



1 **Using SHAP to interpret XGBoost predictions of grassland**
2 **degradation in Xilingol, China**

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8 Abstract

9 Machine learning (ML) and data-driven approaches are increasingly used in many research areas.
10 XGBoost is a tree boosting method that has evolved into a state-of-the-art approach for many ML
11 challenges. However, it has rarely been used in simulations of land use change so far. Xilingol, a
12 typical region for research on serious grassland degradation and its drivers, was selected as a case
13 study to test whether XGBoost can provide alternative insights that conventional land-use models
14 are unable to generate. A set of twenty drivers was analysed using XGBoost, involving four
15 alternative sampling strategies, and SHAP to interpret the results of the purely data-driven approach.
16 The results indicated that, with three of the sampling strategies (over-balanced, balanced and
17 imbalanced), XGBoost achieved similar and robust simulation results. SHAP values were useful for
18 analysing the complex relationship between the different drivers of grassland degradation. Four
19 drivers accounted for 99% of the grassland degradation dynamics in Xilingol. These four drivers
20 were spatially allocated, and a risk map of further degradation was produced. The limitations of
21 using XGBoost to predict future land-use change are discussed.

22 **Key words:** grassland degradation, machine learning, driver-driven method, XGBoost, SHAP
23 values

24 1. Introduction

25 Land-use and land-cover change (LUCC) has received increasing attention in recent years (Aburas
26 et al., 2019; Diouf & Lambin, 2001; Lambin et al., 2003; Verburg et al., 2002). Land-use change
27 includes various land-use processes, such as urbanisation, land degradation, water body shrinkage,
28 and surface mining, and has significant effects on ecosystem services and functions (Sohl &
29 Benjamin, 2012). Grassland is the major land-use type on the Mongolian Plateau; its degradation
30 was first witnessed in the 1960s. About 15% of the total grassland area was characterised as being
31 degraded in the 1970s, which rose to 50% in the mid-1980s (Kwon et al., 2016). In general,
32 grassland degradation (GD) refers to any biotic disturbance in which grass struggles to grow or can
33 no longer exist due to physical stress (e.g. overgrazing, trampling) or changes in growing conditions
34 (e.g. climate; Akiyama & Kawamura, 2007). In this study, grassland degradation is defined as
35 grassland that has been destroyed and subsequently classified as some other land use, or that has
36 significantly decreased in coverage.

37 Grassland is a land use that provides extensive ecosystem services (Bengtsson et al., 2019). When
38 degraded, the consequences are seen in an immediate decline in these services, such as a decrease
39 in carbon storage due to a reduction in vegetation productivity (Li et al., 2017). About 90% of carbon
40 in grassland ecosystems is stored in the soil (Nkonya et al., 2016). Furthermore, GD results in a
41 reduction in plant diversity and above-ground biomass available for grazing (Wang et al., 2014).
42 Likewise, GD leads to soil erosion and frequent dust storms in Inner Mongolia (Hoffmann et al.,
43 2008; Reiche, 2014). Drivers of GD are manifold, and have been analysed in a range of studies (Li
44 et al., 2012; Liu et al., 2019; Sun et al., 2017; Xie and Sha, 2012). However, few studies use
45 sophisticated driver analysis to predict spatial patterns of GD (Jacquin et al., 2016; Wang et al.,
46 2018). A number of studies have addressed the complex relationship between GD and its drivers
47 (Cao et al., 2013a; Feng et al., 2011; Fu et al., 2018; Tiscornia et al., 2019a). However, these studies
48 focus mainly on visualising or describing non-linear relationships between GD and its drivers.

49 The aim of developing various land-use models was to explore the causes and outcomes of land-use
50 dynamics; these models were implemented in combination with scenario analysis to support land
51 management and decision-making (National Research Council, 2014; Ren et al., 2019). Most such
52 models are statistical models, such as logistic regression models or models based on principle



53 component analysis (Li et al., 2013; Lin et al., 2014) or Bayesian belief networks (Krüger and Lakes,
54 2015). Some such models are spatial (e.g. CLUE-S, GeoSOS-FLUS, LTM, Fu *et al.*, 2018; Liang *et*
55 *al.*, 2018; Pijanowski *et al.*, 2002, 2005; Verburg & Veldkamp, 2004; Zhang *et al.*, 2013); others
56 are not (e.g. Markov models; Iacono et al., 2015; Yuan et al., 2015). Hybrid models, which combine
57 different approaches to make the best use of the advantages of each model, are another important
58 variety. This type of model is used to characterise the multiple aspects of LUCC patterns and
59 processes (Li and Yeh, 2002; Sun and Müller, 2013). In most cases of land-use change, it was either
60 assumed that the relationship between the drivers and the resulting land-use change is constant over
61 time (Fu et al., 2018; Samie et al., 2017; Zhan J Y et al., 2007), or the relationships were identified
62 as being linear or non-linear, but were not interpreted (Tayyebi and Pijanowski, 2014a). We
63 hypothesise that the relationships between GD and its drivers are mainly non-linear. We therefore
64 see a need for methods that are capable of analysing and interpreting non-linear relationships
65 between GD and dynamic drivers.

66 With the development of computer science, machine learning (ML) models have been increasingly
67 used in land-use change modelling (Islam et al., 2018; Krüger and Lakes, 2015; Lakes et al., 2009;
68 Tayyebi and Pijanowski, 2014a). ML is superior to the human brain when it comes to pattern
69 recognition in large datasets, e.g. images and sensor fields. Once the task is defined and the data for
70 training is provided, ML operates without any further human assistance. Various ML approaches
71 have been used in the analysis of land-use change processes, the most prominent of which being
72 Support Vector Machines (SVM, Huang *et al.*, 2009, 2010), Artificial Neural Networks (ANN,
73 Ahmadlou *et al.*, 2016; Yang *et al.*, 2016), Classification And Regression Trees (Tayyebi and
74 Pijanowski, 2014b) and Random Forest (RF, Freeman *et al.*, 2016). While the different ML
75 approaches generally perform well in identifying patterns, they remain a black box and make no
76 contribution to our understanding of how the underlying drivers act on the LUCC process.
77 Compared to linear methods such as logistic regression, ML models often achieve higher accuracy
78 and capture non-linear land-use change processes. Likewise, ML models relax some of the rigorous
79 assumptions inherent in conventional models, but at the expense of an unknown contribution of
80 parameters to the outcomes (Lakes et al., 2009). However, the key challenge is to crack the black
81 box and reveal how each driver affects the land-use change pattern or processes in the ML models.

82 The eXtreme Gradient Boosting (XGBoost) method has recently been developed as a supervised
83 machine learning approach (Chen and Guestrin, 2016). XGBoost algorithms have achieved superior
84 results in many ML challenges; they are characterised by being ten times faster than popular existing
85 solutions, and the ability to handle sparse datasets and to process hundreds of millions of examples.
86 XGBoost has already been used in land-use change detection, combined with remote sensing data
87 (Georganos et al., 2018), but has not yet been used in the simulation and prediction of land-use
88 change. SHapley Additive exPlanations (SHAP; Lundberg & Lee, 2016) is a unified approach to
89 explain the output of any ML model and to visualise and describe the complex causal relationship
90 between driving forces and the prediction target. We propose using SHAP to analyse the driver
91 relationships hidden in the black box model of XGBoost when employed for land-use change
92 modelling.

