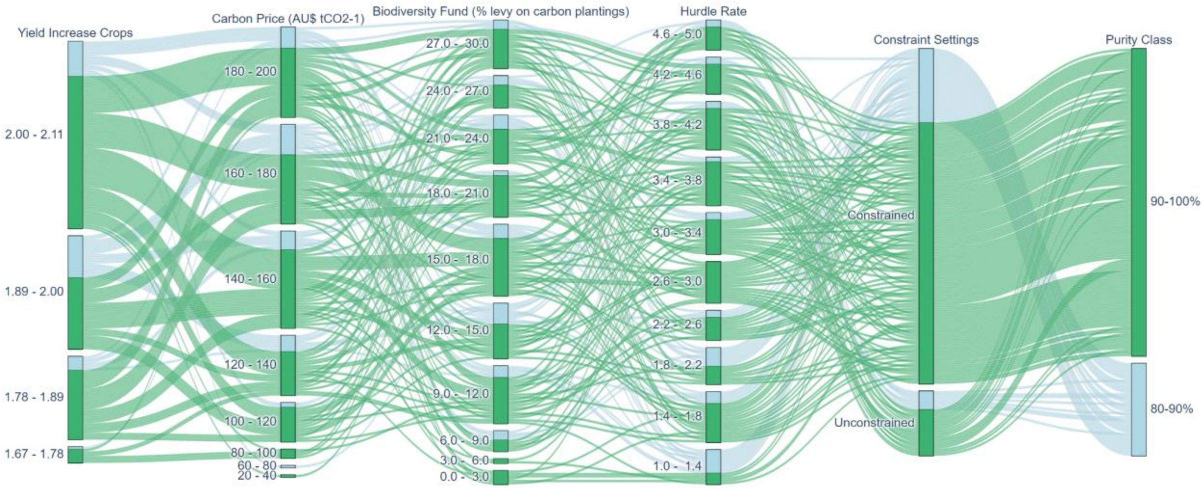

Figure 3: Parameter settings for the five most influential parameters to achieve five targets under Weak 2050 ambition with more than 80% purity.

Investigating further the precise safe operating space settings for pathways to multi-target achievement at >80% purity, complex dependencies between parameter settings were evident. We found that in an unconstrained environment multi-target achievement occurred only at a hurdle rate setting for land-use change above 3.4, whereas in a constrained and regulated environment multi-target achievement was possible at any hurdle rate (Figure 3 and Supplementary Figure 1 and Figure 2). Similarly, at Carbon Price settings between 100 and 120 AU\$ tCO_2^{-1}) a levy on carbon plantings exceeding 12% was required in a constrained environment with a hurdle rate over 1.4 (Supplementary Figure 4).

Table 6: Statistical distribution of the parameter settings to achieve five targets under Weak 2050 ambition (Supplementary Figure 1, Figure 2, Figure 3, and Figure 4).

Rank	Input Variables	Mean	SD	Min	Percentile			Max	Purity >80%
					25th	50th	75th		
1	Yield Increase Crops (multiplier)	1.95	0.10	1.65	1.87	1.96	2.03	2.11	>=1.78
2	Constraint Setting	NA	NA	0	0	0	1	1	0 or 1
3	Carbon Price (AU$ tCO_2^{-1})	146.6	34.9	0.49	123.9	148.75	174	199.7	>=100
4	Hurdle Rate	2.86	1.09	1.00	1.95	2.82	3.71	5.00	>=1.0
5	Biodiversity Fund (% levy on carbon plantings)	18.4	6.7	0.29	12.9	18.6	23.9	29.97	>=9
6	Livestock Price (multiplier)	1.93	0.42	1.07	1.59	2.03	2.29	2.47	>=2.19
7	Crop Price (multiplier)	1.66	0.31	1.06	1.40	1.69	1.93	2.18	>=1.84
8	Electricity Price (AU$/MWh)	78.35	23.6	42.19	57.01	76.02	99.11	122	>=50
9	Oil Price (AUC /litre)	152.3	6.70	140.26	146.5	152.40	158.2	163.3	14>=5
10	Global Outlooks - H3	NA	NA	0	0	0	1	1	0 or 1
11	Global Outlooks - L1	NA	NA	0	0	0	0	1	0 or 1
12	GCM - MPI	NA	NA	0	0	0	1	1	0 or 1
13	GCM - MR5	NA	NA	0	0	0	1	1	0 or 1
14	Global Outlooks - M2	NA	NA	0	0	0	1	1	0 or 1
15	Global Outlooks - M3	NA	NA	0	0	0	1	1	0 or 1
16	Yield Increase Trees (multiplier)	1.19	0.11	1.00	1.10	1.19	1.28	1.37	>=1.15
17	GCM - CE2	NA	NA	0	0	0	1	1	0 or 1

