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Research on Interpretable Machine Learning with Uncertainty Quantification for Ecological Risk Prediction

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Abstract. This study develops an interpretable machine-learning framework with uncertainty quantification for regional ecological risk prediction. The dataset is organized as a county-month panel containing 2,400 observations and 48 predictors from land-use, landscape-pattern, climate, topographic, hydrological, and human-disturbance variables. The ecological risk target is constructed as a three-class label, including low, medium, and high risk, based on a composite ecological risk index. Python 3.11 is used for data cleaning, median imputation, z-score standardization, XGBoost classification, SHAP interpretation, and Bayesian bootstrap interval estimation. The XGBoost model is trained with fixed hyperparameters, while SHAP TreeExplainer produces global and local feature-attribution outputs. Bayesian bootstrap analysis was conducted for 500 iterations for calculating 95% confidence intervals for class probabilities and SHAP importance for features. The findings reveal that the accuracy of the model is 0.872 ± 0.021, the macro F1 score is 0.856 ± 0.026, and the macro AUC score is 0.931 ± 0.018. The average value of the 95% probability intervals width is 0.118 ± 0.027. Among others, the proportion of built-up areas, roads, patches, NDVI, rainfall, and run-off index have the highest SHAP

Keywords: Ecological risk prediction, interpretable machine learning, uncertainty quantification, SHAP, confidence interval

1. Introduction

Ecological risk assessment has become an integral part of environmental management, regional territory planning, ecological restoration, water management, and land use regulation. Ecological risk at the regional level can be estimated based on the interplay between several variables such as land use structure, landscape fragmentation, climate fluctuations, topography, hydrology, and anthropogenic disturbances. These variables are usually measured from remote sensing products, monitoring records, land-cover maps, and regional statistical datasets, which makes ecological risk prediction a typical high-dimensional environmental modeling problem [1, 2].

Machine-learning methods have become useful tools for ecological and environmental prediction because they can handle nonlinear relationships and complex variable interactions. XGBoost, random forest, support vector machines, and ensemble models are frequently applied to air-quality forecasting, land degradation analysis, ecological security assessment, soil contamination prediction, and landscape ecological risk evaluation [3, 4].

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SHAP-based interpretation provides feature-importance ranking, local contribution values, and nonlinear response patterns, but standard SHAP results are often reported as fixed values [5, 6]. This creates a methodological gap because ecological data contain sampling variation, spatial heterogeneity, collinearity, missing-value uncertainty, and model-estimation instability. If interpretation results lack confidence intervals, decision-makers may overtrust unstable feature rankings or treat weak explanatory signals as robust mechanisms [7, 8]. This study proposes an interpretable machine-learning framework with uncertainty quantification for ecological risk prediction.

2. Literature review

2.1. Ecological risk prediction and environmental variable complexity

The ecological risk assessment model includes the use of such parameters as the composition of land use, landscape patterns, climate exposure, topographic limitations, hydrological characteristics, and disturbances from human activities. The variables may have nonlinear dependencies and correlations among each other. The growth in the development of urban areas might lead to increased habitat fragmentation, while precipitation and water runoff will influence wetlands and soil erosion. Therefore, ecological risk modeling requires multidimensional data processing and nonlinear prediction tools [4].

2.2. Interpretability in ecological machine learning

Interpretable machine learning is used to identify how environmental variables contribute to ecological prediction outcomes. SHAP analysis is especially common because it provides both global importance ranking and local instance-level explanation. In ecological applications, SHAP can reveal whether variables such as NDVI, road density, precipitation, or built-up land proportion increase or reduce predicted risk. However, fixed SHAP values may hide sampling instability, variable dependence, and model uncertainty. Interpretation becomes more useful when feature-attribution values are reported with confidence intervals rather than single-point estimates [5, 6].

2.3. Uncertainty quantification in scientific decision models

Uncertainty quantification is essential when machine-learning outputs are used for environmental or ecological decision-making. Prediction uncertainty can be represented through probability intervals, bootstrap distributions, conformal intervals, or Bayesian posterior summaries. Interpretation uncertainty is equally important because feature rankings may change when the sample is perturbed or the model is retrained. In ecological risk analysis, confidence-bounded interpretation helps distinguish stable drivers from noise-sensitive variables. A combined framework should therefore quantify uncertainty for both risk probabilities and SHAP-based feature attribution [9, 10].