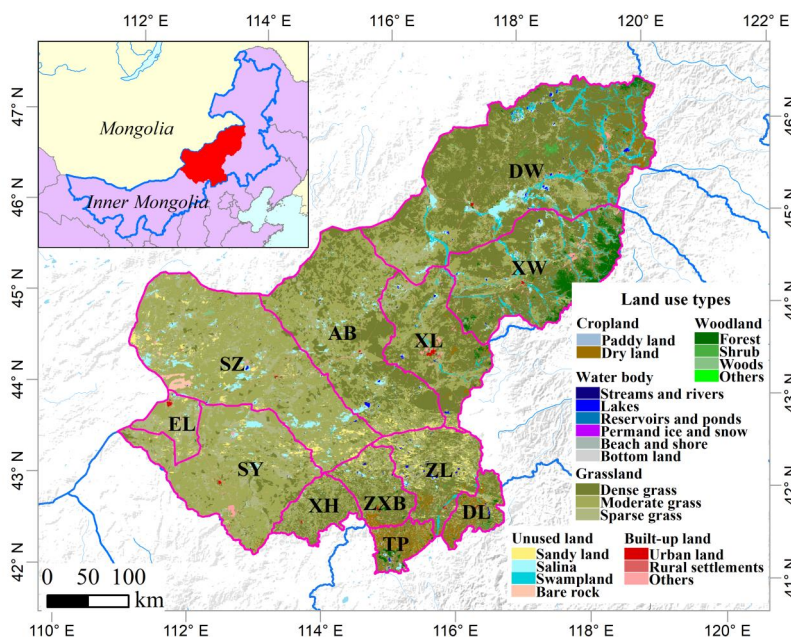
93 Having earlier used a clustering approach to identify drivers of GD in a case study in Inner Mongolia
94 (Xilingol League; Batunacun *et al.*, 2019), we now use XGBoost and SHAP to simulate GD
95 dynamics across the same area. We are primarily interested in learning whether ML models can
96 achieve a better predictive quality than linear methods, in addition to improving our understanding
97 of how grassland degrades in Xilingol. In the intention to identify areas with a high risk of further
98 degradation and to determine the drivers responsible for progressive degradation, we used XGBoost
99 to generate a data-driven model to explore the GD patterns. We then used SHAP to open the non-
100 linear relationships of the black box model stepwise, and transformed these relationships into
101 interpretable rules. The resulting model enabled us to map the primary GD drivers and GD hot spots
102 in Xilingol.



103 2. Materials and Methods

104 2.1 Study area

105 The Xilingol League is located about 600 km north of Beijing (He et al., 2004), in the centre of
106 Inner Mongolia. This administrative unit, covering an area of 206,000 km², spans from 41.4°N to
107 46.6°N and from 111.1°E to 119.7°E (Figure 1). The area is dominated by the continental temperate
108 semiarid climate. The frequent droughts (in summer) and “dzud” (an extremely harsh and snow-
109 rich winter) are the major natural disasters that occasionally lead to catastrophic livestock losses in
110 this region (Allington et al., 2018; Tong et al., 2017; Xu GC et al., 2014). Xilingol possessed about
111 18,104 km² available pasture resources and 1240.4·10⁴ sheep units at the end of 2015 (Xie and Sha,
112 2012). Around 1.044 million people lived in Xilingol in 2015, with ethnic Mongolian minorities
113 accounting for around 31% and the rural population for 37% (Batunacun et al., 2019; Shao et al.,
114 2017). Xilingol is a vast grassland, known for its high-quality meat products, nomadic culture, rich
115 mineral resources and ethnic minorities. The ongoing degradation of grassland is receiving
116 increasing attention. A set of economic stimuli and ecological protection policies launched in
117 Xilingol were viewed as the root cause of GD over the past four decades. Although large-scale
118 ecological restoration policies were implemented after 2000 in a bid to reduce GD, the problem still
119 persists.



120
121 Figure 1: The location of the Xilingol League in Inner Mongolia and its land uses.

122 2.2 Grassland degradation

123 This study defines grassland degradation (GD) based on land-use conversion, involving two kinds
124 of land-use change processes: (i) the complete destruction of grassland by transformation to another



125 type of land use (built-up land, cropland, woodland, water bodies and unused land), and (ii) a decline
126 in grassland coverage, which includes dense grass deteriorating into moderately dense grass and
127 sparse grass, and moderately dense grass deteriorating into sparse grass (see Fig. S 1a). Given that
128 GD is a dynamic process, we intended in this study to find the major drivers of newly added
129 grassland degradation (NGD). NGD refers to the difference in spatial GD extent between two
130 periods. About 13.0% of the total grassland area (176,410 km² in 2015) was degraded between 1975
131 and 2000 (Fig. S 1b); a further 10.6% was degraded in 2000-2015 (Fig. S 1c). Comparing the two
132 periods, approximately 10.2% of the grassland corresponded to the NGD area across the whole
133 region (Fig. S 1d). 18,093 pixels were extracted from the total NGD area, while the pixel number
134 of conversion for other land uses is 178,990 in this study (hereafter: non-NGD).

135 2.3 Data collection

136 In line with previous studies, a checklist of possible drivers (D) of GD was developed from the literature
137 (Cao et al., 2013b; Sun et al., 2017). A total of 19 drivers were grouped into four categories (see Table
138 1). All categories were described as follows: (1) Climate factors, including the annual mean temperature
139 (T) and annual sum of precipitation (P) in the growing season (April to Sep), were extracted from the
140 longest available weather dataset (from 1958-2015), in combination with evaluation data and the kriging
141 algorithm, to produce 1×1 km² raster files. (2) Geographic factors include elevation (DEM), and slope
142 and aspect (extracted from DEM data), which can be treated as the characteristic of each grid cell. The
143 DEM data were extracted from the SRTM 90m resolution and, after resampling, all data were processed
144 into 1×1 km² raster files. (3) Distance measures (the distance of each pixel centre to urban, rural, road
145 and mining, forest, cropland, dense grass, moderately dense grass, sparse grass and unused land pixels)
146 are widely used factors for different land-use models (Khoury, 2012; Samardžić-Petrović et al., 2016,
147 2017; Zhang et al., 2013). All distance measures were extracted from LUCC datasets from the years 2000
148 and 2015 using ArcGIS Euclidean distance, and processed into 1×1 km² grids. (4) Socio-economic
149 factors include the gross domestic product (GDP), sheep density and population density from 2000 and
150 2015. GDP and population density were obtained from a resources and environment data cloud platform,
151 CAS (<http://www.resdc.cn/>); sheep density data were accessed from statistical data; and we converted all
152 livestock data into grassland pixels. (5) Finally, we identified an area in which we assumed a strong
153 policy impact in the past, and developed a proxy for the policy effect on grassland degradation. Here, a
154 range of ecological protection measures were implemented inside and outside the Hunshandake and
155 Wuzhumuqin sand lands (see Fig. S 2), e.g. a livestock ban and the promotion of chicken farming (Su et
156 al., 2015). In a bid to explore policy effects, we assumed that GD is effectively slowed down by various
157 policies inside the sandy area (proxy set as 0), while outside the sandy area, land degradation is more
158 likely to happen in the absence of any policy effect (proxy set as 1, see Fig. S 2).



159 Table 1: Definition and derivation of drivers

Code	Name of driver	Definition of driver	Unit	Measures	Time series	Original format	Process approach	Data sources
Climate factors								
F1	temperature	Difference between average temperature / total precipitation in growth season (April-September) in Phase 1* and Phase 2*	°C	Mean temperature	2000, 2015-2030	Grid	Kriging via ArcGIS and Python language	National Meteorological Information Center (https://data.cma.cn/)
F2	precipitation		mm	cumulative rainfall	2000, 2015-2030			
Geographic factors								
F3	DEM	DEM	m	--		Grid	--	STRM
F4	slope	slope	degree	--		Grid	Reclassification	http://srtm.csi.cgiar.org/SELECTION/inputCoord.asp
F5	aspect	aspect	degree	--		Grid	Reclassification	
Distance measures								
F6	discrop	Change of distance to cropland in 2000 and 2015	m	Distance	2000, 2015	SHP	Euclidean	Extraction from land-use data
F7	disforest	Change of distance to forest in 2000 and 2015	m	Distance	2000, 2015			
F8	disunused	Change of distance to unused land 2000 and 2015	m	Distance	2000, 2015			
F9	disdense	Change of distance to dense grass 2000 and 2015	m	Distance	2000, 2015			
F10	dismode	Change of distance to moderate grass in 2000 and 2015	m	Distance	2000, 2015			
F11	dissparse	Change of distance to sparse grass 2000 and 2015	m	Distance				
F12	disurban	Change of distance to urban in 2000 and 2015	m	Distance	2000, 2015			
F13	disrural	Change of distance to rural in 2000 and 2015	m	Distance	2000, 2015			



F1 4	disroad	Change of distance to road in 2000 and 2015	m	Distance	2000, 2015			
F1 5	dismine	Change of distance to mining in 2000 and 2015	m	Distance	2000, 2015			
F1 6	diswater	Change of distance to water in 2000 and 2015	m	Distance	2000, 2015			
Social-economic factors								
F1 7	population density	Change of population density in 2000 and 2010	Person	Person/ km2	2000, 2010	Grid	Density	Resource and Environment data cloud platform, CAS. (http://www.resdc.cn/)
F1 8	GDP*	Change of GDP in 2000 and 2010	Yuan	Yuan/km2	2000, 2010	Grid	Density	
F1 9	sheep density	Change of sheep density in 2000 and 2015	Sheep Unit	Sheep unit/km2	2000, 2015	Grid	Density	
Scenario setting								
F2 0	policy	--	--	(0,1)	--	Grid	--	Assumption

160 *Note: Phase 1 refers to 1975-2000; Phase 2 refers to 2000-2015. GDP: gross
 161 domestic product.