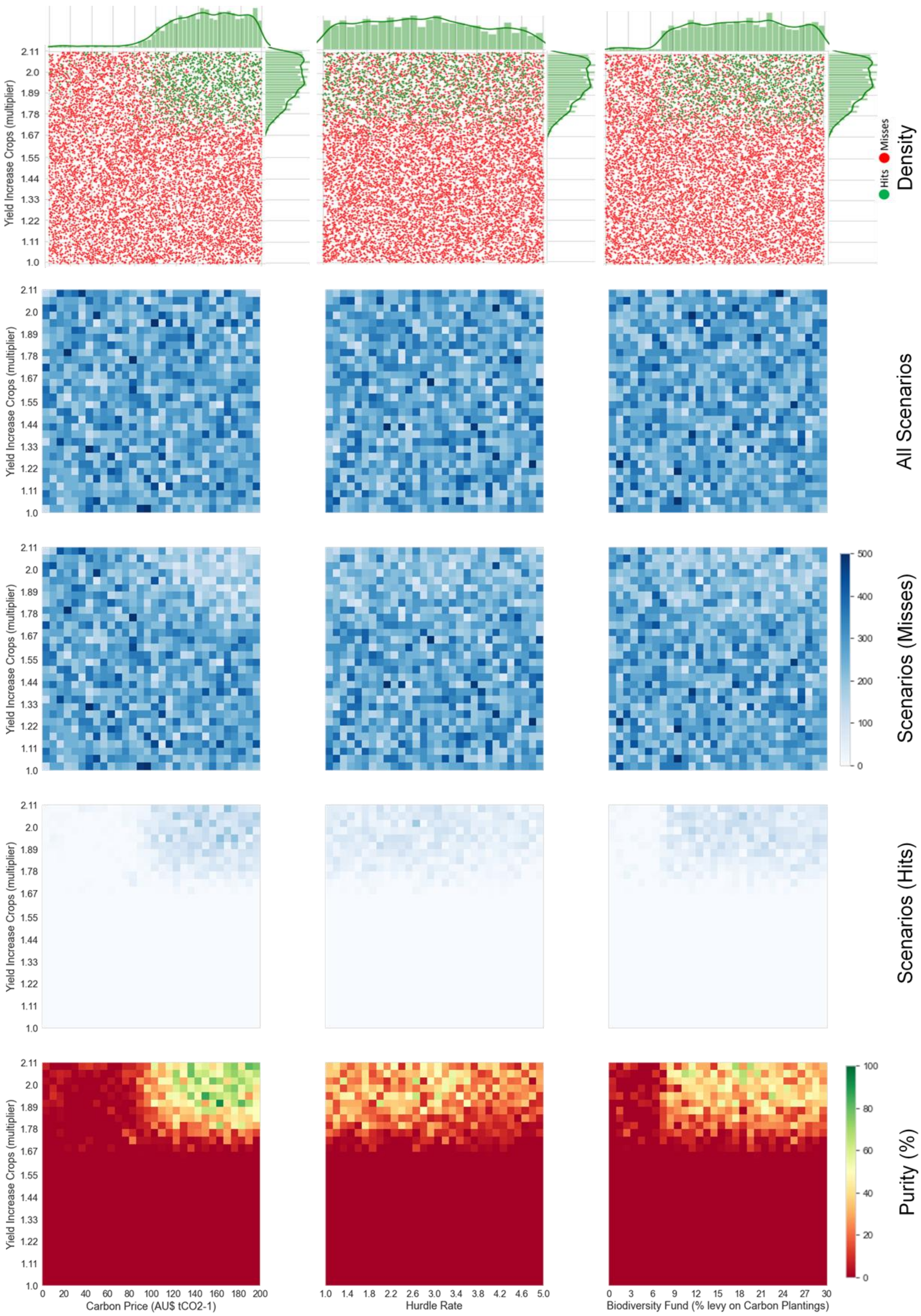

Figure 4: Target achievement in relation to the input parameter space for four of the most influential parameters. Density subplots illustrated the number of scenarios meeting the Weak 2050 multi-target combinations (5 targets in green) and the number of scenarios not meeting the targets is shown in red. All Scenarios shows the density of all 240,000 scenarios. Scenarios (Misses) and Scenario (Hits) shows the density of hits and misses, and Purity (%) shows the density ratio as a percentage of hits to misses in each bin.

4 Discussion

Using a machine learning approach we developed a meta-model which accurately mimicked the behaviour of a complex, non-linear, national-scale land-system model. Once trained, we were able to run hundreds of thousands of scenario outputs in minutes with little computational effort. This fast and accurate meta-model enabled the exploratory modelling of scenario configurations across a dense sampling of the input parameter uncertainty space and produce outputs spanning the complete space of potential futures across a range of sustainability indicators. Scenario discovery enabled the identification of the input parameters and policy settings which are essential for achieving the Sustainable Development Goals in Australia's land system but which were not evident in previous scenario analyses (Gao and Bryan, 2017).

4.1 Implications of the results for meta-modelling

Integrated assessment models of complex social-ecological systems have helped provide a glimpse of the future considering plausible changes in climatic, socio-economic, and technological conditions. With the improvements and extension of these models over the years the computational complexity has increased while transparency has decreased (Keppo et al., 2021). Over the same period, significant advances in exploratory modelling including techniques such as scenario discovery have occurred specifically to address the uncertainty in complex social-ecological systems. However, the increased computational demands of integrated assessment models have limited their ability to explore uncertainty using these techniques due to the challenges in producing the many scenario runs required. We have demonstrated here that machine learning based meta-models which provide a fast, accurate surrogate for complex, integrated, computationally-intensive models can effectively bridge this gap. Our results add to the momentum of machine learning based meta-modelling (Razavi et al., 2021).