3. Experimental methodology

3.1. Dataset construction and ecological risk variable matrix

The experimental dataset was compiled to forecast ecological risk on a county basis and includes 2,400 county-month observations with 48 predictors. The raw data were obtained from the monitoring system of environmental conditions, land use maps, digital elevation model,

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hydrometeorological databases, meteorological observations, and statistical databases of regions. In each observation, there is only one county and month, while the dependent variable is a three-level classification of ecological risk-low, moderate, and high risk. The predictors were divided into six groups: land use, landscape structure, climate, topography, hydrology, and anthropogenic disturbance. The land use variables include forest cover, cropland, urbanization, grassland, bareland, and intensity of land use change. Landscape pattern variables include patch density, edge density, contagion, Shannon diversity index, fragmentation, mean patch size, and aggregation. Variables related to climate, topography, hydrology, and anthropogenic disturbances include air temperature, precipitation, elevation, slope, river density, runoff, road density, population density, and nighttime light. Data cleaning was performed in Python 3.11. Missing values were filled in with group-year median values, and continuous variables were standardized with z-score normalization.

3.2. Prediction model and interpretable analysis configuration

The predictive model is built based on XGBoost 2.0 where the values for each hyperparameter are defined as follows: max_depth = 6, learning_rate = 0.05, n_estimators = 300, subsample = 0.8, colsample_bytree = 0.8, objective = multi:softprob, eval_metric = mlogloss, and random_state = 42. The predictive model uses as its input an encoded matrix with 48 features and predicts the output class probabilities for low, medium, and high risk ecological classes.

The multi-class ecological risk prediction function is specified as shown in Equation (1):

$$\widehat{\mathbf{p}}_i = softmax\left[\sum_{m=1}^{M} f_m\left(\mathbf{x}_i\right)\right]$$

$$\mathscr{L} = -\frac{1}{N}\sum_{i=1}^{N}\sum_{c=1}^{3}\mathbb{I}\left(y_i = c\right)\log\left(\widehat{p}_{ic}\right) + \lambda\sum_{m=1}^{M}\Omega\left(f_m\right) \tag{1}$$

where $\mathbf{x}_i$ denotes the environmental predictor vector of county-month observation i, f_m denotes the m-th regression tree, $\widehat{\mathbf{p}}_i$ is the predicted class-probability vector, L, M, and H denote low, medium, and high ecological risk classes, $\mathscr{L}$ is the multi-class log-loss objective, and $\Omega\left(f_m\right)$ is the tree-complexity regularization term.

For interpretability, SHAP TreeExplainer is used to calculate mean absolute SHAP values, instance-level SHAP values, and SHAP dependence patterns for selected variables. Global interpretation is based on average absolute SHAP values across the testing set. Local interpretation is performed for high-risk county-month observations. The top explanatory variables are reported with their mean SHAP contribution and confidence interval after Bayesian bootstrap estimation.

3.3. Uncertainty quantification and confidence-bound construction

Uncertainty quantification is implemented through a Bayesian bootstrap procedure with 500 iterations. At each iteration, sampling weights are generated from a Dirichlet distribution. The XGBoost classifier is retrained on the weighted training data, and predicted class probabilities are generated for the test observations. For each county-month observation, the 500 predicted probabilities are collected for low, medium, and high risk classes. The 2.5th and 97.5th percentiles are used as the 95% confidence interval of class probability.

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The bootstrap confidence-bound construction is specified as shown in Equation (2):

$$\mathbf{w}^{(b)} \sim Dirichlet\left(1,\ldots,1\right),\quad \widehat{\mathbf{p}}_i^{(b)} = F_{\theta(b)}\left(\mathbf{x}_i\right),\quad CI_{i,c}^{0.95} = \left[Q_{0.025}\left(\widehat{p}_i^{(1:B)}\right), Q_{0.975}\left(\widehat{p}_i^{(1:B)}\right)\right],$$

$$CI_j^{SHAP} = \left[Q_{0.025}\left(\overline{|\phi_j|}^{(1:B)}\right), Q_{0.975}\left(\overline{|\phi_j|}^{(1:B)}\right)\right] \tag{2}$$

where $\mathbf{w}^{(b)}$ is the Bayesian bootstrap weight vector at iteration b, $F_{\theta(b)}$ is the XGBoost model trained under weighted sampling, B=500, $CI_{i,c}^{0.95}$ is the confidence interval of predicted probability for class c, and CI_j^{SHAP} is the confidence interval of the mean absolute SHAP value for feature j.