162 2.3.1 XGBoost and logistic regression

163 Two algorithms were selected in this study: logistic regression (LR) and XGBoost. LR is a linear
164 method involving two parts: the statistic LR and the classification LR. Both methods have already
165 been used to simulate land use (Lin et al., 2011; Mustafa et al., 2018) and to define the relationship
166 between land-use change and its drivers (Gollnow and Lakes, 2014; Mondal et al., 2014; Verburg et
167 al., 2002; Verburg and Chen, 2000). Here, we use LR as a benchmark model to compare linear and
168 non-linear methods in the simulation of land-use change. The optimised parameters of LG are $C =$
169 0.1 , $\text{penalty} = \text{l2}$, $\text{solver} = \text{'lbfgs'}$, $\text{multi_class} = \text{'multinomial'}$.

170 Boosting algorithms have been implemented in many past studies, where they often outperformed
171 other ML algorithms (Ahmadlou et al., 2016; Filippi et al., 2014; Freeman et al., 2016; Keshtkar et
172 al., 2017; Tayyebi and Pijanowski, 2014a). However, traditional boosting algorithms are often
173 subject to overfitting (Georganos et al., 2018). To overcome this problem, Chen and Guestrin (2016)
174 presented a new, regularised implementation of gradient boosting algorithms, which they called
175 XGBoost (eXtreme Gradient Boosting). XGBoost was built as an enhanced version of the gradient
176 boosting decision tree algorithm (GBDT), a regression and classification technique developed to
177 predict results based on many weak prediction models – the decision tree (DT) (Abdullah et al.,
178 2019; Freeman et al., 2016). XGBoost provides strong regularisation by adopting a stepwise
179 shrinkage process instead of the traditional weighting process provided by GBDT. This process
180 limits overfitting, minimises training losses and reduces classification errors while developing the
181 final model (Abdullah et al., 2019; Hao Dong et al., 2018).

182 The XGBClassifier uses the following parameters: `learning_rate` (controls learning itself);
183 `max_depth` (control depth of the RF); the `n_estimators` (controls the number of estimators used for
184 the model); the `min_child_weight` (controls the complexity of a model, defines the minimum sum
185 of weights of all observations required in a child); and `lambda` (L2 regularisation term on weights).
186 The parameters were optimised using a simple grid search algorithm provided by scikit (Pedregosa
187 et al., 2011) to estimate the optimal parameters (`learning_rate = 0.1`, `max_depth = 9`, `n_estimator =`
188 `500`, `min_child_weight = 3`, `lambda = 10`).

189 2.3.2 Sampling methods

190 Data are often distributed unevenly among different classes (Vluymans, 2019). Such imbalanced
191 class distribution generally induces a bias. Canonical ML algorithms assume that data is roughly
192 balanced in different classes. In real situations, however, the data is usually skewed, and smaller
193 classes often carry more important information and knowledge than larger ones (Krawczyk, 2016).
194 It is therefore important to develop learning from imbalanced data to build real-world models
195 (Krawczyk, 2016; Vluymans, 2019). To ensure a highly accurate GD model, we introduced four
196 different sampling methods in this study (Fig. S 3).

197 **Balanced sampling:** Random data sampling, resulting in equal sized samples.

198 **Imbalanced sampling:** Random data sampling, but with the same share of the sampled class,
199 resulting in unequal sized samples.

200 **Over-sampling:** Artificial points are added to the minority class of an imbalanced sampling set,
201 making it equal to the majority class and resulting in equal sized samples.

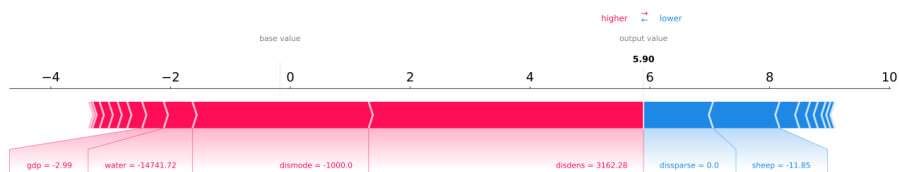
202 **Under-sampling:** Points are removed from a majority class of an imbalanced sampling set,
203 making it equal to the minority class and resulting in equal sized samples (He and Garcia, 2009).



204 In the present study, we used these four sampling methods to evaluate the model in the context of
205 the sampling method and its performance in the training process and the simulation process (see Fig.
206 S 3). In our case study, 18,190 pixels (about 10% of the total) were selected by different sampling
207 methods (Fig. S 3) to train (66% of the sample size) and test (34% of the sample size) the model.

208 2.3.3 SHAP values

209 SHAP (SHapley Additive exPlanations) is a novel approach to improve our understanding of the
210 complexity of predictive model results and to explore relationships between individual variables for
211 the predicted case (Lundberg and Lee, 2017). SHAP is a useful method to sort the driver's effects,
212 and break down the prediction into individual feature impacts. Feature selection is of primary
213 concern when using ML methods to process land-use change (Samardžić-Petrović et al., 2015, 2016,
214 2017). SHAP values show the extent to which a given feature has changed the prediction, and allows
215 the model builder to decompose any prediction into the sum of the effects of each feature value and
216 explain – in our case – the predicted NGD probability for each pixel (see Figure 3). In this study,
217 we used SHAP values to sort the driver's attributions; capture the relationship between drivers and
218 NGD; and map the primary driver for NGD at the pixel level.



219

220 Figure 2: Decomposed SHAP values for the individual prediction of an example pixel.

221 In our study, we define the *base value* as the value that would be predicted by the model if no feature
222 knowledge were provided for the current output (mean prediction); we define the output value as
223 the prediction for this particular observation. SHAP values are calculated in log odds. Features that
224 increase the value of the prediction (to the left in Fig. 2) are always shown in red; those that lower
225 the prediction value are shown in blue (to the right in Fig. 2, Dataman, 2019). In this instance (Figure
226 2), *disdense* (change of distance to dense grass) is the primary driver of NGD at this pixel level
227 (largest value). The fact that the value is positive means that the risk of NDG increases in line with
228 an increase in distance to dense grass areas.

229 2.3.4 Validation of the model

230 Two validation steps are required for ML models: validation of the training process, and validation
231 of the simulation process. For the training process, a robust model was selected using overall
232 classification accuracy, precision, recall and the kappa index. Accuracy, precision and recall were
233 calculated based on a confusion matrix (CM) (He and Garcia, 2009). For the simulation process, the
234 final model was validated using the kappa index, the area under the precision-recall curve, and recall.
235 The validation indicators are defined as follows.

236 Overall classification accuracy (ACC) is the correct prediction of NGD and other pixels in the whole
237 region. This indicator was used to evaluate the accuracy of the model. Precision is the proportion of
238 correctly predicted positive examples (refers to NGD in this study) in all predicted positive examples.
239 Recall is the proportion of correctly predicted positive examples in all observed positive examples
240 (the observed NGD) (Sokolova and Lapalme, 2009). In general, high precision predictions have a
241 low recall, and vice versa, depending on the predicted goals. Here, since we focus on NGD and
242 other land-use changes, we use both indicators to evaluate our models.



243 Table 2: Confusion matrix for binary classification of newly added grassland degradation (NGD) and
 244 other changes, including four indicators: false positives (FP), cells that were predicted as non-change but
 245 changed in the observed map; false negatives (FN), cells that were predicted as change, but did not
 246 change in the observed map for disagreement; true positives (TP), cells that were predicted as change
 247 and changed in the observed map; and true negatives (TN), cells that were predicted as non-change and
 248 did not change in the observed map for agreement.