The accuracy of the meta-model in estimating the outputs of the original model is a key factor underlying the success of the methods used here. Our results show that machine learning methods were able to accurately mimic the behaviour of the complex LUTO model of Australian land-use change. We evaluated five different machine learning methods to test the sensitivity to the choice of method. While XGBoost was selected as the most accurate, other methods also performed well and consideration also needs to be given to the requirements for hyper-parameter tuning and compute time. For example, RF had a training time required of 4.9 minutes and only 2 hyperparameters needed tuning but the accuracy was only 83%, whereas

XGBoost tuning involved 6 hyperparameters and 5.5 minutes of training time but had a 96% accuracy. The performance and choice of machine learning methods are likely to be dependent upon the specific characteristics of the data and the model being mimicked and we recommend the evaluation of multiple machine learning methods in future meta-modelling exercises.

The current process-based LUTO model involves several thousand lines of computer code, depends upon a licensed version of the Cplex solver, and even with advanced heuristics and a high-performance compute cluster still takes around one hour to run a single scenario. Conversely, the meta-model is much more accessible, has no proprietary software limitations, and can run many scenarios in seconds on modest compute resources. This makes the meta-model deployable to online platforms and publishable as open source so that the users can easily access and understand the approximate behaviour of LUTO without heavy computational requirements.

4.2 Implications for land system sustainability

We used a fast, accurate, machine learning based meta-model to comprehensively explore plausible future uncertainty space and find the dominant variables within the model. By producing many thousands of scenario runs, the meta-model revealed futures spanning broad combinations of model parameter settings including socio-economic and environmental forcing data, land-use policy, and global outlooks. This was not previously possible with the full LUTO model due to the heavy resource requirement and computational overhead (Nazari et al., 2015). The meta-modelling approach enabled a dense sampling of the input parameter and scenario space. This in turn, allowed the specification of precise regions of interest in the output space (i.e., achieving multiple downscaled SDGs for Australia) and indicated highly resolved input parameter settings which gave rise to these regions of interest as the *safe operating space* necessary for charting future pathways to sustainability. Exploring the full range of potential futures for Australia's land system, the meta-model revealed new pathways and insights into the requirements for meeting multiple SDG targets, complementing a previous landmark assessment (Gao and Bryan, 2017).