4. Experimental procedure

4.1. Data preparation, label assignment, and sample splitting

The dataset is first cleaned by removing duplicate county-month records, invalid county codes, missing administrative identifiers, and environmental values outside physically meaningful ranges. The ecological risk index is calculated from standardized ecological pressure, landscape disturbance, ecological sensitivity, and human disturbance components. The resulting index is classified into three risk categories, low, moderate, and high, using certain thresholds. After preprocessing, the data set is divided into training, validation, and testing subsets at a ratio of 70:15:15. Stratified sampling is applied to preserve the distribution of the three risk categories. Standardization parameters are fitted only on the training set and then applied to the validation and testing sets. The final data files include feature matrices, risk labels, county identifiers, month identifiers, and feature-group labels.

4.2. Model training, SHAP computation, and bootstrap execution

The XGBoost classifier is trained on the training set and monitored on the validation set. SHAP TreeExplainer computes global feature importance and local explanation values for selected observations. Global SHAP ranking is calculated from the mean absolute SHAP value of each feature. Bayesian bootstrap execution is then performed on the combined training and validation data. For each of the 500 iterations, Dirichlet weights are generated, the XGBoost model is retrained, test-set probabilities are predicted, and SHAP values are recalculated. Probability intervals and SHAP intervals are stored in structured output tables. Each table records mean value, lower bound, upper bound, interval width, and feature or observation identifier.

4.3. Evaluation metrics and output generation

Model performance is evaluated using accuracy, macro F1, macro AUC, and log loss on the testing set. Prediction uncertainty is measured by the average width of the 95% class-probability interval. Interpretation uncertainty is measured by the interval width of global SHAP importance and local SHAP values. Top-10 environmental drivers are reported with mean SHAP values and 95% confidence intervals. All result processing is completed in Python and R 4.4. Python is used for

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bootstrap execution, SHAP computation, and interval extraction. R is used for final result checking and table formatting. Output files include classification performance tables, probability uncertainty summaries, feature-attribution rankings, SHAP confidence-interval tables, and local high-risk explanation records.

5. Experimental results

5.1. Descriptive statistics of ecological risk samples and environmental predictors

The final sample data contains 2,400 observations on a county-month level. The number of observations in low risk, moderate risk, and high risk samples was 812, 1,046, and 542, respectively. Higher percentages of built-up area were found in high-risk samples, namely, 0.386 ± 0.071 vs. 0.214 ± 0.058 for low-risk samples. The road density is higher in the case of high-risk samples, namely, 1.82 ± 0.44 km/km² for low-risk samples vs. 3.67 ± 0.69 km/km² in high-risk samples. The NDVI index decreases from 0.641 ± 0.083 to 0.472 ± 0.076, while patch density increases from 18.6 ± 4.7 to 31.4 ± 6.2 (see Table 1).

Table 1. Descriptive statistics of selected environmental predictors across ecological risk classes

Predictor	Low Risk	Medium Risk	High Risk
Built-Up Land Proportion	0.214 ± 0.058	0.297 ± 0.064	0.386 ± 0.071***
Forest Proportion	0.482 ± 0.091	0.391 ± 0.086	0.286 ± 0.074***
NDVI	0.641 ± 0.083	0.553 ± 0.079	0.472 ± 0.076***
Road Density (km/km²)	1.82 ± 0.44	2.74 ± 0.58	3.67 ± 0.69***
Patch Density	18.6 ± 4.7	24.8 ± 5.3	31.4 ± 6.2***
Runoff Index	0.318 ± 0.052	0.374 ± 0.061	0.431 ± 0.068**