Simulated values	Observed values			Recall=TP/(TP+FN)
	Others NGD	Others	NGD	
		True negatives (TN)	False positives (FP)	
False negatives (FN)	True positives (TP)			
ACC=(TP+TN)/(TP+FN+FP+TN)				

249 The precision-recall curve (PR curve) provides more information about the model’s performance
 250 than, for instance, the Receiver Operator Characteristic curve (ROC curve), when applied to skewed
 251 data (Davis and Goadrich, 2006). The PR curve shows the trade-off of precision and recall, and
 252 provides a model-wide evaluation. The area under the PR curve (AUC-PR) is likewise effective in
 253 the classification of model comparisons. The baseline for the PR curve (y) is determined by positives
 254 (P) and negatives (N). In our study, $y = 0.09$ ($y = 18374/200652$), which means when AUC-PR =
 255 0.09, the model is a random model (Brownlee, 2018; Davis and Goadrich, 2006).

256 The kappa index (κ) is a popular indicator used to measure the proportion of agreement between
 257 observed and simulated data, especially to measure the degree of spatial matching. When $\kappa > 0.8$,
 258 strong agreement is yielded between the simulation and the observed map; $0.6 < \kappa < 0.8$ describes
 259 high agreement; $0.4 < \kappa < 0.6$ describes moderate agreement; and $\kappa < 0.4$ represents poor agreement
 260 (Landis and Koch, 1977).

261 In this study, κ was used to evaluate the agreement and disagreement between observed NGD and
 262 simulated NGD. Kappa should be the primary validation measure, followed by AUC-PR (used to
 263 evaluate model performance) and recall (used to evaluate model sensitivity). Features and
 264 definitions of these indicators are given below.

265 2.3.5 The structure of the ML model

266 The ML methodology of simulating GD involves six steps (Fig. S 4): (1) Target definition and data
 267 collection and processing; the targets of this study are to build a robust ML model for simulating
 268 NGD, as well as visualising these complex relationships between various variables and the dynamics
 269 of GD. A total of 20 drivers (D) of GD were collected. All dynamic drivers were processed by GIS
 270 into raster files and exported into ASCII files as final inputs for the ML model. (2) Data organisation:
 271 the ML model simulates land-use change as a classification task (Samardžić-Petrović et al., 2015,
 272 2017). In the present study, we organise this task as a binary classification Y (value 1 and 0, stand
 273 for NGD and Non-NGD); related drivers are x ($x_1, x_2, x_3, \dots, x_n$), n is the driver identifier, and x
 274 denotes the change in value of each driver. The process of data standardisation is usually necessary
 275 for most ML models, but since XGBoost is a tree-based method, it does not require standardisation
 276 or normalisation. In this case, we performed standardisation only for the logistic regression model.
 277 (3) Data sampling: this is a necessary step to avoid overfitting or the loss of important information.
 278 The sampling method generally includes balanced and imbalanced sample strategies. In this study,
 279 we tested various balanced sampling strategies to identify the most suitable one. (4) Model building
 280 and selection: a ranking was used to find the best model in each specific case. In our study, we
 281 defined a model with $\kappa > 0.8$ and AUC-PR>0.09 as robust, while $0.6 < \kappa < 0.8$ and AUC-PR>0.09
 282 represents an acceptable model. (5) Model validation and feature ranking: after tuning the model,
 283 the most robust model and the driver with most useful information are selected. (6). The last step is



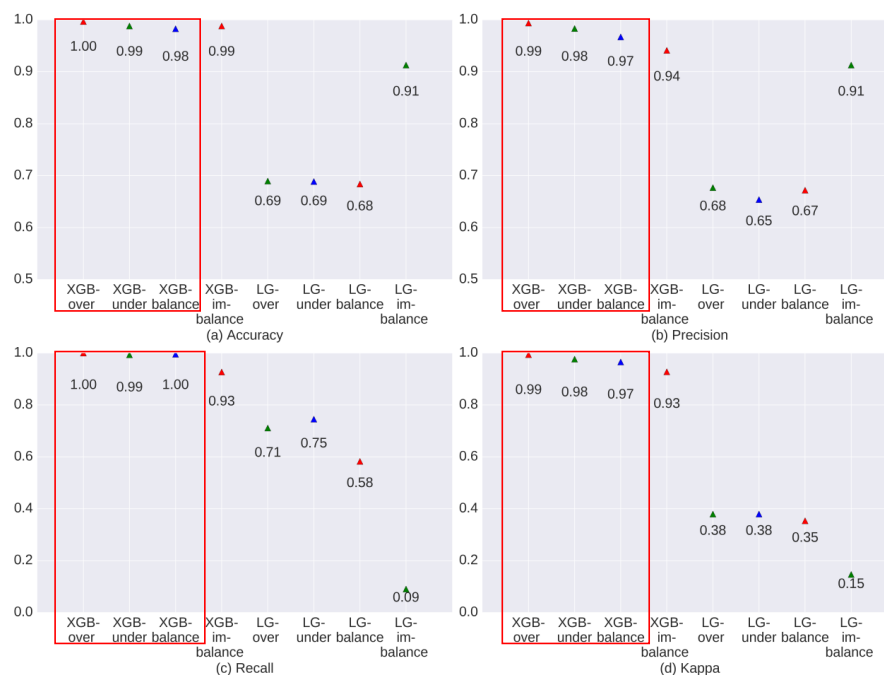
284 explaining the model and the simulation.

285 3. Results

286 3.1 Model validation

287 The XGBoost model outperformed the LG model in both training and simulation (Figure 3 and 4).
 288 The LG model seems to be an inappropriate model for understanding NGD in this case. XGBoost
 289 yielded robust results in both training and simulation, with indicator values almost entirely above
 290 90%.

291 Figure 3 indicates that XGBoost performed very well across all balanced sampling methods (over-
 292 sampling, under-sampling and balanced sampling, red rectangle in Figure 3) in the training process.
 293 Only the imbalanced sampling exhibited a slightly weaker performance in the training process. This
 294 is mainly due to the balanced sampling datasets, which provided more information for the model.
 295 In addition, the model was affected less than the imbalanced sampling method by the majority class
 296 or unchanged cells (Mileva Samardzic-Petrovic et al., 2018).



297

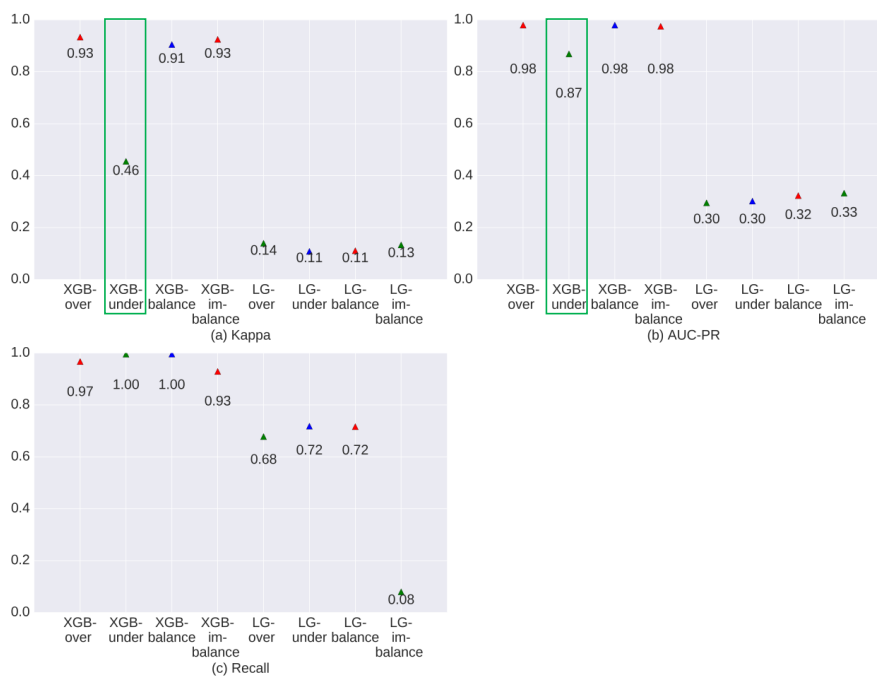
298 Figure 3: Evaluation of model performance during the training process.