After running 240,000 scenario simulations for 2050, we identified via scenario discovery the most prospective pathway where five weak SDG targets (all but Water Resource Use) were achieved under just 5.82% of all possible future scenarios. The safe operating space was defined as the scenario setting configuration where the future pathways were more likely to achieve these 5 targets (with a purity > 80%). Target achievement required specific parameter setting combinations, but typically Yield Increase (Crops) needed to more than 1.78 times of the 2013 levels, Carbon Price above 100 AU\$ tCO_2^{-1}, and a Biodiversity Fund levy on carbon plantings above 9%. In addition, multiple targets were more likely to be met in when land-use change was constrained and regulated, although achievement was also possible when unconstrained with hurdle rates exceeding 3.4 (Supplementary Figure 1-4). This indicates that for a sustainable future for Australia's land sector we must focus on the research and development to improve productivity, manage the pace of land-use change via regulation, fund carbon sequestration in land systems, and implement the biodiversity fund levy policy such that some of the proceeds from carbon plantings go towards restoring Australia's native ecosystems.

4.3 Limitations

Several factors limited the application of the meta-model in this study. First, the machine learning methods evaluated and used require the tuning of several hyper-parameters which affect their performance. We used a grid-search algorithm to find the most suitable hyper-parameter values to maximise meta-model accuracy. Second, although our approach showed that a close approximation of a complex, process-based, land systems model is possible with machine learning methods, the behaviour of the model is learned only for one particular point in time. However, in reality, most large systems models are constantly being improved and extended. If the process-based model is modified via the incorporation of new variables, data, or scenarios, the meta-model also needs to be re-trained to capture this new behaviour. While the time required to retrain the machine learning is short, it still takes a significant amount of time and expertise to incorporate the changes to the process-based model and reanalyse the outputs. Third, future projections using the meta-model are also limited to the range of input data used in the original process-based model runs. Predicting beyond the range of these known values is likely to produce unreliable results. Hence, the great utility of the meta-model approach is to produce many model runs at a dense sampling of the input parameter uncertainty space and to provide a comprehensive coverage of the output space.

5 Conclusion

We created a machine learning based meta-model which was able to accurately mimic the performance of LUTO, a complex land systems model for Australia. Of the five machine learning methods evaluated, XGBoost was relatively quick to train, most accurate, and fast to run. The meta-model was used to simulate many land-use futures across a dense sampling of the input uncertainty space via Latin hypercube sampling. We used the resulting future land-use simulation dataset in an exploratory process of scenario discovery to identify the input parameter settings required to achieve six downscaled UN Sustainable Development Goal targets for Australia. We found pathways where five of the six desired sustainability targets (Food Production, Economic Returns, Biodiversity Services, Biofuels Use, and Emissions Abatement) were achieved by 2050 under just 5.82% of the total number of scenarios. Using scenario discovery we identified the safe operating space under which these pathways could be achieved defined by settings for influential model input variables. The production of many simulation runs densely spanning the input uncertainty space helped accurately understand the input parameter settings to achieve the outputs of interest. The approach in this study can be used to understand any complex model and increase the understanding of the uncertainty space, influential variables, and identify key input parameter settings required to achieve specific model outputs. In our case, it generated insights into the requirements for sustainable futures for Australia's land sector that have not been possible using traditional integrated modelling approaches.

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Open Research

The authors can declare that the data and the developed LUTO model code is publicly available in GitHub repository. The input data as a raw format was attained from CSIRO's open data portal and can be accessed via **https://doi.org/10.4225/08/5756169E381CC** (Bryan et al., 2015b).

All the prepared input data is prepared in CSV format and the model development was done in python environment using notebooks and can be accessed via **ML-Based-Surrogate-LUTO-Model-V1**. The trained models are saved as .sav format and can be loaded to reproduce the results.

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