5.2. Prediction performance and probability uncertainty of the interpretable xgboost model

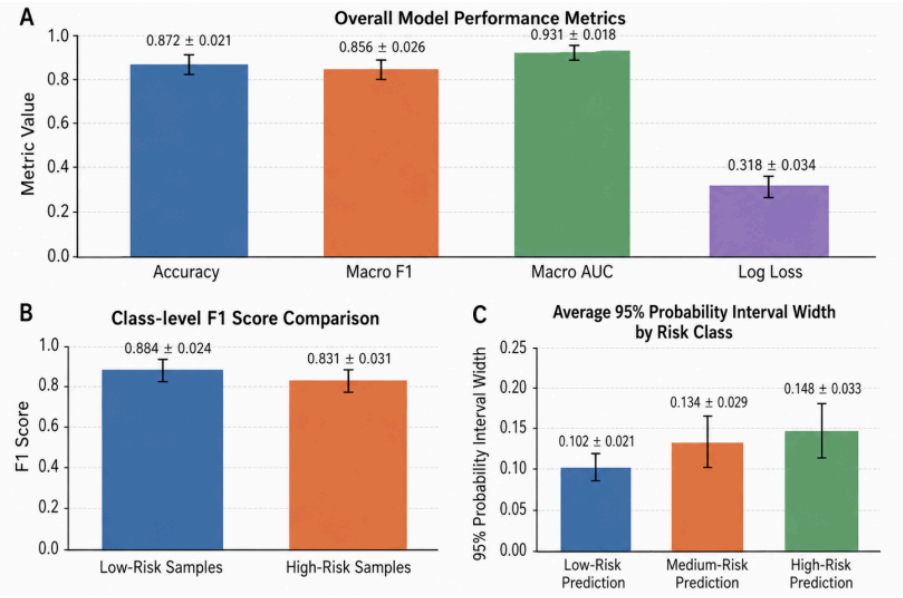

Figure 1. Prediction performance and probability uncertainty of the interpretable XGBoost model

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XGBoost produces accuracy = 0.872 ± 0.021, macro-F1 = 0.856 ± 0.026, macro-AUC = 0.931 ± 0.018, and log-loss = 0.318 ± 0.034. Regarding individual classes, prediction accuracy is higher among low-risk samples (macro-F1 = 0.884 ± 0.024) and lower among high-risk samples (macro-F1 = 0.831 ± 0.031). For the mean width of the 95% probability interval, the values obtained are as follows: low risk = 0.102 ± 0.021; medium risk = 0.134 ± 0.029; and high risk = 0.148 ± 0.033. The findings reveal that there is more uncertainty associated with high-risk predictions,

5.3. Shap-based feature attribution with confidence intervals and local explanation stability

SHAP analysis recognizes the following as the primary factors contributing to ecological risk assessment: the ratio of land covered by built-up areas, road density, patch density, NDVI, forest ratio, precipitation, runoff index, Shannon's diversity index, slope, and nighttime light intensity. The ratio of built-up land shows the highest mean absolute SHAP value, namely, 0.186 ± 0.024; the second and third most influential variables are road density, 0.163 ± 0.021, and patch density, 0.142 ± 0.019, respectively. The intervals for built-up land and road density are shorter than those of precipitation and runoff (refer to Table 2).

Table 2. Prediction performance, uncertainty, and SHAP attribution results

Indicator	Result
Accuracy	0.872 ± 0.021
Macro F1	0.856 ± 0.026
Macro AUC	0.931 ± 0.018
Log Loss	0.318 ± 0.034
Average Probability CI Width	0.118 ± 0.027
Mean Local SHAP CI Width	0.041 ± 0.012
Top Feature: Built-Up Land Proportion	0.186 ± 0.024***
Top Feature: Road Density	0.163 ± 0.021***
Top Feature: Patch Density	0.142 ± 0.019***
Top Feature: NDVI	0.137 ± 0.018**

6. Conclusion

This study establishes an interpretable machine-learning framework with uncertainty quantification for ecological risk prediction. The framework integrates ecological risk label construction, XGBoost classification, SHAP-based interpretation, Bayesian bootstrap uncertainty estimation, and confidence-bounded result reporting. It provides prediction outputs together with probability intervals and feature-attribution confidence intervals. The results show that the model achieves strong classification performance and produces interpretable ecological drivers. Built-up land proportion, road density, patch density, NDVI, forest proportion, precipitation, runoff index, and nighttime light intensity are identified as major contributors to ecological risk.

Author contribution

Zhuoxi Chu and Ling Zhai contributed equally to this paper.

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