299 Figure 4 and Figure 5 show the model evaluation results in the simulation process and the spatial
 300 prediction maps. XGBoost with under-sampling (green rectangle in Figure 4) yielded the weakest
 301 performance compared to the other three sampling methods. This is mainly due to the smaller
 302 sample size, which prevents the model from extracting sufficient experience. As can be seen in
 303 Figure 5b, XGBoost used with the under-sampling method produced the error map with the highest



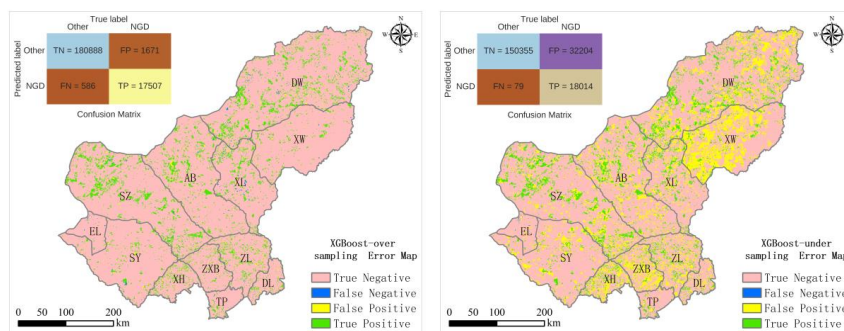
304 FP values, where the model predicted non-change points as change points. The under-sampling
 305 method is unable to identify NGD points sufficiently well. XGBoost used with the over-sampling
 306 method caused balanced and imbalanced sampling to have similar and strong prediction abilities
 307 (see Figure 4), differing only slightly in their CM indicators (see Figure 5). We finally selected
 308 XGBoost combined with the over-sampling strategy for our study, mainly because of its relatively
 309 higher values in κ , AUC-PR and recall (see Figure 4).

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312 Figure 4: Evaluation of model performance during the prediction process.

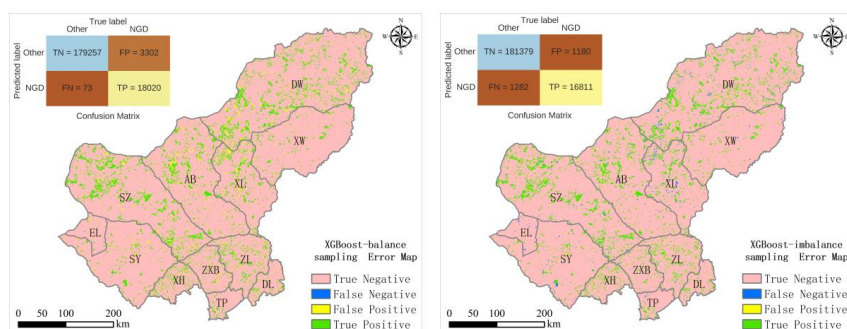


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(a) Over-sampling

(b) Under-sampling



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(c) Balanced sampling

(d) Imbalanced sampling

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Figure 5: Error map of different sampling methods using the XGBoost model.

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3.2 Driver selection

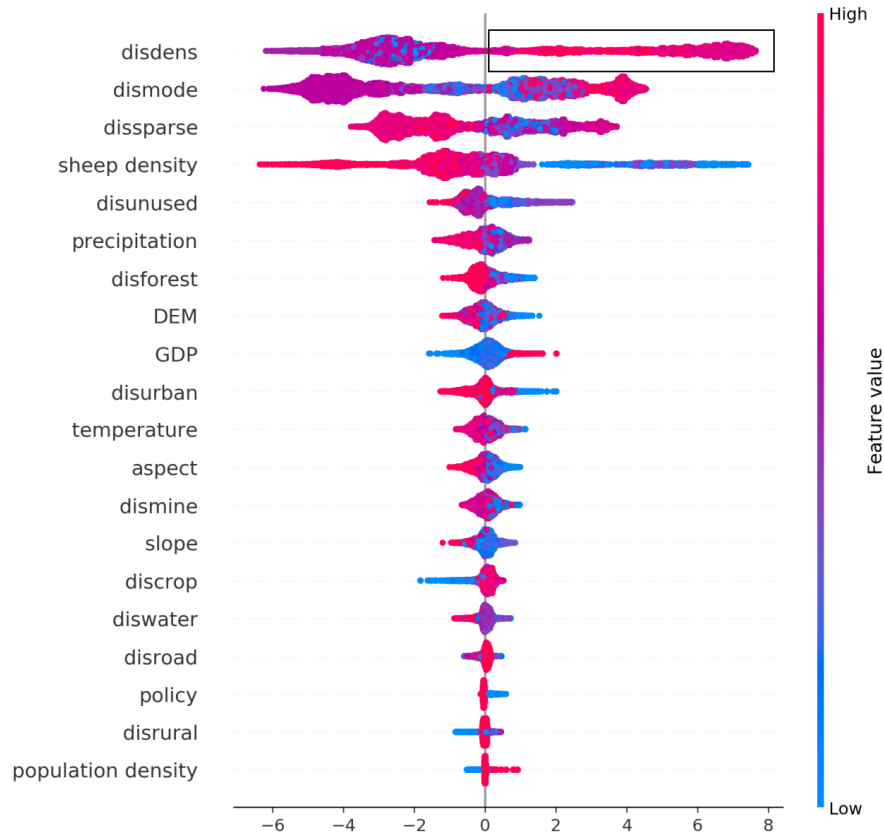
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Figure 6 is a summary plot produced from the training dataset; it includes approximately 13,200 points (66% of the sample size). This plot combines feature importance (drivers are ordered along the y-axis) and driver effects (SHAP values on the x-axis), which describe the probability of NGD having occurred. Positive SHAP values refer to a higher probability of NGD. The gradient colour represents the feature value from high (red) to low (blue), as previously introduced in Figure 2. As Figure 6 shows, *disdense* was the primary driver for NGD in the study region. The relationship between *disdense* and NGD is non-linear, which can be seen from the SHAP values being both positive and negative (black rectangle in Figure 6). The interpretation of the effects of *disdense* can be summarised as a higher probability of NGD with increasing distance from dense grassland (see black rectangle in Figure 6 with pink colour on the right).

329

Figure 6 shows that driver effects include both linear-dominated relationships, such as *sheep*, *GDP* and others, and non-linear-dominated relations, such as *disdense*, *dismode* and others. In addition, the figure shows that the most important drivers for NGD are the changes of distance to dense, moderately dense and sparse grassland, then followed by sheep density and the distance to unused land. The effect of policies comes almost at the bottom, indicating that policies implemented outside sandy areas seem to have little effect on GD. The geographical factors DEM and slope are also positioned mid-field. The effect of geographical drivers does not appear to be as strong as the effect of other drivers. The change of distance to mining, located at the bottom for all drivers, does not have a strong effect on NGD compared to other drivers.

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339 Figure 6: Driver ranking by SHAP values based on the training dataset (66% of sample size) using the
340 over-sampling method.

341 Note: The top rank indicates the most significant effects across all predictions. Each point in the cloud to
342 the left represents a row from the original dataset. The colour code denotes high (red) to low (blue) feature
343 values. Positive SHAP values represent a higher likelihood of NGD, while negative values indicate lower
344 likelihoods. The range across the SHAP value space indicates the degradation probability, expressed as
345 the logarithm of the odds.

346 A recursive attribute elimination method was performed to determine how attribute reduction affects
347 modelling performance using XGBoost with the oversampling method (see Fig. S 5; for more details,
348 refer to Samardžić *et al.*, 2015). The results indicate that the first three drivers may already produce
349 a satisfactory model ($\kappa = 0.74$, AUC-PR = 0.85, recall = 0.92), while adding the fourth driver can
350 produce a robust model ($\kappa = 0.94$, AUC-PR = 0.98, recall = 0.98). This means that XGBoost used
351 with the oversampling strategy can predict NGD with very high accuracy using a relatively small
352 amount of data. Fig. S 6 shows the simulation result using the first four drivers, and compares the
353 results with the observed map.

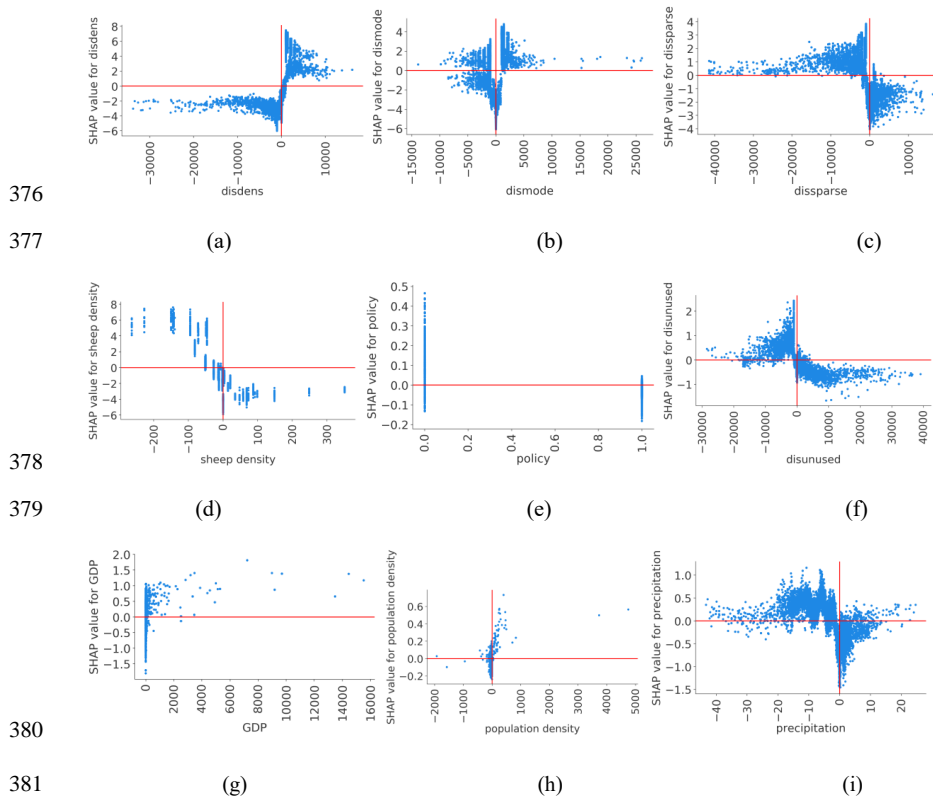
354 3.3 Relationship between NGD and drivers in the XGBoost model

355 SHAP values and spread (Figure 7) indicate that no linear relationship between driver and prediction



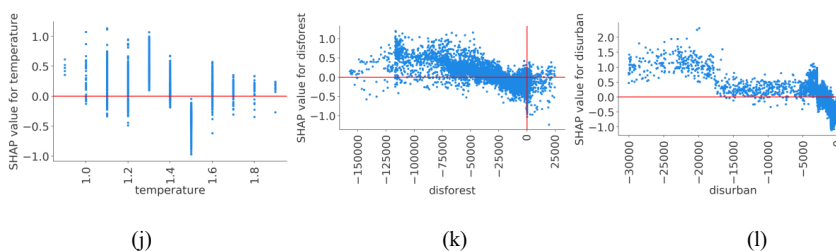
356 could be found for any of the individual features. Change of distance to dense, moderately dense
 357 and sparse grass pixels, and change of sheep density were the dominant drivers for NGD. Figure 7a
 358 indicates that when $disdense < 0$, the SHAP value is negative, and when the distance to dense grass
 359 areas is small, the likelihood of degradation is also small. The relationship seems to be more
 360 complex for distance to moderately dense grass ($dismode$, Figure 7b); here, no simple linear
 361 interpretation is obvious. For distance to sparse grass ($disparse$, Figure 7c), the pattern again
 362 suggests a rather linear interpretation, which is that the likelihood of degradation increases with
 363 decreasing distance. For sheep density, Figure 7d indicates that when sheep density decreased, the
 364 probability of GD obviously increased. Policy was not identified as a major driver of GD (Figure
 365 6). However, policy effects obviously have a different impact inside and outside sandy zones. Figure
 366 7e shows that our initial assumption is invalid: the probability of GD increased inside the sandy
 367 areas where we assumed effective policy measures to be in place (value 0). This result is also in line
 368 with Figure 7g, which shows that the closer to unused land, the more likely degradation will occur.

369 We can identify three groups for the remaining 14 drivers. For GDP and population density (Figure
 370 7g and Figure 7h), the likelihood of NGD increases with increasing values. Figure 7i-j indicate that
 371 warmer and drier climate conditions increase the probability of GD. Figure 7k, l, m and n indicate
 372 that the probability of GD rises with closer distances to forest, urban, rural and water areas. Figure
 373 7o shows a slight SHAP value pattern, in which the closer to cropland, the more unlikely degradation
 374 will occur. This is mainly due to transformation from cropland to grassland. Figure 7p-t do not show
 375 any interpretable spatial pattern.

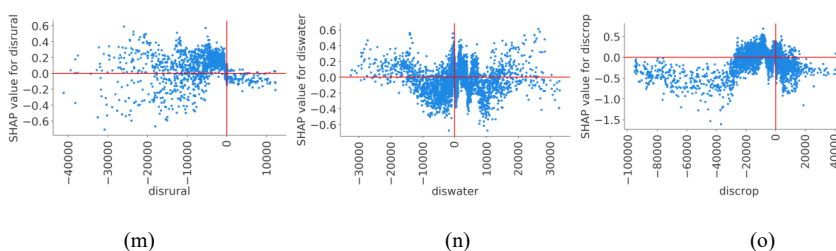




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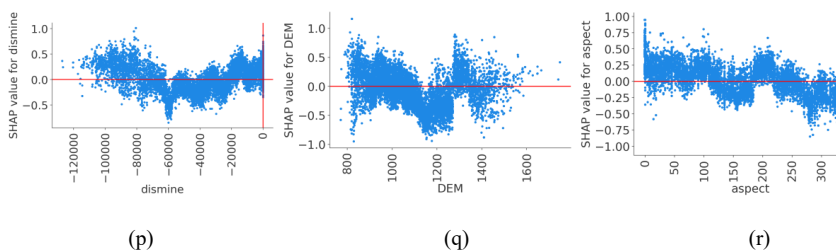


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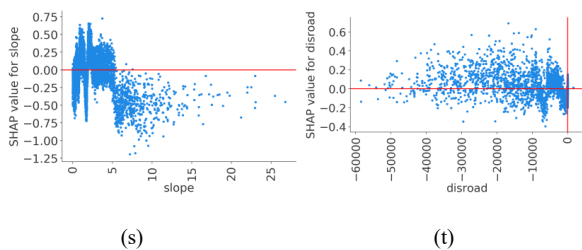
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Figure 7: The SHAP dependence plot for each driver.

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3.4 Mapping the primary drivers of NGD

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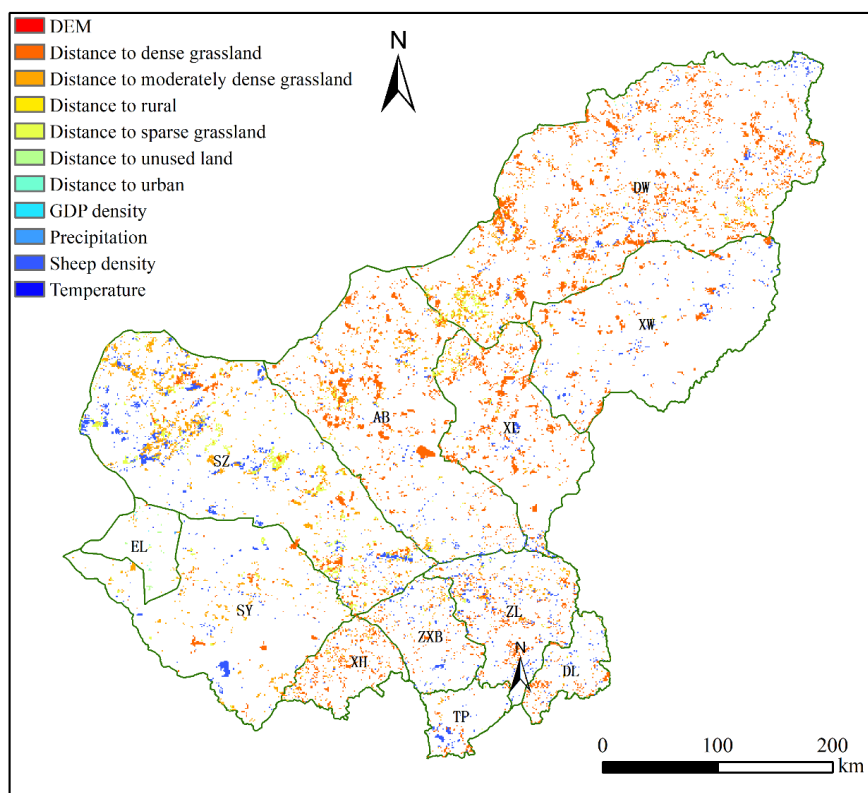
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All drivers' contributions to NGD were ranked according to their SHAP values for each pixel in this study. Figure 8 shows the primary driver for each NGD pixel. Distance to grassland pixels (dense, moderately dense and sparse grass) were the major drivers of NGD, responsible for 9,478, 3,892 and 1,629 NGD pixels, respectively. Sheep density was responsible for 3,042 NGD pixels, ranking third among all drivers. This order differs to that in Figure 6 and Figure 8 because in those cases, ranking is based on the total contribution of all drivers. Fig. S 7 shows the number of NGD pixels in which a driver was dominant or primary. The change of distance to any type of grassland was the primary driver for about 82.8% of the total NGD pixels; sheep density accounted for 16.8%. The



400 remaining seven drivers caused less than 1% of the total NGD. We can see from the spatial pattern
401 that the change of distance to grassland was the major driver for GD in the dense grassland region
402 (counties of DW, XL and AB), while in the counties of SZ, SY, ZXB, ZL and TP, sheep density was
403 often identified as the major driver.



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Figure 8: Spatial patterns of primary drivers for each pixel.

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3.5 Regions of high risk for grassland degradation

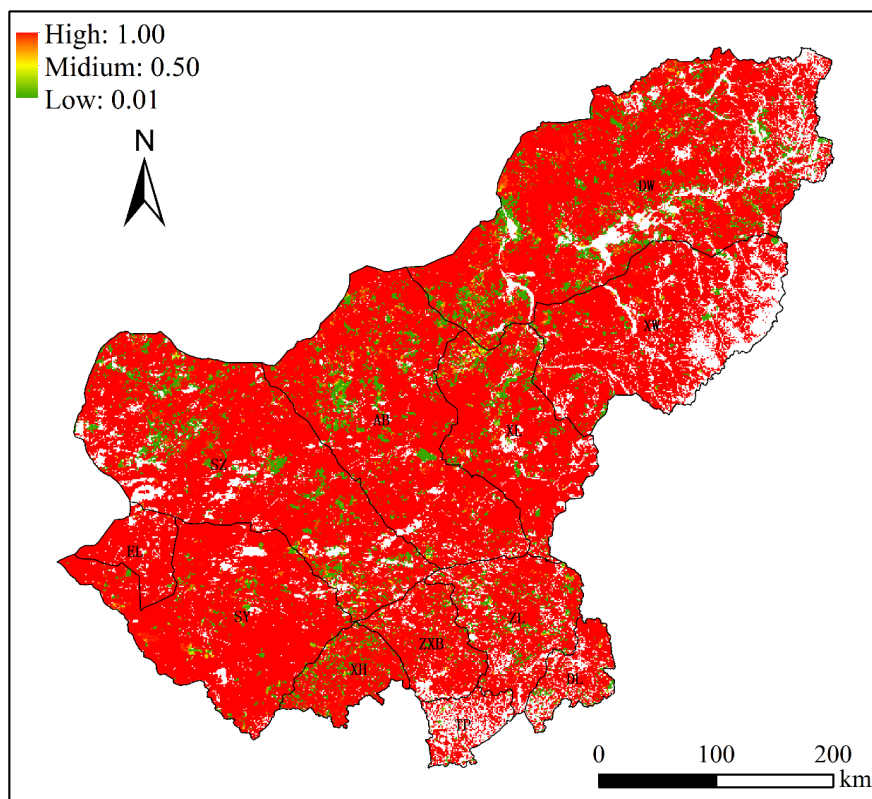
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A probability map of NGD was produced (Figure 9). Low probabilities of NGD were found in the central and northern counties (DW, XL, AB, SZ, ZL, ZXB and XH), while high probability regions were EL, SY and XW. TP and DL in the south were categorised as low probability regions, due to their lower share of grassland area.



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Figure 9: Degradation probability map for grassland in Xilingol.

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4. Discussion

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4.1 ML model building and evaluation

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In this study, we defined a general framework for creating an ML model using the XGBoost algorithm for the purpose of analysing and predicting land-use change. XGBoost obtained a κ of 93% and a recall value of $> 99\%$ when used to simulate and predict GD in this study. Compared to other popular ML learning algorithms, XGBoost exhibited a strong prediction ability. In studies where ANN, SVM, RF, CART, Multivariate Adaptive Regression Spline (MARS) or LR were used in combination with Cellular Automata (CA), the recall value is usually 54%-60% (Shafizadeh-Moghadam et al., 2017). Ahmadlou *et al.* (2019) stated that MARS and RF only yield high accuracy in training runs, but do not prove very accurate in the validating process when simulating land-use change.

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Concerning the four sampling strategies we used to test the imbalance issue, we found that all strategies performed satisfactorily in the training runs. In the simulation, the under-sampling strategy yielded a relatively low accuracy ($\kappa = 0.46$) model. We assume that removal of data from the majority class causes the model to lose the important concepts pertaining to the majority class



428 (He and Garcia, 2009). XGBoost used with the under-sampling method always produced similar
429 results, irrespective of the size of the dataset (see Fig. S 8). We conclude from this pattern that
430 XGBoost is also able to use sparse data to reflect real-world problems (Chen and Guestrin, 2016).

431 4.2 SHAP values and drivers of grassland degradation

432 The general idea of introducing SHAP values as a further tool to analyse XGBoost ranking is to
433 provide a method to evaluate the ranking with respect to causal relationships. The original XGBoost
434 ranking is based on the in-built feature selection functions *Gain* (refers to the improvement in
435 accuracy provided by a feature), *Weight* (or frequency, refers to the relative number of a feature
436 occurrence in the trees of a model) and *Coverage* (refers to the relative numbers of observations
437 related to this feature). However, these functions always produce different rankings of drivers (Abu-
438 Rmoleh, 2019) due to random components in the algorithms. SHAP values introduce two further
439 properties of feature importance measures: *consistency* (whenever we change a model such that it
440 relies more on a feature, the attributed importance for that feature should not decrease) and *accuracy*
441 (the sum of all feature importance values should equate to the total importance of the model;
442 Lundberg, 2018; Lundberg & Lee, 2017). Consistency is required to stabilise the ranking throughout
443 the analysis, reducing the change of order in the ranking to a minimum when the number of
444 identified drivers changes. The accuracy property of SHAP makes sure that each driver's
445 contribution to overall accuracy remains the same, even when drivers are excluded from analysis.
446 Other methods usually compensate for the withdrawal of a driver from the analysis, which makes
447 the determination of a single driver's contribution difficult.

448 The feature ranking based on SHAP values indicated that the change of distance to any type of
449 grassland (dense, moderately dense and sparse grass) is the most important driver for any newly
450 added grassland degradation. In this context, dense and moderately dense grassland areas are more
451 easily degraded than other land-use types, followed by sparse grass. These results are in line with
452 previous studies (Li et al., 2012; Xie and Sha, 2012). Good-quality grassland is more likely to be
453 degraded through increasing human disturbance. An explanation for this can be derived from local
454 people's living strategies. People who live in good-quality grassland areas are more likely to use
455 grassland for livestock production with higher animal densities, risking overgrazing. Furthermore,
456 Li et al. (2012) indicated that good-quality grassland is more likely to be converted to other land-
457 use types, such as cropland. In contrast, people who have lived in sparse grassland regions for
458 centuries have long adapted to low productivity, reducing their livestock numbers accordingly. They
459 have also developed strategies to cope with variability in weather conditions, e.g. by preparing and
460 storing more fodder and forage.

461 Sheep density was identified as the fourth major driver. However, the SHAP values indicate that
462 when sheep density decreases, the probability of grassland degradation increases. Overgrazing has
463 been the dominant driver for grassland degradation on the Mongolian plateau before, which has
464 changed the grassland ecosystem significantly towards lower grass coverage (Nkonya et al., 2016;
465 Wang et al., 2017). However, there is recent evidence that this causal relationship has changed. It
466 now appears that farmers increasingly select their livestock numbers according to the carrying
467 capacity of the grazing land (Cao et al., 2013b; Tiscornia et al., 2019b). By passing the "Fencing
468 Grassland and Moving Users" policy (FGMU), the Chinese government issued a law that regulates
469 livestock numbers based on a previously calculated carrying capacity. This development has
470 upturned the causal relationship between livestock numbers and NGD, reflected by the SHAP value
471 pattern in Figure 6.

472 Besides the four main drivers, seven other drivers also occasionally appear as the main driver for
473 some pixels (Figure 8). This highlights the fact that, at the local level, other drivers apart from the
474 four drivers identified as being major can also play a significant role. For example, in the county of
475 EL, the remaining seven drivers were mainly responsible for NGD. EL has less NGD after 2000



476 compared with other counties in Xilingol (Fig. S 1), and most of the EL area is covered by sparse
477 grass. EL is the most frequented border control point to Mongolia, and is subject to intensive tourism.

478 In the sparse grassland and agro-pastoral regions (SZ, SY, ZXB, ZL and TP), sheep density was
479 identified as the important driver. This indicates that, even though livestock numbers have decreased,
480 grassland is still experiencing serious degradation in this region. Here we see additional potential
481 for installing further grassland conservation measures, such as adjusting the livestock number to the
482 grassland carrying capacity.

483 **4.3 The current risk of grassland degradation in Xilingol**

484 Three regions of different risk classes were identified in the probability map of NGD (Fig. 9). The
485 low-risk region (DW, XL, AB, SZ, ZL ZXB and XH) is dominated by good-quality grassland (dense
486 and moderately dense grass). In recent decades, this region has suffered from increasing human
487 disturbance, e.g. overgrazing and mining development. However, after 2000, grassland in this region
488 has recovered, mainly as the result of ecological protection projects (Sun et al., 2017). Even though
489 this region is predicted as being less exposed to the risk of land degradation in the future, attention
490 is still required for the restoration process. The high-risk region includes the counties of EL, SY and
491 XW. EL and SY are covered by a large share of low-quality grassland, which – due to its own
492 fragility – is likely to be affected by extreme climate and human disturbance, more than, e.g. higher-
493 quality grasslands. The recent change in grassland property rights and the establishment of
494 ecological protection projects have also limited the mobility of nomadic herders throughout Xilingol.
495 As a consequence, herders cannot easily change grazing spots if extreme weather occurs; they are
496 then bound to have their cattle graze at the same spots, increasing the pressure on low-quality
497 grasslands in particular (Qian, 2011). For a long time, fragile grassland remained in an equilibrium
498 state with the extreme weather (frequent droughts, “dudz”) to which it was exposed, and with the
499 nomadic livestock husbandry that the region’s inhabitants practised. However, when the property
500 rights of grassland and livestock were changed from collective to private, the nomadic lifestyle was
501 largely abandoned.

502 **4.4 The limitations of XGBoost for scenario exploration**

503 XGBoost has already scored top in a range of algorithm competitions in the data scientists
504 community (Kaggle, 2019) due to its high accuracy and speed (Chen and Guestrin, 2016). ML
505 models extract patterns from data, without considering any existing expert knowledge, which is why
506 they are increasingly used to identify non-linear relationships (Ahmadlou et al., 2016; Samardžić-
507 Petrović et al., 2015; Tayyebi and Pijanowski, 2014b). However, ML models require specific data
508 structures for each problem to which they are applied. In this study, we simulated grassland
509 degradation in two different phases (1975-2000 and 2000-2015). All time series of driver data were
510 organised as model inputs, while grassland degradation dynamics were organised as prediction
511 targets. Although the model achieved high accuracy in predicting NGD in Phase 2, it was not
512 possible to achieve acceptable results in simulating both Phase 1 and Phase 2 separately. Second,
513 compared with conventional models, the XGBoost model cannot be easily transferred to other
514 regions for the same research question. Models like CLUE-S and GeoSOS-FLUS have been widely
515 used in different regions across the world (Fuchs et al., 2017; Liang et al., 2018a; Liu et al., 2017;
516 Verburg et al., 2002). When ML models are used in other regions, driver data must be collected and
517 structures adapted. Thirdly, ML models always need to learn sufficiently before they are able to
518 make predictions. This requires a sufficient amount of data covering historical periods or different
519 land-use change patterns.

520 XGBoost alone is unable to project any scenarios of land-use change based on historical data.
521 However, the methodology presented here can be applied to quantify alternative scenarios produced
522 using other approaches, such as conventional, rule-based models (Verburg et al., 2002) or cellular



523 automata (Islam et al., 2018; Shafizadeh-Moghadam et al., 2017).

524 **5 Conclusion**

525 Machine learning and data-driven approaches are becoming more and more important in many
526 research areas. The design and development of a practical land-use model requires both accuracy
527 and predictability to predict future land-use change, a well-fitted model that reflects and monitors
528 the real world (Ahmadlou et al., 2019). The method framework presented here for building an ML
529 model and explaining the relationship between drivers and grassland degradation identified
530 XGBoost as a robust data-driven model for this purpose. XGBoost showed higher accuracy in
531 training and simulation compared to existing ML models. Combined with over-sampling, it slightly
532 outperformed in the simulation process. The simulated map has a high agreement with the observed
533 values ($\kappa=93\%$).

534 We identified six basic steps that should be included in ML model building, and they are also similar
535 for other research applications (Kiyohara et al., 2018, 2018; Kontokosta and Tull, 2017;
536 Subramaniyan et al., 2018). However, different validation measures can be introduced in both the
537 training process and the simulation process. In this study, we tested different evaluation measures
538 to evaluate the ML model, e.g. a typical confusion matrix to evaluate the training process, AUC-PR
539 to evaluate the goodness of the ML model, and the kappa index to measure the degree of matching
540 between observed and simulated values. These validation indicators consider both the research
541 object and data characteristics. For example, when the data size is unbalanced, AUC-PR is a better
542 choice than AUC-ROC (Brownlee, 2018; Davis and Goadrich, 2006; Saito and Rehmsmeier, 2015).

543 SHAP was introduced in this context to provide a causal explanation of the patterns identified by
544 the ML model. In our case, SHAP was used to explain how drivers contribute to grassland
545 degradation processes at the pixel and regional level, despite their non-linear relationship.
546 According to the analysis, the distance to dense, moderately dense, and sparse grass, and sheep
547 density, were the most important drivers that caused new grassland degradation in this region. In
548 addition, individual SHAP values of sheep density indicated that the causal relationship between
549 grassland degradation and livestock pressure has changed over time: the increase in sheep density
550 was not the major driver for NGD in Phase 2 of the land degradation trajectory. Instead, the decrease
551 in the grazing capacity of grassland caused a decrease in livestock numbers. The primary driver map
552 of NGD provided a more detailed picture of NGD drivers for each pixel, as an important support
553 for grassland management in the Xilingol region. The individual SHAP values of each driver may
554 be an important prerequisite for rule-based scenario-building in the future.

555 **Author contribution:**

556 Batunacun prepared the manuscript with contribution from all co-authors, and Batunacun performed
557 the simulation. Ralf Wieland develop the model code.

558 **Code and data availability**

559 The development of XGBoost and SHAP values, graphs and model validation presented in this
560 paper were conducted in Python language. The original source code for XGBoost was obtained from
561 website (<https://xgboost.readthedocs.io/en/latest/>) and the explanation of XGBoost could be
562 obtained from Chen et al (2016). The original source code of SHAP values could be found in GitHub
563 (<https://github.com/slundberg/shap>), while the explanation could be obtained from Lundberg et al
564 (2017). The land use data in this manuscript can be downloaded Resource and Environment data
565 cloud platform, CAS (<http://www.resdc.cn/>), the statistical data could be obtained form Inner



566 Mongolia statistic year book. Other data get from various data sources, please check Table 1.
567

568 **Competing interests:**

569 The authors declare that they have no conflict of interest

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